Thermal segregation beyond Navier–Stokes

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Abstract. A dilute suspension of impurities in a low-density gas is described by the Boltzmann and Boltzman–Lorentz kinetic theories. Scaling forms for the species distribution functions allow the determination of the space dependence of the hydrodynamic fields without restriction to small thermal gradients or Navier–Stokes hydrodynamics. The thermal diffusion factor characterizing segregation is identified in terms of collision integrals as a function of the mechanical properties of the particles and the temperature gradient. An evaluation of the collision integrals using Sonine polynomial approximations is discussed. The conditions for segregation both along and opposite to the temperature gradient are obtained and contrasted with the leading order Navier–Stokes approximation.

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1. Introduction

Consider a granular mixture of two mechanically different species in a steady state with number densities $n_0(r)$ and $n(r)$, respectively. One component is dilute with respect to the other, $n_0(r)/n(r) \ll 1$, such that this component has negligible effect on the host gas. Moreover, the latter is at sufficiently low density such that the granular Boltzmann kinetic theory applies to its intra-species collisions. The dilute component has negligible intra-species collisions and its collisions with the host gas are described by the granular Boltzmann–Lorentz kinetic theory. The objective here is to provide a description of segregation induced by a temperature gradient without restriction on its size in this context. The motivation is the description some years ago of a solution to the Boltzmann equation for a steady state with constant temperature gradient [2, 3]. That analysis is extended here to include the presence of the dilute component with a complementary description of the solution to the Boltzmann–Lorentz equation. Since there is no limitation on the size of the temperature gradient, the results given here are an extension of previous results on thermal segregation obtained from the Navier–Stokes equation restricted to small gradients [4]. In the dilute conditions considered here and in the absence of gravity, no segregation occurs for the leading Sonine approximation at Navier–Stokes order, in contrast to the results obtained here.

The particles of the dilute component will be referred to as the ‘impurities’. The hydrodynamic fields obtained for the host gas are zero flow velocity, constant temperature gradient in the $x$-direction, $dT(x)/dx = \theta$, and a constant uniform pressure $p$, such that the density is $n(x) = p/T(x)$. The impurities have a temperature profile $T_0(x)$ proportional to the host temperature $T_0(x) = \gamma T(x)$ and a nontrivial density $n_0(x)$ expressed in terms of the host temperature field. In the dilute limit, the concentrations are $\rho_0(x) \simeq n_0(x)/n(x)$ and $\rho(x) = 1 - \rho_0(x)$. They have the relationship $d\rho_0/dx = -d\rho/dx$, so any spatial variation in $\rho_0(x)$ implies that the opposite variation in $\rho(x)$ and segregation occurs. Here, segregation is predicted for $g = 0$ at Navier–Stokes order if the transport coefficients are calculated beyond first order (see [5]).

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4 Segregation is predicted for $g = 0$ at Navier–Stokes order if the transport coefficients are calculated beyond first order (see [5]).
induced by the temperature gradient, and it is common to introduce a thermal diffusion factor \( \Lambda \) defined by

\[
\Lambda = \frac{\frac{1}{\rho_0} \frac{d \ln T}{dx} - \frac{d \ln \rho_0}{dx}}{\frac{d \ln T}{dx}}.
\]  

(1)

This dimensionless factor depends on the properties of the two components, \( \Lambda = \Lambda(\alpha, \alpha_0, \sigma/\sigma_0, m/m_0, \theta^*) \), where \( \alpha \) and \( \alpha_0 \) are the restitution coefficients of the host–host and impurity–host collisions, \( \sigma, \sigma_0 \) and \( m, m_0 \) are the species diameters and masses, and \( \theta^* = \theta/p \sigma d^{-1} \) is the dimensionless temperature gradient, \( d \) being the geometrical dimension of the system. In principle, \( \Lambda \) can be positive or negative within this parameter space. The case \( \Lambda = 0 \) implies no segregation, while \( \Lambda \) positive (negative) implies that the impurities increase in concentration against (along) the temperature gradient. This is the thermal analogue of the Brazil nut and reverse Brazil nut effects for gravitational segregation [6–9].

The distribution functions of the two species are of a ‘normal’ form, meaning that their dependence on space and time occurs only through the hydrodynamic fields \( n(x), T(x) \) and \( n_0(x) \) [10, 11]. Thus, boundary conditions do not occur explicitly but occur only through the determination of these fields. For example, no external driving source is required in the kinetic equation for a stationary state, since this is implicit in the time independence of the fields. Instead, the stationary form of the fields is determined self-consistently from moments of the kinetic equations. This self-consistency also shows the temperature of the impurities as being proportional to the host temperature, \( T_0(x) = \gamma T(x) \), with \( \gamma \neq 1 \) in general. No reference to hydrodynamics is made, although these moment equations are equivalent to the balance equations forming the basis for a hydrodynamical description.

The steady state obtained occurs by establishing a gradient of the heat flux to compensate for local energy loss due to collisional cooling. Thus, it is exclusive to granular fluids and links the temperature gradient to the degree of inelasticity rather than to boundary conditions. This is similar to steady uniform shear flow where the steady state is possible due to a balance of viscous heating and collisional cooling, such that the velocity gradient (shear rate) is linked to the degree of inelasticity. In both cases, the control needed to ensure that Navier–Stokes hydrodynamics is lost. In the present case, smaller gradients entail smaller pressure at a constant restitution coefficient or smaller inelasticity at a constant pressure. Such non-Newtonian steady states are a characteristic of granular flows, and segregation for such states can be qualitatively different from that for Navier–Stokes hydrodynamics. This has been illustrated recently for thermal segregation under uniform shear flow [12].

