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Granular thermal diffusion in flows of binary-sized mixtures

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Summary. The revised Enskog theory was employed to analyze granular flows of binary-sized mixtures. The governing equations and constitutive relations were used to investigate granular thermal diffusion – a diffusion process resulting from the granular temperature gradient. The granular thermal diffusion causes the smaller or the lighter particles to concentrate in the region of the flow with higher granular temperature, and causes the larger or the heavier particles to concentrate in a region of lower granular temperature. A granular flow of binary mixtures in an oscillatory no-flow system and in a sheared system was examined, and indicated a complete segregation when the granular thermal diffusion was sufficiently large.

1 Introduction

A granular material is an assembly of a large number of discrete solid components that are dispersed in a fluid. This class of two-phase flow occurs in many industrial situations such as the transport of ore, coal, mineral concentrate, sand, powders, food products or tablets. In the chemical industry more than 30% of products are formed as particles [1].

In granular flows, the particles are much denser than the interstitial fluid or are closely packed, so the interstitial fluid is neglected in the bulk flow behavior. The particle-to-particle collisions are dominant in these flows [2], [3], and result in a random motion of the particles. The similarity between the random motion of the particles in a granular flow and the motion of molecules in a gas has prompted researchers to use the term granular temperature to quantify the mean-square value of the fluctuating velocities [4]. Although the granular temperature plays a similar role to the thermal temperature in the gas kinetic theory, it does not have the dimension of thermodynamic temperature but has the dimension of specific energy. In granular flows, similar to dense gases, two mechanisms influence the transport properties: the streaming or kinetic mode and the collisional mode [3]. The streaming or kinetic mode accounts for the transfer of particle properties as the particles freely move between collisions. The collisional mode accounts for the transfer of the properties during collisions. The streaming mode is dominant for the dilute flows that have larger mean-free path. The collisional mode is more important for the high-solid-fraction flows because of the higher collisional frequency.

Most granular flow analyses assume the particles are identical. However, in real applications, the particle sizes are usually not uniform. Because of the complications involved in the transport of multicomponent mixtures, this topic receives less attention except for the following studies. Shen [5] used mixing-length kinetic theory concepts to study binary-sized mixtures in a highly-concentrated simple-shear flow. The particles were of the same material, frictionless, inelastic and spherical. Farrell, Lun and Savage [6] followed the dense-gas kinetic theory for mixtures to derive the governing equations for a binary-mixture of smooth, slightly inelastic, spherical granular particles. They also calculated the stresses generated in a simple shear flow with high solid fraction. The results were compared with Shen's [5] theoretical and Savage and Sayed's [7] experimental results. Both of these theoretical studies only considered the collisional mode of the stresses. Jenkins and Mancini [8] used the more rigorous kinetic theory to derive the balance laws and the constitutive relations for a plane flow of a dense binary mixture of smooth nearly-elastic circular disks. In this study, both the kinetic and the collisional modes were considered. Jenkins and Mancini [9] used revised Enskog theory to develop a kinetic theory for binary mixtures of smooth nearly-elastic spheres. The current study follows the approach by Jenkins and Mancini [9] but focuses on granular thermal diffusion as a mechanism that may result in particle segregation.

In binary or multi-size mixtures, a segregation of particles may occur due to differences in particle size, particle mass, properties of materials, and angle-of-repose of the material [10], which has been reported in several experimental studies. In Bagnold's 1954 work, Bagnold observed that in particle mixtures the larger grains drifted toward the region of the flow of the lowest shear strain, such as to the free surface in a gravity flow [11]. Similar results were found by Savage and Lun [12] for flows of binary mixtures down inclined chutes. They measured the degree of segregation between the large and small particles as a function of downstream position and chute inclination angle. Two mechanisms were proposed: the random fluctuating sieve mechanism and the squeeze expulsion mechanism. The first mechanism results from the voids opening within the flow and the smaller particles dropping into the voids or sieve openings more readily than the larger particles. The squeeze expulsion mechanisms describes the process in which a particle may be squeezed to another layer because of an imbalance in the contact forces. This mechanism does not show a preferential direction for the migration of large or small particles. In a separate experiment that used a shear cell with a rotating bottom and side surfaces and a stationary upper surface, Savage and Sayed [7] found that the smaller particles migrated toward the outer bottom corner of the shear cell and the larger particles tended to locate in the top inner corner. Their observation was that the smaller particles moved in the direction of the resultant of the gravitational and centrifugal forces, and that the movement was linked to the probability of void spaces opening that could be filled only by the smaller particles.

In addition to these studies, there are also vibrating bed experiments as reviewed by Savage [13]. In general, the vibratory motion caused the larger particles to rise to the top of the bed. A recent study by Knight, Jaeger and Nagel [14] indicated that the particle segregation resulted from a convective motion and not from the smaller particle filling the voids within the bed. This study, however, was limited to beds in which the particles were primarily one particle size, and only a single or a few tracer particles of different diameter.

Although segregation is routinely observed in experimental studies and is important in many industrial processes [10], there is little fundamental understanding of the processes. In the present study, the focus is on segregation that is caused by granular thermal diffusion, a transport mechanism that depends on the gradient in the granular temperature.

2 Revised Enskog theory and governing equations

The first examination of the collisional transfer mechanism in dense gases was done by Enskog, but that work only considered single-sized particles. Enskog's theory and work in this field are fully described in Chapman and Cowling [15]. Throne extended the Enskog theory to binary mixtures of hard spheres [15].