The next section defines the system and its kinetic theory description. In section 3, scaling forms for the distribution functions are introduced and the implications for the hydrodynamic fields are obtained. Three constants must be determined self-consistently. One of these, the temperature gradient \( \theta \), has been obtained in [2, 3]. Collision integrals for the other two are obtained here. The form of the thermal diffusion factor \( \Lambda \) is given in terms of these constants, and the sign of \( \Lambda \) is discussed based on approximate evaluations of the collision integrals given in the appendices.

2. Kinetic theory

Consider a one-component gas of \( N \) smooth, inelastic hard spheres (\( d = 3 \)) or discs (\( d = 2 \)) with diameter \( \sigma \) and mass \( m \) at low density. Their distribution for position \( \mathbf{r} \) and velocity \( \mathbf{v} \) at
time \( t \), \( f(\mathbf{r}, \mathbf{v}, t) \), is determined from the Boltzmann equation (without external forces) [13]

\[
\left( \partial_t + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \right) f = J[\mathbf{v} | f, f],
\]

(2)

where the collision operator \( J[\mathbf{v} | f, f] \) is

\[
J[\mathbf{v} | f, f] = \sigma^{-1} \int d\mathbf{v}_1 \int d\hat{\mathbf{\sigma}} \Theta(\hat{\mathbf{\sigma}} \cdot \mathbf{g})(\hat{\mathbf{\sigma}} \cdot \mathbf{g}) \left[ \alpha^{-2} f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}', t) - f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_1, t) \right].
\]

(3)

Here, \( \mathbf{g} = \mathbf{v} - \mathbf{v}_1 \) is the relative velocity of the colliding pair, \( \Theta \) is the Heaviside step function, \( d\hat{\mathbf{\sigma}} \) is the solid angle element about the direction of the unit vector \( \hat{\mathbf{\sigma}} \), and \( \alpha \) is the restitution coefficient characterizing the degree of inelasticity \((0 < \alpha \leq 1)\). The velocities \( \mathbf{v}', \mathbf{v}_1' \) denote the restituting velocities for the pair \( \mathbf{v}, \mathbf{v}_1 \),

\[
\mathbf{v}' = \mathbf{v} - \frac{1 + \alpha^{-1}}{2} (\hat{\mathbf{\sigma}} \cdot \mathbf{g})\hat{\mathbf{\sigma}}, \quad \mathbf{v}_1' = \mathbf{v}_1 + \frac{1 + \alpha^{-1}}{2} (\hat{\mathbf{\sigma}} \cdot \mathbf{g})\hat{\mathbf{\sigma}}.
\]

(4)

Now consider \( M \) additional impurity particles in this gas, all of which are identical but mechanically different from the fluid particles. When \( M \ll N \), the primary collisions for the impurity particles are with the host gas particles, and impurity–impurity collisions and the effects of the impurities on the gas distribution function \( f \) can be neglected. The distribution function of the impurities, \( F(\mathbf{r}, \mathbf{v}_0, t) \), is governed by the corresponding Boltzmann–Lorentz equation,

\[
\left( \partial_t + \mathbf{v}_0 \cdot \frac{\partial}{\partial \mathbf{r}} \right) F = I[\mathbf{v}_0 | F, f],
\]

(5)

where the operator \( I[\mathbf{v}_0 | F, f] \) describes changes in \( F \), due to binary collisions between the impurity and gas particles,

\[
I[\mathbf{v}_0 | F, f] \equiv \sigma^{-1} \int d\mathbf{v}_1 \int d\hat{\mathbf{\sigma}} \Theta(\hat{\mathbf{\sigma}} \cdot \mathbf{g}_0)(\hat{\mathbf{\sigma}} \cdot \mathbf{g}_0) \left[ \alpha_0^{-2} F(\mathbf{r}, \mathbf{v}_0, t) f(\mathbf{r}, \mathbf{v}_1, t) - F(\mathbf{r}, \mathbf{v}_0, t) f(\mathbf{r}, \mathbf{v}_1, t) \right],
\]

(6)

and \( \mathbf{g}_0 = \mathbf{v}_0 - \mathbf{v}_1 \). The restituting velocities \( \mathbf{v}_0', \mathbf{v}_1' \) in this case are

\[
\mathbf{v}_0' = \mathbf{v}_0 - \frac{m_0 (1 + \alpha_0^{-1})}{m + m_0} (\hat{\mathbf{\sigma}} \cdot \mathbf{g}_0)\hat{\mathbf{\sigma}}, \quad \mathbf{v}_1' = \mathbf{v}_1 + \frac{m_0 (1 + \alpha_0^{-1})}{m + m_0} (\hat{\mathbf{\sigma}} \cdot \mathbf{g}_0)\hat{\mathbf{\sigma}}.
\]

(7)

In the above expressions, \( \sigma \equiv (\sigma + \sigma_0) / 2 \) and \( \sigma_0, m_0 \) and \( \alpha_0 \) are the hard sphere diameter, mass and restitution coefficient of the impurity particles, respectively.