Similar to the single species of dense gases, a radial distribution function describing the probability of the collisions between two particles must be evaluated. Since the particles are of different size and mass in the mixture, it is difficult to define the local density to evaluate the radial distribution function in a non-equilibrium flow. Barajas et al. [16] evaluated the radial distribution function at three different locations: the midpoint of the line connecting the two colliding particles, the contact point, and the mass center of the two colliding particles. They found that these choices were not satisfactory because the diffusion force was in conflict with irreversible thermodynamics.

Instead of using a specific point to evaluate the radial distribution function in the standard Enskog theory (SET), van Beijeren and Ernst [17] proposed a modified Enskog theory (referred by López de Haro et al. [18] as revised Enskog theory – RET), which takes the radial distribution function at the contact point as a non-local functional of the density field. The results from the RET were found to be consistent with irreversible thermodynamics. López de Haro et al. [18] employed the RET to the multicomponent mixtures and derived equations for the linear transport theory. Jenkins and Mancini [9] extended this theory to binary mixtures of smooth nearly-elastic spheres.

Much of the theoretical analysis in this paper reflects the presentation by Jenkins and Mancini [9]. Since the details of the derivation are available in the literature, only the basic nomenclature, the governing equations and some of the constitutive relations that are needed for the diffusion calculations are presented.

The subscripts α and β represent two different species in the binary-mixture, and the indices i, j are either α or β. Similar to that for a single species [19], the fluctuating velocities of the particle i are assumed to follow the singlet distribution function, $f_i^{(1)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t)$. Since the particle motion is not self-sustaining, the velocity distribution function is not Maxwellian. In this case, the singlet velocity distribution function $f_i^{(1)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t)$ is assumed to be

$$f_i^{(1)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t) = f_i^{(0)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t)\,(1 + \Phi_i), \tag{1}$$

where $\boldsymbol{c}_i$ is the particle's local velocity, $\boldsymbol{r}_i$ is the particle location, t is the time, Φ_i is a perturbation term where $\Phi_i \ll 1$, and $f_i^{(0)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t)$ is the well-known Maxwellian distribution function:

$$f_i^{(0)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t) = \frac{n_i}{(2\pi \Upsilon_i)^{3/2}} \exp\left(-\frac{(\boldsymbol{c}_i - \boldsymbol{u})^2}{2\Upsilon_i}\right). \tag{2}$$

In the Maxwellian distribution function, n_i is the number density, Υ_i is the granular temperature of species i defined by $\Upsilon_i \equiv \langle C_i^2 \rangle/3$, $\boldsymbol{u}_i$ is the mean velocity, $\boldsymbol{u}_i = \langle \boldsymbol{c}_i \rangle$. The fluctuating velocity $\boldsymbol{C}_i$ is the local velocity deviation from the mass average velocity, $\boldsymbol{C}_i = \boldsymbol{c}_i - \boldsymbol{u}$, where $\boldsymbol{u} = (\varrho_\alpha \boldsymbol{u}_\alpha + \varrho_\beta \boldsymbol{u}_\beta)/(\varrho_\alpha + \varrho_\beta)$, and ϱ_α and ϱ_β are the densities for the two species in the flows, $\varrho_i = \varrho_{pi} v_i = m_i n_i$. The symbol $\langle\,\rangle$ represents the ensemble-average quantity. The ensemble-average of the local property Ψ is determined by averaging the single-particle properties over the entire velocity space:

$$\langle \Psi_i \rangle = \frac{1}{n_i} \int \Psi_i f_i^{(1)}(\boldsymbol{r}_i, \boldsymbol{c}_i; t)\, d\boldsymbol{c}_i, \tag{3}$$

where $d\boldsymbol{c}_i = dc_{ix}\, dc_{iy}\, dc_{iz}$.

The granular temperature of the mixture is defined by

$$\Upsilon = \frac{1}{m_0 n} (\varrho_\alpha \Upsilon_\alpha + \varrho_\beta \Upsilon_\beta), \tag{4}$$

where n is the total number density, $n = n_\alpha + n_\beta$, and m_0 is the sum of the masses of particles α and β, $m_0 = m_\alpha + m_\beta$. Note that this definition of granular temperature differs from that used by Jenkins and Mancini [9]. For a binary mixture, an equipartition of fluctuating energy is assumed [5], [6]:

$$\frac{3}{2} m_\alpha \Upsilon_\alpha = \frac{3}{2} m_\beta \Upsilon_\beta . \tag{5}$$

The conservation equations are derived by examining the time rate of change of the mass, momentum or energy due to an influx of particles into the control volume, to external forces acting on the particles, and to collisional exchanges between particles. The resulting diffusion equation for species i is [9]:

$$\frac{\partial \varrho_i}{\partial t} + \nabla \cdot (\varrho_i \boldsymbol{u}_i) = 0 . \tag{6}$$