The macroscopic state of this system is described by the fluid number density \( n(\mathbf{r}, t) \), temperature \( T(\mathbf{r}, t) \), and flow velocity \( \mathbf{u}(\mathbf{r}, t) \), defined in terms of the distribution function by

\[
\begin{pmatrix}
n(\mathbf{r}, t) \\
\frac{1}{2} n(\mathbf{r}, t) T(\mathbf{r}, t) \\
n(\mathbf{r}, t) \mathbf{u}(\mathbf{r}, t)
\end{pmatrix} \equiv \int d\mathbf{v} \begin{pmatrix} 1 \\ \frac{1}{2} m V^2 \\ \mathbf{v} \end{pmatrix} f(\mathbf{r}, \mathbf{v}, t),
\]

(8)
with \( V(\mathbf{r}, t) \equiv v - u(\mathbf{r}, t) \). It is convenient to introduce corresponding fields for a macroscopic description of the impurity particles,

\[
\begin{pmatrix}
\frac{1}{2}n_0(\mathbf{r}, t) \\
\frac{1}{2}n_0(\mathbf{r}, t)T_0(\mathbf{r}, t) \\
j_0(\mathbf{r}, t)
\end{pmatrix}
\equiv 
\int d\mathbf{v}_0 
\begin{pmatrix}
1 \\
\frac{1}{2}m_0V_0^2 \\
v_0
\end{pmatrix}
F(\mathbf{r}, \mathbf{v}_0),
\tag{9}
\]

with \( V_0(\mathbf{r}, t) = v_0 - u_0(\mathbf{r}_0, t) \). Instead of an impurity velocity, the more usual number flux notation \( j_0 = n_0u_0 \) has been used.

### 3. Scaling solutions

In [2], a solution to the Boltzmann equation was described for the special case of a scaling form in terms of the hydrodynamic variables,

\[
f(x, v) = n(x) \left[ \frac{m}{2T(x)} \right]^{d/2} \phi (c), \quad c \equiv \left[ \frac{m}{2T(x)} \right]^{1/2} v.
\tag{10}
\]

Such a solution, where the space and time dependence of the distribution function occurs only through the hydrodynamic fields, is called ‘normal’. The definitions of the fields in (8) and the choice of \( u = 0 \) give the self-consistency conditions on \( \phi (c) \),

\[
\left( \frac{d}{2} \right) = \int dc \left( \frac{1}{c^2} \right) \phi (c).
\tag{11}
\]

Here, a similar scaling solution for the impurities is sought,

\[
F(x, \mathbf{v}_0) = n_0(x) \left[ \frac{m_0}{2T_0(\mathbf{x})} \right]^{d/2} \Phi (c_0), \quad c_0 \equiv \left[ \frac{m_0}{2T_0(\mathbf{x})} \right]^{1/2} \mathbf{v}_0.
\tag{12}
\]

The definitions (9) then give the conditions on \( \Phi \),

\[
\left( \frac{d}{2} + \frac{m_0j_0^2}{2T_0n_0^2} \right) = \int dc_0 \left( \frac{1}{c_0^2} \right) \Phi (c_0).
\tag{13}
\]

In order for (12) to be ‘normal’, it should depend only on the hydrodynamic fields for the gas and impurities, i.e. on \( n_0(x), n(x) \) and \( T(x) \). Dimensional analysis then requires that \( T_0(x) \) must be proportional to \( T(x) \),

\[
T_0(x) = \gamma T(x).
\tag{14}
\]

The constant \( \gamma \) must be determined in the course of solving the kinetic equation (as discussed below). Further comments on the implications of normal solutions are provided in the last section.
In terms of these scaling solutions and dimensionless velocity variables, the Boltzmann and Boltzmann–Lorentz equations become

\[
\begin{align*}
& c_x \left\{ \frac{1}{n\sigma^{d-1}} \frac{d \ln n}{dx} \phi (c) - \frac{1}{2n\sigma^{d-1}} \frac{d \ln T}{dx} \frac{\partial}{\partial c} [c\phi (c)] \right\} = J [c|\phi , \phi ] , \\
& c_0x \left\{ \frac{1}{n\sigma^{d-1}} \frac{d \ln n_0}{dx} \Phi (c_0) - \frac{1}{2n\sigma^{d-1}} \frac{d \ln T}{dx} \frac{\partial}{\partial c_0} [c_0\Phi (c_0)] \right\} = I [c_0|\phi , \phi ] ,
\end{align*}
\]

(15) (16)

with the dimensionless collision operators

\[
J [c|\phi , \phi ] \equiv \int dc_1 \int d\hat{\sigma} \Theta (\hat{\sigma} \cdot w)(\hat{\sigma} \cdot w) \left[ \alpha^{-2} \phi (c') \phi (c_1) - \phi (c) \phi (c_1) \right] ,
\]

(17)

\[
I [c_0|\phi , \phi ] = \int dc_1 \int d\hat{\sigma} \Theta (\hat{\sigma} \cdot w_0)(\hat{\sigma} \cdot w_0) \left[ \alpha^{-2} \Phi (c_0, c') - \Phi (c_0) \phi (c_1) \right] .
\]

(18)

The relative velocities \( w \) and \( w_0 \) are now

\[
w \equiv c - c_1 , \quad w_0 \equiv c_0 - \left( \frac{m_0}{m_y} \right)^{1/2} c .
\]

(19)

The expressions of the dimensionless restituting velocities in equation (18) are given in equation (A.3). Since the right-hand sides of equations (15) and (16) are independent of \( x \), the left-hand sides must be as well. This will be true if the hydrodynamic fields \( n(x), n_0(x) \), and \( T(x) \) satisfy the equations

\[
\frac{1}{n\sigma^{d-1}} \frac{d \ln n}{dx} = A , \quad \frac{1}{n\sigma^{d-1}} \frac{d \ln T}{dx} = B , \quad \frac{1}{n\sigma^{d-1}} \frac{d \ln n_0(x)}{dx} = C ,
\]

(20)

where \( A, B \) and \( C \) are constants. The constants \( A \) and \( B \) are determined by taking moments of the Boltzmann equation (15). Namely, multiplication of the equation by 1, \( c_s \), and \( c^2 \) and integration over \( c \) yields

\[
\begin{align*}
\left( A + \frac{B}{2} \right) \int dc c_s \phi (c) & = 0 , \quad (A + B) \int dc c^2_s \phi (c) = 0 , \\
\left( A + \frac{3B}{2} \right) \int dc c^2_s \phi (c) & = \int dc c^2 J [c|\phi , \phi ] .
\end{align*}
\]

(21) (22)

The zeros on the right-hand side of (21) result from the conservation of particle number and momentum by the collision operator. The first equation of (21) is satisfied because of conditions (11) required on \( \phi (c) \), while the second equation gives \( A = -B \). Finally, equation (22) determines \( B \),

\[
B = \frac{2 \int dc c^2 J [c|\phi , \phi ]}{\int dc c^2 c_s \phi (c)} .
\]

(23)
The hydrodynamic fields of the gas are now given by $u = 0$ and
\[
\frac{dp}{dx} = 0, \quad \frac{dT}{dx} = \theta, \tag{24}
\]
where $p = n(x)T(x)$ is the uniform pressure and $\theta = Bp\sigma^{d-1}$ is the constant temperature gradient.

A similar analysis applies to the impurity constants $C$ and $\gamma$. Taking moments of the Boltzmann–Lorentz equation (16) with respect to $1$, $c_{0x}$ and $c_{0}^2$ gives
\[
(C + \frac{\sigma^{d-1}}{2\sigma^{d-1}} B) j_{0x} = 0, \tag{25}
\]
\[
C + \frac{\sigma^{d-1}}{\sigma^{d-1}} B = \frac{\int dc_{0} c_{0x} I[c_{0}|\Phi, \phi]}{\int dc_{0} c_{0x} \Phi(c_{0})}, \tag{26}
\]
\[
C + \frac{3\sigma^{d-1}}{2\sigma^{d-1}} B = \frac{\int dc_{0} c_{0x}^2 I[c_{0}|\Phi, \phi]}{\int dc_{0} c_{0x}^2 \Phi(c_{0})}. \tag{27}
\]
The right-hand sides of equations (26) and (27) depend on $\gamma$ explicitly through $w_{0}$ (see (19)) and implicitly on both $\gamma$ and $C$ through $\Phi$. Since $B$ is known independently from equation (23), the two unknowns $\gamma$ and $C$ are determined by using equations (26) and (27). Equation (25) has two solutions, $j_{0x} = 0$ and $C = -\sigma^{d-1} B / 2\sigma^{d-1}$. The latter gives an additional equation for $\gamma$ and $C$ and the problem is overdetermined. Probably, this choice is not consistent with the assumption (12). Here, it is assumed that the boundary conditions enforce the choice $j_{0x} = 0$.

In summary, the description of the gas and impurities is completely specified by the kinetic equations for $\phi(e)$ and $\Phi(c_{0})$,
\[
-Bc_{x} \left\{ \phi(e) + \frac{1}{2} \frac{\partial}{\partial e} \cdot [e\phi(e)] \right\} = \mathcal{J} [c|\phi, \phi], \tag{28}
\]
\[
c_{0x} \left\{ C \Phi(c_{0}) - \frac{\sigma^{d-1}}{2\sigma^{d-1}} B \frac{\partial}{\partial c_{0}} \cdot [c_{0} \Phi(c_{0})] \right\} = \mathcal{I} [c_{0}|\Phi, \phi], \tag{29}
\]
and the constants $B$, $C$ and $\gamma$ are determined self-consistently from equations (23), (26), and (27). The corresponding collision integrals are further simplified in appendix A. The hydrodynamic fields have the simple spatial forms,
\[
T(x) = T(0) + \theta x, \quad n(x) = \frac{p}{T(0) + \theta x}, \tag{30}
\]
\[
T_{0}(x) = T_{0}(0) + \gamma \theta x, \quad n_{0}(x) = n_{0}(0) \left[ 1 + \frac{\theta x}{T(0)} \right]^{\sigma^{d-1} C / \sigma^{d-1} B}. \tag{31}
\]
4. Segregation

The segregation of impurity particles relative to the host gas is described by the inhomogeneity of the composition \( \rho_0(x) \approx n_0(x) / n(x) \), which follows from (30) and (31),

\[
\rho_0(x) = n_0(0) \left[ \frac{1 + \frac{\theta}{T(0)} x}{1 + \sigma/d} \right]^{1 + \sigma/d - 1 B}.
\]

The thermal diffusion factor of (1) is therefore

\[
\Lambda = - \left( 1 + \frac{\sigma}{d - 1} C \frac{1}{\sigma} \right) = - \frac{\sigma}{2 \sigma - 1} \int dc_0 c_0 I[c_0|\Phi, \phi] \frac{1}{dc_0 c_0^2} \int dc c^2 \phi(c). \]

If the impurities are mechanically equivalent to the host particles, then \( I[c_0|\Phi, \phi] = J[c_0|\phi, \phi] \), \( \Phi = \phi \) and \( \Lambda = 0 \), since the first integral in the numerator of (33) vanishes by conservation of momentum.