The conservation of mass equation is

$$\frac{d\varrho}{dt} = -\varrho \nabla \cdot \boldsymbol{u}, \tag{7}$$

where ϱ is the (total) bulk flow density, $\varrho = \varrho_\alpha + \varrho_\beta$. The conservation equations for momentum and fluctuating energy are as follows:

$$\varrho \frac{d\boldsymbol{u}}{dt} = -\nabla \cdot \boldsymbol{P} + \varrho_\alpha \boldsymbol{F}_\alpha + \varrho_\beta \boldsymbol{F}_\beta \tag{8}$$

and

$$\frac{3}{2} m_0 n \frac{d\Upsilon}{dt} - \frac{3}{2} m_0 \Upsilon \nabla \cdot (n_\alpha \boldsymbol{v}_\alpha + n_\beta \boldsymbol{v}_\beta) = -\nabla \cdot \boldsymbol{\Gamma} - \boldsymbol{P} \colon \nabla \boldsymbol{u} + \varrho_\alpha \boldsymbol{v}_\alpha \cdot \boldsymbol{F}_\alpha + \varrho_\beta \boldsymbol{v}_\beta \cdot \boldsymbol{F}_\beta - \gamma , \tag{9}$$

where $\boldsymbol{v}_i$ is the diffusion velocity of species i,

$$\boldsymbol{v}_i = \langle \boldsymbol{C}_i \rangle , \tag{10}$$

and $\boldsymbol{F}_i$ is the specific external force on particles of species i.

The relations for the pressure tensor, $\boldsymbol{P}$, and the fluctuating energy flux $\boldsymbol{\Gamma}$, and the energy dissipation due to the inelastic collisions per unit volume, γ, are derived in the work by Jenkins and Mancini [9]. The relations are given here because the formulations are slightly different from those in [9].

The normal stress or the granular pressure in the mixture P is

$$P = m_0 \Upsilon \left(n + \sum_{i=\alpha,\beta} \sum_{j=\alpha,\beta} \frac{2}{3} \pi n_i n_j \sigma_{ij}^3 g_{cij} \right) . \tag{11}$$

The diameters of the two species are σ_i and σ_j and the average diameter is $\sigma_{ij} = (\sigma_i + \sigma_j)/2$. In (11), g_{cij} is the equilibrium value of the radial distribution function of particles i and j at contact, which is found by substituting the local density as the equilibrium density and is expressed as [9], [20]

$$g_{cij} = \left[Z^2 + \frac{3\sigma_i \sigma_j}{\sigma_i + \sigma_j} Z Z_2 + 2 \left(\frac{\sigma_i \sigma_j}{\sigma_i + \sigma_j} \right)^2 Z_2{}^2 \right] \Big/ Z^3 , \tag{12}$$

where

$$Z_l = \frac{\pi}{6} \sum_{j=\alpha,\beta} n_j \sigma_j^l, \quad l = 1, 2, 3; \quad Z = 1 - Z_3. \tag{13}$$

Note that Z_3 is equal to the total solid fraction, $Z_3 = \nu = \nu_\alpha + \nu_\beta$. This equilibrium radial distribution function is originally derived by Mansoori et al. [21] and is known as the Carnahan-Starling approximation. The first term of the pressure in (11) is the contribution from the kinetic or streaming mode of energy transfer and the second is from the collisional mode.

When there is no net diffusion indicating a balance between particle diffusion and granular thermal diffusion, the shear stress and the fluctuating energy flux are given by

$$P_{nl} = -\mu \frac{\partial u_n}{\partial r_l}, \quad n, l, r_l = x, y, z, \quad k \neq l, \tag{14}$$

and

$$\Gamma_l = -\lambda \frac{\partial \Upsilon}{\partial r_l}, \quad l, r_l = x, y, z, \tag{15}$$

where μ is the mixture viscosity and λ is the granular thermal conductivity, which can be found in [9]. The energy dissipation due to the inelastic collisions per unit volume is derived as

$$\gamma = \sum_{i=\alpha,\beta} \sum_{j=\alpha,\beta} 4 g_{cij} \sigma_{ij}^2 n_i n_j M_{ji} \frac{1 - e_{p,ij}^2}{2} \sqrt{\frac{2\pi m_{ij} m_0{}^3 \Upsilon^3}{m_i m_j}}. \tag{16}$$

From (10), the difference between the diffusion velocities of the two species is determined from

$$\boldsymbol{v}_\alpha - \boldsymbol{v}_\beta = -\frac{n^2}{n_\alpha n_\beta} D_{\alpha\beta} \left(\boldsymbol{d}_\alpha + k_\Upsilon \frac{1}{\Upsilon} \nabla \Upsilon \right), \tag{17}$$

where $D_{\alpha\beta}$ is the diffusion coefficient given by

$$D_{\alpha\beta} = \frac{3}{2n} \sqrt{\frac{2\Upsilon}{\pi M_{\alpha\beta} M_{\beta\alpha}}} \frac{1}{8 \sigma_{\alpha\beta}^2 g_{c\alpha\beta}}, \tag{18}$$

k_Υ is granular-thermal-diffusion ratio expressed as

$$k_\Upsilon = \frac{4}{3} \sqrt{\pi}\, \sigma_{\alpha\beta}^2 \frac{n_\alpha n_\beta}{n} [M_{\beta\alpha}^{3/2} a_{\alpha 1} - M_{\alpha\beta}^{3/2} a_{\beta 1}], \tag{19}$$

and $\boldsymbol{d}_i$ is the diffusion force:

$$\begin{aligned} \boldsymbol{d}_i = {} & \frac{-\varrho_i}{m_0 n \varrho \Upsilon} \left[\nabla P + \sum_{j=\alpha,\beta} \varrho_j (\boldsymbol{F}_i - \boldsymbol{F}_j) \right] \\ & + \sum_{j=\alpha,\beta} \frac{n_i}{n} \left(\delta_{ij} + \frac{4}{3} \pi n_j \sigma_{ij}^3 M_{ij} g_{cij} \right) \nabla \ln \Upsilon \\ & + \sum_{j=\alpha,\beta} \frac{n_i}{m_0 n \Upsilon} \left(\frac{\partial \mu_i}{\partial n_j} \nabla n_j \right). \end{aligned} \tag{20}$$