The corresponding result on the thermal diffusion factor obtained from the Navier–Stokes order Chapman–Enskog solutions to the Boltzmann and Boltzmann–Lorentz equations, evaluated to leading order Sonine approximation, gives \( \Lambda = 0 \) for all values of the parameters \( \alpha, \alpha_0, \sigma/\sigma_0, m/m_0, \theta/\rho \sigma - 1 \). If the Navier–Stokes calculation is extended to include effects of gravity, the condition becomes

\[
\left( \Lambda \frac{\partial T}{\partial x} \right)_{NS} = mg \left( \frac{T_0}{T} - \frac{m_0}{m} \right). \]

Thus thermal segregation can occur, facilitated by gravity, and it depends on the sign of \( (T_0/T - m_0/m) \) and the direction of \( \partial T/\partial x \) relative to the gravitational force (see, however, [5]). This is in sharp contrast to the results obtained in the next section.

5. Approximate determination of \( T_0/T \) and \( \Lambda \)

To determine the coefficients \( B, C \) and \( \gamma = T_0/T \), the distribution functions \( \phi \) and \( \Phi \) are represented as truncated Sonine polynomial expansions,

\[
\phi(c) \simeq \pi^{-d/2} e^{-c^2} \left[ 1 - a_{01} (c^2 - d c_x^2) + \left( \frac{d - 1}{2} \right) b_{01} + \frac{3}{2} b_{10} \right] c_x - b_{01} c^2 c_x - (b_{10} - b_{01}) c_x^3.
\]

\[
\Phi(c_0) \simeq \pi^{-d/2} e^{-c_0^2} \left[ 1 - A_{01} (c_0^2 - d c_{0x}^2) + \left( \frac{d - 1}{d} \right) B_{01} + \frac{3}{2} B_{10} \right] c_{0x} - B_{01} c_0^2 c_{0x} - (B_{10} - B_{01}) c_{0x}^3.
\]

The method for determining the coefficients in these expansions is described in [3] and summarized for the present case in appendix B. The numerical solutions for the case of a two-dimensional (2D) system \( (d = 2) \) with \( m = m_0 \) and \( \sigma = \sigma_0 = \sigma \) are shown in figures B.1–B.3.
Figure 1. Temperature of the impurity $T_0$ divided by the temperature of the host gas $T$ as a function of the coefficient of normal restitution of the gas particles $\alpha$, for several values of the restitution coefficient for collisions between the gas particles and the impurities, $\alpha_0$, as indicated in the inset. In all cases, $d = 2$, $m_0 = m$ and $\sigma = \sigma_0 = \bar{\sigma}$.

as a function of $\alpha$ for several values of $\alpha_0$. An important general feature is that all coefficients in (35) and (36) vanish as $\alpha \to 1$. Thus the non-uniform steady state described here exists only as a consequence of the inelasticity of the host gas. Further comments on this are given in the last section below.

In the following, attention is restricted to $\sigma = \sigma_0 = \bar{\sigma}$ and $d = 2$ for several values of $m_0/m$, $\alpha$, and $\alpha_0$. It is well established that different species of granular mixtures have different partial temperatures, even in their homogeneous cooling state (i.e. equipartition of energy does not occur) [6, 14, 15]. Figures 1 and 2 show the behavior of $T_0/T$ when $m_0/m = 1$ and 2, respectively, as a function of $\alpha$ for several values of $\alpha_0$. The common feature is the increase in $T_0/T$ with decreasing $\alpha$, increasing $\alpha_0$ and decreasing $m_0/m$. Figure 3 shows a broader range of $m_0/m$. Even at the relatively weak dissipation values of this figure, it is clear that the largest values of $T_0/T$ occur in the cases of a small mass ratio, the maximum host dissipation and the weakest impurity dissipation.

The existence of segregation for the same weak dissipation values of figure 3 is demonstrated in figure 4. The thermal diffusion factor $\Lambda$ is positive when $m_0/m > 1$. This means that the impurity concentration is higher at the colder part of the host fluid. This is similar to the host fluid density that behaves as $n = p/T$ with constant $p$. For a smaller mass ratio, segregation goes in the opposite direction with the impurity concentration being highest in the hotter part of the host fluid. This effect is enhanced for stronger host fluid dissipation and weaker impurity dissipation, as illustrated in figures 5 and 6 for $m_0/m = 1$ and 2, respectively.

It is interesting to note that for $m_0/m = 1$, the border between the two types of segregation, $\Lambda = 0$, occurs for $\alpha = \alpha_0$. Referring to figure 4, these values also correspond to $T_0/T = 1$. Similarly, for $m_0/m = 2$, comparing figures 2 and 6 it is seen that $\Lambda = 0$ for $T_0/T = 2$. These limited data suggest the possibility that the segregation criterion $\Lambda = 0$ occurs at $m_0/m = T_0/T$. Surprisingly, this is the same as the Navier–Stokes criterion in the presence of gravity, (34).
A further analysis of this potential relationship across a larger data set is necessary. In the case of larger $m_0/m$, it was found that $T_0/T \leqslant 1$ and that segregation occurs only for $\Lambda > 0$.

5.1. Weakly inelastic host gas

A simpler description occurs in the limit of weak inelasticity for a host gas, $1 - \alpha \ll 1$. The analysis is described in appendix B, where explicit expressions for the coefficients $B$, $C$ and $\gamma$ are given. To leading order, the temperature ratio is the same as that for an impurity in an isolated gas in its homogeneous cooling state. Also $B$ and $C$ are proportional to $\sqrt{1 - \alpha}$,
Figure 4. The dimensionless thermal diffusion factor $\Lambda$ as a function of the mass ratio $m_0/m$ for the same system as that in figure 3.