In the above equations, δ_{ij} is the Kronecker delta and $M_{ij} \equiv m_i/m_{ij} = m_i/(m_i + m_j)$, and $a_{\alpha,1}$ and $a_{\beta,1}$ are two coefficients that are dependent on the particle diameters, densities and the radial distribution function and are found in [9]. The granular chemical potential of species i, μ_i, depends on the radial distribution function. Corresponding to the form of equilibrium distribution function derived by Mansoori et al., the granular chemical potential μ_i is derived by Reed and Gubbins [22] and can also be found in [9], [20]. The diffusion force is the main difference that results from using RET instead of SET. Since there is no mass transfer during collisions, the mutual diffusion only depends on the kinetic mode.

The self-diffusion process in a single species granular flow was studied by Hsiau and Hunt [23], [24] and by Savage and Dai [25]. For binary mixtures, the granular thermal diffusion results from the granular temperature gradient as indicated in (17). The granular-thermal-diffusion ratio k_T is the ratio of the granular thermal diffusion coefficient, D_T, to the mutual-diffusion coefficient, $D_{\alpha\beta}$. From (19), k_T is 0 if the two species are identical, meaning there is no granular thermal diffusion for a single-species granular flow. The granular-thermal-diffusion ratio in (19) is positive if species α is more massive, or if α is of larger size than species β. The effect of the granular thermal diffusion is that the lighter or the smaller particles move to the position with higher granular temperature, and the heavier or the larger particles move in the opposite direction. This phenomenon has been demonstrated in the theoretical development and in some experiments for gases and liquids [15].

The diffusion coefficient given by (18) has the same form as derived by Throne for the perfectly-elastic dense gases. Since the present theory neglects the higher order terms, the inelasticity does not enter the equation. If the two species are identical, then (18) is the same as the diffusion coefficient derived by Hsiau and Hunt [24] and by Savage and Dai [25] when their expressions are evaluated for $e_p = 1$. Although the diffusion coefficient derived by RET is the same as that derived by SET, the diffusion force is different, resulting in a different diffusion flux.

3 Granular thermal diffusion in flows of binary mixtures

In the previous Sections, the governing equations and the constitutive relations for a binary mixture of granular materials are presented. Unlike transport in single-sized materials, the pressure gradient, the number density gradient, and the granular temperature gradient all influence the diffusion process. In this work, the former effects are referred to as particle diffusion (mass diffusion), and the latter effect is called granular thermal diffusion.

The rigorous theory about thermal diffusion in gases was first analyzed by Enskog and Chapman [15]. Frankel [26] and Furry [27] offer elementary explanations of the physical meaning of thermal diffusion for dilute gases. A similar explanation can be applied to granular flows in which the contribution to the pressure is mainly from the kinetic mode of transfer.

Consider a system in which the total pressure is constant, but in which there is a gradient in partial pressures due to granular thermal diffusion. The gradient of the partial pressure of one species is equal in magnitude and opposite in sign of the partial pressure gradient of the second species. In addition, the gradient of the partial pressure of one species, i, in a particular direction y equals the y component of momentum for the i particles in that direction,

$$\frac{dP_{ii,y}}{dy} = -\Xi_{ij,y}, \tag{21}$$

where $\Xi_{ij,y}$ is the average momentum transfer in y direction per unit volume per unit time. Since collisions between like particles do not alter the net momentum, only collisions between particles of type i and j are included in (21). Since collisions between particles with the greatest relative velocity determine the direction of the momentum transfer, consider a collision between a light particle coming from a region of high granular temperature and a heavier particle coming from a region of the low granular temperature. This kind of collision results in a net momentum transfer from the lighter particle to the heavier particle, which is the direction opposite to that of the granular temperature gradient. Hence, from (21), the partial pressure of the lighter species increases in the opposite direction of that of the momentum transfer, which is in the direction of granular temperature gradient. Since the partial pressure depends on the partial number density as given in (11), this effect causes the lighter particles to concentrate in the place with higher granular temperature.

The present study considers two-dimensional (in xy-plane) flows of binary granular materials in a steady state. The gradients only exist in y-direction, since the flow is assumed to be fully developed in x-direction. From (8) and (9), the governing equations can be simplified as:

$$-\frac{\partial P_{yy}}{\partial y} + \varrho_\alpha F_{\alpha,y} + \varrho_\beta F_{\beta,y} = 0, \tag{22}$$

$$-\frac{\partial P_{xy}}{\partial y} + \varrho_\alpha F_{\alpha,x} + \varrho_\beta F_{\beta,x} = 0, \tag{23}$$

and

$$-\frac{\partial \Gamma_y}{\partial y} - P_{xy}\left(\frac{\partial u_x}{\partial y}\right) - \gamma = 0, \tag{24}$$

where $F_{i,x}$ and $F_{i,y}$ are the specific external forces acting on particle i in the x and y directions. For zero net diffusion of particles, the diffusion velocities $\boldsymbol{v}_i$ are zero, and (19) simplifies to

$$d_{\alpha,y} + k_\Upsilon \frac{\partial \ln \Upsilon}{\partial y} = 0, \tag{25}$$

where $d_{\alpha,y}$ is the y component of the diffusion force $\boldsymbol{d}_\alpha$.