Figure 5. The dimensionless thermal diffusion factor $\Lambda$ as a function of the coefficient of normal restitution of the gas particles $\alpha$, at several values of the restitution coefficient of collisions between the gas particles and the impurities, $\alpha_0$, as indicated in the inset. In all cases, $d = 2$, $m_0 = m$ and $\sigma = \sigma_0 = \bar{\sigma}$.

so that the thermal diffusion factor $\Lambda$ is independent of $\alpha$. For $d = 2$, the explicit result is

$$\Lambda = -\frac{8}{27h^2 - 80h + 96} \left( h + \frac{\bar{\sigma}}{\sigma} (2 - h)^{3/2} (5h - 6) \right).$$

(37)

It is seen that $\Lambda$ is linear in $\bar{\sigma}/\sigma$ and depends on $\alpha_0$ and $m/m_0$ only in the combination $h = m(1 + \alpha_0)/(m + m_0)$. For all values of $\bar{\sigma}/\sigma$, the thermal diffusion factor takes on both positive and negative values, with the latter occurring for larger $h$ (note that $0 \leq h \leq 2$). The

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border between the two types of segregation, $\Lambda = 0$, is now expressed by the value of $\sigma/\bar{\sigma}$ as a function of $h$,

$$\frac{\sigma}{\bar{\sigma}} = h^{-1} (2 - h)^{3/2} (6 - 5h).$$

(38)

As expected, $\bar{\sigma}/\sigma = 1 = h$ is a solution corresponding to identical particles. For $h > 6/5$, there are no positive solutions and segregation occurs in all cases.

6. Discussion

The description of a low-density granular gas with a dilute concentration of impurities has been given in terms of solutions to the coupled Boltzmann and Boltzmann–Lorentz kinetic equations. These are normal solutions whose space and time dependences are entirely specified in terms of the hydrodynamic fields $n, n_0$ and $T$. The special case of a steady state in which the host gas has a constant temperature gradient and constant pressure, described earlier in [2] and [3], has been generalized to include a corresponding steady state of the impurities. In this way, the thermal segregation factor is identified in terms of the constants of the hydrodynamic fields, without the limiting approximations of small spatial gradients. The self-consistent kinetic equations (28) and (29) determining these constants were solved using a low-order Sonine polynomial approximation for the velocity dependence of the host and impurity distributions. The resulting thermal diffusion factor was found to identify the conditions for segregation along the temperature gradient as well as segregation against the temperature gradient. Such normal solutions are typically constructed by the Chapman–Enskog method whose practical application typically entails limitation to small spatial gradients, e.g. the Navier–Stokes order. The application of the Navier–Stokes hydrodynamics obtained in this way and specialized to the steady state with constant temperature gradient and constant pressure leads to the prediction of absence of segregation. The effects described here are therefore due to the contributions from the Chapman–Enskog method beyond the small gradient approximation. In fact, there are no limitations on the temperature gradient in the present analysis.
There are two important clarifications to note. First, the validity of a normal solution both for granular and molecular gases is limited to domains away from the initial preparation time and confining boundaries. For the steady state considered here, this means that there is typically a boundary layer to which the normal solution does not apply. Additional information is then required to connect the physically specified values of the fields or their gradients at the boundary with those values associated with the normal solution. These are the familiar ‘slip’ boundary conditions. The existence of the normal solution described here for a system with finite confinement and the associated boundary layer has been demonstrated in [2] and [3] by molecular dynamics simulation. Typically, the size of the bulk interior relative to the boundary layer decreases as the temperature gradient increases. An investigation of this problem for the case of a molecular gas has shown that the bulk normal solution domain still exists beyond the Navier–Stokes limit [16].

A second clarification is that the special nature of the steady state described here is unique to a granular gas. The analysis of Brey et al [2] shows that it results from the balance between the heat flux gradient and the cooling rate due to inelastic collisions. In the absence of the latter, there is no steady-state solution of the type considered here. In contrast to normal fluids, the gradients of such steady states are controlled by internal processes rather than by boundary sources. External control of the gradients is therefore lost. In the present case, the magnitude of the dimensionless temperature gradient $\theta / \rho a^{d-1} = B(\alpha)$ monotonically decreases to zero as $\alpha \to 1$, vanishing in the elastic limit. Consequently, for example, it is not possible for the Navier–Stokes to apply here to strong dissipation.

The truncation of the Sonine polynomial expansion used here is expected to fail for the distribution functions at velocities much larger than the thermal velocity. However, here these distributions are only used to calculate coefficients that are low order polynomials that are insensitive to the large velocity behavior. This is consistent with past experience in using such truncated expansions to calculate transport coefficients. Nevertheless, retention of all polynomials through cubic order is required for correct $\alpha$ dependence, as illustrated by comparison with the simple single polynomial approximation at the end of appendix B.