As mentioned earlier, granular thermal diffusion is caused by a granular temperature gradient. From (17), the conduction of granular temperature is influenced by the shear work and the energy dissipation. To investigate clearly the influence of the granular temperature on the diffusion process, an oscillatory system without any bulk motion of perfectly-elastic materials is first examined in Section 3.1. The more complicated system of a sheared flow is studied in Section 3.2. In both studies the emphasis is on the extent of particle segregation that results from thermal diffusion. To solve for the distribution in number density, boundary conditions are needed for the velocity and the granular temperature in order to integrate the governing equations. However, in granular flows analytical representations for the boundary conditions are problematic because the standard no-slip conditions used in conventional fluid mechanics cannot be imposed. As shown in the work by several studies such as that by Richman [28] and by Jenkins [29], the boundary conditions result from detailed balances of momentum and energy at the solid surfaces. As a result, the boundary conditions depend on the entire flow field, so the velocity and the granular temperature cannot be specified independently. By considering the interaction between the boundary and the flow field, these studies derived the boundary conditions for granular flows of single-species spheres interacting with bumpy surfaces or with flat frictional surfaces. However, these boundary conditions are only for single-sized particles and not for mixtures. The extension of these studies to include binary-mixtures is a formidable task. As a result, the boundary conditions used in this work are not based on the detailed balances of momentum and energy. Instead, granular thermal diffusion is the emphasis of this work.

3.1 Oscillatory no-flow system

Consider a steady system without mean motion between two parallel boundaries as shown in Fig. 1. The body forces are neglected. The momentum equation in the x direction disappears since there is no shearing of the flow. From (15), the momentum equation is:

$$\frac{\partial P}{\partial y} = 0, \tag{26}$$

and using (11), the momentum equation is rewritten as

$$\frac{\partial}{\partial y}\left[\Upsilon\left(n + \sum_{i=\alpha,\beta}\sum_{j=\alpha,\beta}\frac{2}{3}\pi n_i n_j \sigma_{ij}^3 g_{cij}\right)\right] = 0. \tag{27}$$

From (15) and (24), the balance equation for the fluctuating energy is

$$\frac{\partial}{\partial y}\left(\lambda\frac{\partial \Upsilon}{\partial y}\right) = 0. \tag{28}$$

Note that since the particles are assumed perfectly-elastic ($e_{p,ij} = 1$), the energy dissipation γ is zero.

Using (19) and (20), the diffusion equation (25) becomes

$$\left[k_\Upsilon + \sum_{j=\alpha,\beta}\frac{n_\alpha}{n}\left(\delta_{\alpha j} + \frac{4}{3}\pi n_j \sigma_{\alpha j}^3 M_{\alpha j} g_{c\alpha j}\right)\right]\frac{\partial \ln \Upsilon}{\partial y} + \frac{n_\alpha}{m_0 n \Upsilon}\sum_{j=\alpha,\beta}\frac{\partial \mu_\alpha}{\partial n_j}\frac{\partial n_j}{\partial y} = 0. \tag{29}$$

The granular temperature Υ and the channel location y can be normalized by the granular temperature at $y = 0$, Υ_0, and by the channel width L, $\Upsilon^* = \Upsilon/\Upsilon_0$ and $Y = y/L$. Then Eqs. (26)–(29) can be rewritten as four first-order ordinary differential equations for dv_α/dY, dv_β/dY, $d\Upsilon^*/dY$ and $d^2\Upsilon^*/dY^2$. As mentioned in the previous Section, the boundary conditions are chosen to demonstrate the diffusion process and may not be representative of physical boundary conditions. The four boundary conditions used to solve the equations are:

$$\Upsilon^*(Y = 0) = 1, \tag{30}$$

$$\Upsilon^*(Y = 1) = \Upsilon_L^*, \tag{31}$$

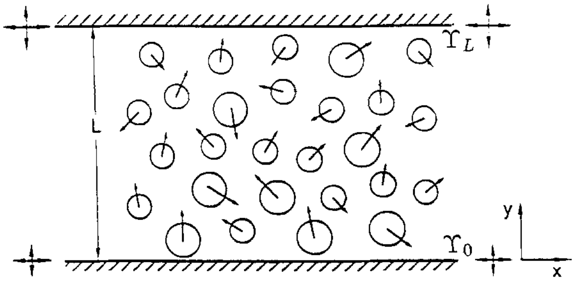

Fig. 1. Configuration of an oscillatory no-flow system

$$\int_0^1 \nu_\alpha(Y)\, dY = \overline{\nu_\alpha}, \tag{32}$$

$$\int_0^1 \nu_\beta(Y)\, dY = \overline{\nu_\beta}. \tag{33}$$

By a Runge-Kutta method, this system of equations can be solved. For the current calculations, the average solid fractions of species α and β of 0.1 and 0.25 are used, and the solid fractions are selected as $\overline{\nu_\alpha} = 0.1$ and $\overline{\nu_\beta} = 0.25$. The dimensionless granular temperature at $Y = 1$ is chosen to be 2 for the calculations, $\Upsilon_L{}^* = 2$. The calculations are performed for four different sizes of α: (a) $\sigma_\alpha = 1$ mm, (b) $\sigma_\alpha = 1.2$ mm, (c) $\sigma_\alpha = 1.5$ mm, (d) $\sigma_\alpha = 2$ mm; and the particle diameters of species β are 1 mm in the four cases and the particle densities of both species are 2490 kg/m^3.

Figure 2 shows the solid fraction distributions for case (a) where species α and β are identical. Since the two species are identical, there is no granular thermal diffusion and hence the solid fractions of both species decrease in the positive y direction in a similar ratio. To balance the momentum equation, the granular pressure is constant in the channel, so the solid fractions decrease with the increase of granular temperature. To check the numerical integration, this case is calculated by the theory of Lun et al. [19] for the single-species material, and the resulting granular temperature profiles are nearly identical. The solid fraction profiles are compared in Fig. 2 and the difference is less than 2%. The difference is because the RET is employed in the present theory.

Figure 3 presents the solid fraction distributions for case (d). As indicated by the figure, the smaller particles (β) tend to move to the region with higher granular temperature and the larger particles (α) tend to move in the opposite direction. For the smaller (lighter) particles, the granular thermal diffusion causes a diffusive flux in the direction of the granular temperature gradient and results in the increase of the partial number density n_β. Due to the partial number density gradient, particle diffusion causes the smaller particles to diffuse to the opposite direction of the gradient of the partial number density, that is the direction in which the granular temperature decreases. Hence, a balance is established between particle diffusion and granular

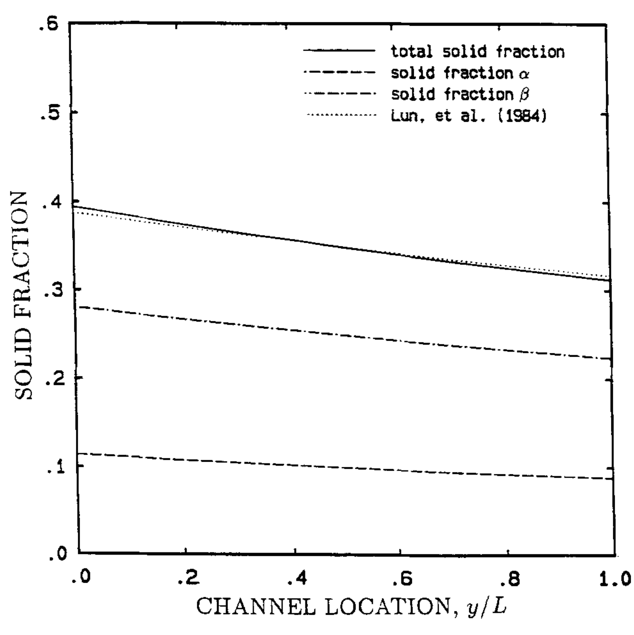

Fig. 2. The distributions of solid fractions when two species are identical (case (a)). The dotted line is calculated from the theory of Lun et al. [19] for the single-size material.

thermal diffusion so that there is no net diffusive flux. A similar diffusive balance occurs for the larger particles.

In Fig. 4, the four curves are the granular temperature distributions for the four cases. The differences in the granular temperature profiles result from the variations in the solid fractions which are due to granular thermal diffusion.

Figure 5 shows the ratios of the solid fractions v_β/v_α in the channel for the four cases in log scale. Due to the granular thermal diffusion, the ratio increases with the granular temperature. The ratio of v_β/v_α increases faster for higher ratio of $\sigma_\alpha/\sigma_\beta$, which indicates the larger size difference causes an increase in the granular thermal diffusion. For case (a), since there is no granular thermal diffusion, the distribution of v_β/v_α is flat.

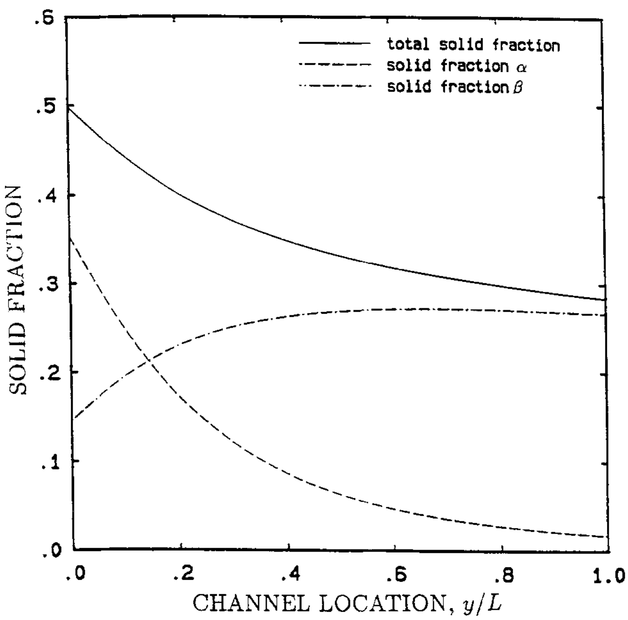

Fig. 3. The distributions of solid fractions for case (d): $\sigma_\alpha = 2$ mm, $\sigma_\beta = 1$ mm