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Appendix A. Reduction of collision integrals

The Boltzmann collision integral appearing on the right-hand side of equation (23) is simplified further in [2], with the result

$$B = -\frac{(1 - \alpha^2) \pi^{(d-1)/2}}{2\Gamma \left(\frac{d+1}{2}\right)} \int \frac{\int d^3c_1 |c - c_1|^3 \phi(c) \phi(c_1)}{\int d^2c_1 \phi(c)}.$$  \hspace{1cm} (A.1)
The Boltzmann–Lorentz collision integrals can be simplified in a similar way. Consider first the collision integral appearing in equation (26),

$$\int \mathrm{d} e_0 \mathcal{L} [c_0] \Phi, \phi = \int \mathrm{d} c_1 \int \mathrm{d} e_0 c_0 \int \mathrm{d} \hat{\sigma} \Theta(\hat{\sigma} \cdot w_0)(\hat{\sigma} \cdot w_0) \left[ \alpha_0^{-2} \Phi(c_0) \phi(c_1) - \Phi(c_0) \phi(c_1) \right],$$

(A.2)

where $w_0$ is defined in equation (19) and the dimensionless restituting velocities following from equation (7) are

$$c'_0 = c_0 - \frac{m}{m + m_0} \left( 1 + \alpha_0^{-1} \right) (\hat{\sigma} \cdot w_0) \hat{\sigma}, \quad c' = c + \frac{m_0}{m + m_0} \left( 1 + \alpha_0^{-1} \right) \left( \frac{m \gamma}{m_0} \right)^{1/2} (\hat{\sigma} \cdot w_0) \hat{\sigma}.$$  

(A.3)

It is easily verified that

$$dc'_0 \cdot c'_0 = \alpha_0^{-1} dc_1 dc_0, \quad \hat{\sigma} \cdot g_0 = -\alpha_0 \hat{\sigma} \cdot g'_0.$$  

(A.4)

Also, equations (A.3) can be inverted to obtain the collision rule in dimensionless units,

$$c_0^* = c_0 - \frac{m (1 + \alpha_0)}{m + m_0} (\hat{\sigma} \cdot w_0) \hat{\sigma},$$

(A.5)

$$c_1^* = c_1 + \frac{m (1 + \alpha_0)}{m + m_0} \left( \frac{m \gamma}{m_0} \right)^{1/2} (\hat{\sigma} \cdot w_0) \hat{\sigma}.$$  

(A.6)

Returning to equation (A.2), change variables in the first term in brackets in the right-hand side to integrate over the restituting velocities. Using the above relations, the equation becomes

$$\int \mathrm{d} e_0 \mathcal{L} [c_0] \Phi, \phi = \int \mathrm{d} c_1 \int \mathrm{d} e_0 \Phi(c_0) \phi(c_1) \int \mathrm{d} \hat{\sigma} \Theta(\hat{\sigma} \cdot w_0)(\hat{\sigma} \cdot w_0) (c_{0x} - c_{0x})$$

$$= - \frac{m (1 + \alpha_0)}{m + m_0} \int \mathrm{d} c_1 \int \mathrm{d} e_0 \Phi(c_0) \phi(c_1) w_0 w_0 \int \mathrm{d} \hat{\sigma} \Theta(\hat{\sigma} \cdot w_0)(\hat{\sigma} \cdot \hat{w}_0)^3$$

$$= - \frac{m (1 + \alpha_0) \pi^{(d-1)/2}}{m + m_0} \int \mathrm{d} c_1 \int \mathrm{d} e_0 \Phi(c_0) \phi(c_1) w_0 w_0.$$  

(A.7)

Finally, (26) becomes

$$C + \frac{\sigma^{d-1}}{\sigma^{d-1}} B = - \frac{m (1 + \alpha_0) \pi^{(d-1)/2}}{m + m_0} \int \mathrm{d} c_1 \int \mathrm{d} e_0 \Phi(c_0) \phi(c_1) w_0 w_0.$$  

(A.8)

The analysis of equation (27) is similar, with the result

$$C + \frac{3 \sigma^{d-1}}{2 \gamma^{d-1}} B = \frac{m (1 + \alpha_0) \pi^{(d-1)/2}}{m + m_0} \left[ \frac{m (1 + \alpha_0)}{m + m_0} w_0^3 - 2 w_0 w_0 \cdot c_0 \right].$$  

(A.9)
Appendix B. Solutions to kinetic equations

The solution to the kinetic equation for $\phi(c)$ and the self-consistent determination of $B$ are a problem that is independent of the impurities and can be solved first. The method is described in [3]. First, $B$ is given the representation as a collision integral using equation (23), so the kinetic equation (28) becomes

$$-2c_x \left\{ \phi(c) + \frac{1}{2} \frac{\partial}{\partial c} \cdot [c \phi(c)] \right\} \int dc c^2 \mathcal{J}[c | \phi, \phi] = \mathcal{J}[c | \phi, \phi]. \tag{B.1}$$

Next, $\phi(c)$ is approximated by a truncated Sonine polynomial expansion,

$$\phi(c) \simeq \pi^{-d/2} e^{-c^2} \left[ 1 - a_{01} \left( c^2 - d c_x^2 \right) + \left( \frac{d - 1}{2} b_{01} + \frac{3}{2} b_{10} \right) c_x - b_{01} c_x^2 - (b_{10} - b_{01}) c_x^3 \right]. \tag{B.2}$$

This form ensures the conditions given in equation (11). The coefficients $a_{01}, b_{01}$ and $b_{10}$ are then obtained from three equations obtained by taking velocity moments in (B.1). Namely, the equation is multiplied by $c_x^2, c_x^3$ and $c_x^4$, respectively, and afterwards integrated over $c$. With these coefficients determined, $B$ is calculated from equation (23).

To determine $\Phi(c_0), C$ and $\gamma$, a similar procedure is followed. First, express $C$ as a collision integral from equations (26) and (27),

$$C = 2 \left[ 3 \int dc_0 c_{0x} \mathcal{I}[c_0 | \Phi, \phi] - \int dc_0 c_{0x}^2 \Phi(c_0) \right], \tag{B.3}$$

and use this in the kinetic equation (29). Next, express $\Phi(c_0)$ as a truncated Sonine polynomial expansion,

$$\Phi(c_0) \simeq \pi^{-d/2} e^{-c_0^2} \left[ 1 - A_{01} \left( c_0^2 - d c_{0x}^2 \right) + \left( \frac{d - 1}{2} B_{01} + \frac{3}{2} B_{10} \right) c_{0x} - B_{01} c_{0x}^2 - (B_{10} - B_{01}) c_{0x}^3 \right], \tag{B.4}$$

which satisfies conditions (13) with $j_0 = 0$. The coefficients, $A_{01}, B_{01}$ and $B_{10}$, are determined from three equations obtained by taking moments of (29) with respect to $c_{0x}^2, c_{0x}^3$ and $c_{0x} c_{0x}^2$. However, these equations also depend on $\gamma$, so they are supplemented by an additional equation relating the above coefficients to $\gamma$. This equation is obtained from a new combination of equations (26) and (27),

$$B = \frac{2 \sigma^{d-1}}{\sigma^{d-1}} \left[ \int dc_0 c_{0x}^2 \mathcal{I}[c_0 | \Phi, \phi] - \int dc_0 c_{0x} \Phi(c_0) \right] \left[ \int dc_0 c_{0x}^2 \Phi(c_0) \right]. \tag{B.5}$$

Since $\phi$ and $B$ are known at this point, this gives four independent equations for the coefficients $A_{01}, B_{01}, B_{10}$ and $\gamma$. With these determined, $C$ is calculated from equation (B.3).
Figure B.1. The dimensionless parameters $a_{01}$ and $A_{01}$ as a function of the coefficient of normal restitution of the host gas particles $\alpha$ for several values of the coefficient of restitution for the collisions between the gas particles and the impurities, $\alpha_0$. The coefficient $a_{01}$ does not depend on the latter. The other (fixed) parameters are $d = 2$, $m_0 = m$ and $\sigma_0 = \sigma$.

Figure B.2. The same as in figure 1 but for the coefficients $b_{10}$ and $B_{10}$.

In practice, the above procedure leads to highly nonlinear equations for the coefficients and the collision integrals. In the numerical results to be presented in the following, only terms up to the second degree in the coefficients have been kept [3]. As an example, in figures B.1–B.3, the parameters obtained for a two-dimensional system ($d = 2$) with $m = m_0$ and $\sigma = \sigma_0 = \bar{\sigma}$ are plotted as a function of $\alpha$ for several values of $\alpha_0$. For small values of $\alpha$, the numerical solutions for the $B$ parameters constructed as described above seem to disappear.
Nearly elastic host gas

The above method for solving the kinetic equations simplifies when the host gas is nearly elastic \(|1 - \alpha| \ll 1\), but with \(\alpha_0, m/m_0\), and \(\sigma/\bar{\sigma}\) still arbitrary. The solution is given by the forms (B.2) and (B.4), with \(a_{01} = A_{01} = 0\), \(b_{01} = b_{10}\) and \(B_{01} = B_{10}\). The coefficients \(b_{01}, B_{01}, B, C\) and \(\gamma\) can then be determined explicitly.

For the special case of two dimensions (\(d = 2\)), to lowest order in \(1 - \alpha\), the properties of the host fluid are given by

\[
b_{01} \simeq 2\sqrt{(1 - \alpha)}, \quad B \simeq \sqrt{2\pi (1 - \alpha)},
\]

while the properties of the impurities are given by

\[
B_{01} \simeq \sqrt{(1 - \alpha)} \left( B_1(h) + B_2(h) \frac{\sigma}{\bar{\sigma}} \right), \quad C \simeq \sqrt{(1 - \alpha)} \left( C_1(h) + C_2(h) \frac{\sigma}{\bar{\sigma}} \right).
\]

The dependence of these quantities on \(\sigma/\bar{\sigma}\) is linear, while the dependence on \(\alpha_0\) and \(m/m_0\) occurs in the combination \(h \equiv m(1 + \alpha_0)/(m + m_0)\), with

\[
B_1(h) = \frac{54h(2 - h)^{3/2}}{\sqrt{h} \left( 27h^2 - 80h + 96 \right)}, \quad B_2(h) = \frac{32}{\sqrt{h} \left( 27h^2 - 80h + 96 \right)}, \quad \text{(B.8)}
\]

\[
C_1(h) = \frac{8\sqrt{2\pi} (2 - h)^{3/2} (5h - 6)}{27h^2 - 80h + 96}, \quad C_2(h) = -\frac{\sqrt{2\pi} \left( 27h^2 - 88h + 96 \right)}{27h^2 - 80h + 96}.
\]

The temperature ratio to lowest order in \(1 - \alpha\) is the same as that for an impurity in a homogeneously cooling gas,

\[
\gamma \simeq \frac{1 + \alpha_0 - h}{2 - h}.
\]

\(\text{(B.10)}\)
The thermal diffusion factor $\Lambda$ is given by equation (33),

\[
\Lambda = -\left(1 + \frac{\sigma C}{\sigma B}\right) = -\frac{8}{27h^2 - 80h + 96} \left(h + \frac{\sigma}{\sigma} (2 - h)^{3/2} (5h - 6)\right).
\] (B.11)

Finally, the critical value $\Lambda = 0$ is determined from

\[
\frac{\sigma}{\sigma} = h^{-1}(2 - h)^{3/2} (6 - 5h).
\] (B.12)

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