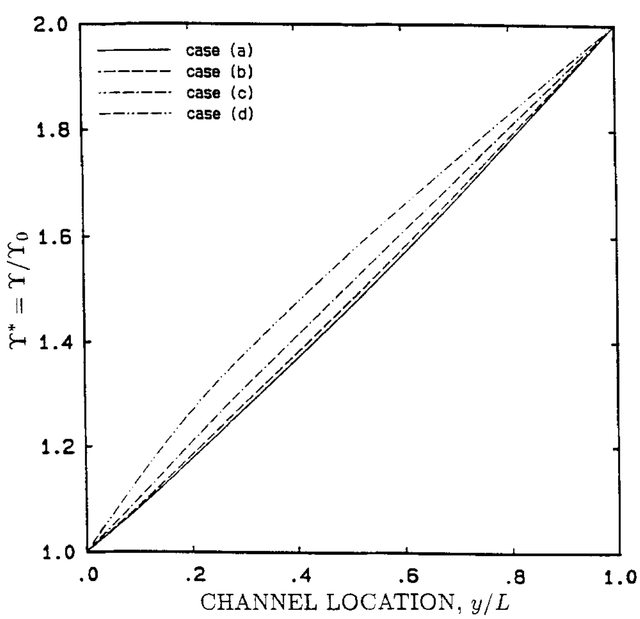

Fig. 4. Granular temperature distributions for four different sizes of α: (a) $\sigma_\alpha = 1$ mm, (b) $\sigma_\alpha = 1.2$ mm, (c) $\sigma_\alpha = 1.5$ mm, (d) $\sigma_\alpha = 2$ mm

In Fig. 6, the ratio of ν_β/ν_α is presented in a log scale for the same particle diameters but different particle densities. The particle density of species α is 2490 kg/m^3 but the ratios of particle densities vary for the four cases: $\varrho_{p\alpha}/\varrho_{p\beta} = 1, 2, 3, 4$. The case of $\varrho_{p\alpha}/\varrho_{p\beta} = 1$ means identical species as discussed above. The higher ratio of $\varrho_{p\alpha}/\varrho_{p\beta}$ indicates a larger mass difference, which results in enhanced granular thermal diffusion; hence the ratio of ν_β/ν_α increases faster.

When the difference in size or mass of the two species is increased or the granular temperature gradient is increased, transport due to granular thermal diffusion becomes more significant. If any factor is large enough, the two species can be completely segregated. One example is shown in Fig. 7 plotted for the solid fraction distributions for the case of $\Upsilon_L{}^* = 3$, $\sigma_\alpha/\sigma_\beta = 2$, and $\varrho_{p\alpha}/\varrho_{p\beta} = 4$.

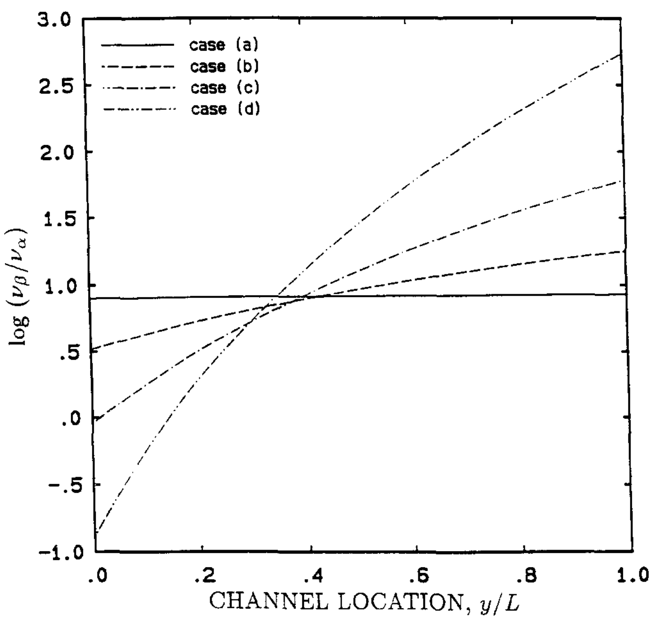

Fig. 5. The distributions of the ratio of ν_β/ν_α for the four cases

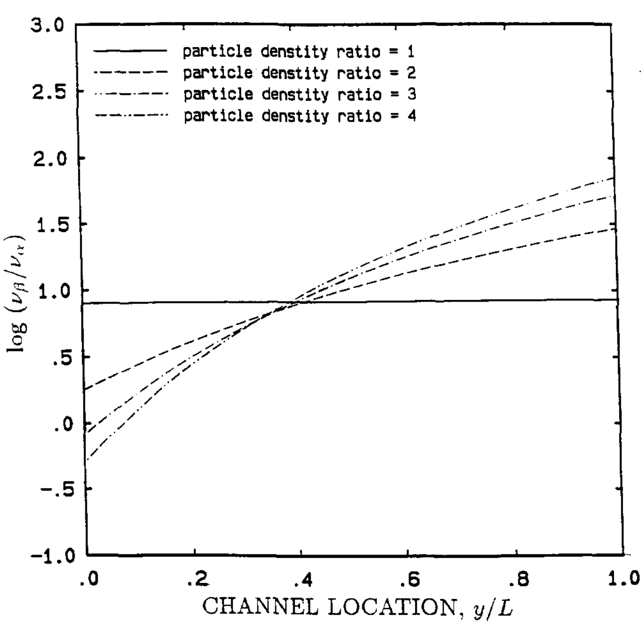

Fig. 6. The distributions of the ratio of ν_β/ν_α for four different $\varrho_{p\alpha}/\varrho_{p\beta}$

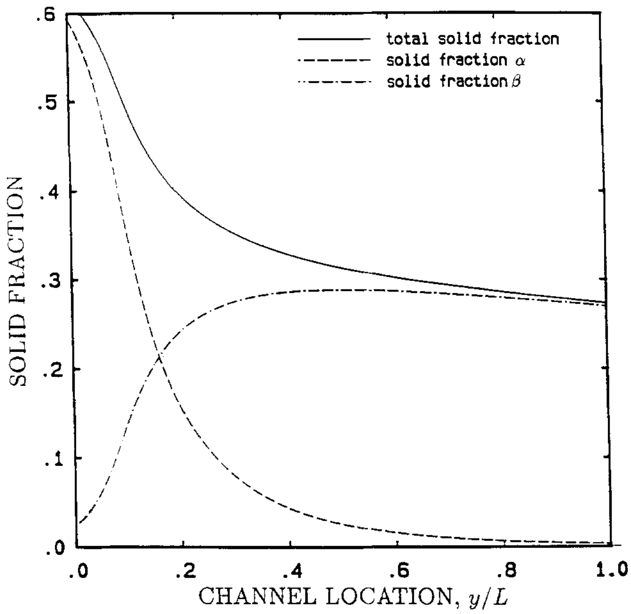

Fig. 7. The distributions of the solid fractions for $\Upsilon_L/\Upsilon_0 = 3$, $\sigma_\alpha/\sigma_\beta = 2$, and $\varrho_{p\alpha}/\varrho_{p\beta} = 4$

3.2 Sheared granular flows

In this part, a steady and fully developed sheared flow of a binary mixture between two parallel boundaries is studied. The configuration of this system is shown in Fig. 8. The external forces are neglected. The momentum equation in y direction and the equation for zero diffusion velocity remain the same as (26), (27) and (29) for the oscillatory no-flow system. From (23) and (14), the momentum equation in x-direction is written as:

$$\frac{\partial}{\partial y}\left(\mu \frac{\partial u_x}{\partial y}\right) = 0. \tag{34}$$

Using (14) and (15) in (24), the conservation equation for energy is

$$\frac{\partial}{\partial y}\left(\lambda \frac{\partial \Upsilon}{\partial y}\right) + \mu \left(\frac{\partial u_x}{\partial y}\right)^2 = \gamma. \tag{35}$$

The first term in (35) is the fluctuating energy added to the system by the conduction of the granular temperature and the second term is the shear work done to the system. The sum of these two terms is equal to the energy dissipation due to the inelastic collisions. Equation (35) can be nondimensionalized to

$$\frac{\partial}{\partial Y}\left(\lambda^* \frac{\partial \Upsilon^*}{\partial Y}\right) + R_1{}^2 R_2{}^2 \mu^* \left(\frac{\partial u_x{}^*}{\partial Y}\right)^2 = R_2{}^2 \gamma^*. \tag{36}$$

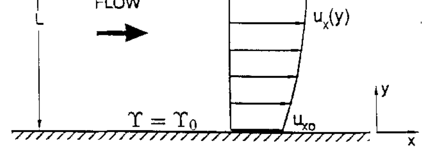

Fig. 8. Configuration of a shear flow

The dimensionless variables Υ^*, u_x^*, λ^*, μ^* and γ^* are defined as $\Upsilon^* = \Upsilon/\Upsilon_0$, $u_x^* = (u_x - u_{x0})/(u_{xL} - u_{x0}) = (u_x - u_{x0})/\Delta u_x$, $\lambda^* = \lambda/(\sqrt{\Upsilon_0}\, \varrho_{p\beta}\sigma_\beta)$, $\mu^* = \mu/(\sqrt{\Upsilon_0}\, \varrho_{p\beta}\sigma_\beta)$, $\gamma^* = \gamma\sigma_\beta/(\Upsilon_0^{3/2}\varrho_{p\beta})$ and $Y = y/L$, where Υ_0 and u_{x0} are the granular temperature and the velocity at $y = 0$ respectively, u_{xL} is the velocity at $y = L$, and L is the channel width. The dimensionless parameter R_1 is defined by

$$R_1 = \frac{\sigma_\beta(\Delta u_x/L)}{\sqrt{\Upsilon_0}}, \tag{37}$$

and R_2 is the ratio of the channel width to the smaller particle diameter, $R_2 = L/\sigma_\beta$.

Equations (27), (34), (36) and (29) can then be rewritten as six first-order ordinary differential equations for dv_α/dY, dv_β/dY, $d\Upsilon^*/dY$, $d^2\Upsilon^*/dY^2$, du_x^*/dY and $d^2u_x^*/dY^2$. Six boundary conditions are used to solve the equations. The first four boundary conditions are the same as that used in the oscillatory no-flow system and the other two are

$$u_x^*(Y = 0) = 0, \tag{38}$$

and

$$u_x^*(Y = 1) = 1. \tag{39}$$

As discussed before, the boundary conditions for the sheared granular flows should be determined by the whole flow field. However, due to the lack of information regarding boundary conditions for binary-mixture flows, the imposed boundary conditions are used.

The Runge-Kutta method is employed to solve these equations. Due to the effect of granular thermal diffusion, the solid fraction of the smaller or the lighter particles (β) is found to increase with the positive gradient of granular temperature and to decrease when the granular temperature decreases. The only exception occurs when the solid fraction of the larger or the heavier species is close to 0; in order to maintain the constant mixture pressure, the solid fraction of the smaller (lighter) particles has to decrease with the increase of granular temperature.

In the current calculations, $\sigma_\alpha = 2$ mm, $\sigma_\beta = 1$ mm, $\varrho_{p\alpha} = \varrho_{p\beta} = 2490$ kg/m^3, $e_{p,ij} = 0.95$ and $R_2 = 20$ are used. According to the computer simulation results for simple shear flows of a granular material by Campbell [30], the parameter $(\sigma_i\, du_x/dy)/\sqrt{\Upsilon_i}$ ranges from 0 to 1. The present calculation uses R_1 from 2 to 3 so that $(\sigma_i\, du_x/dy)/\sqrt{\Upsilon_i}$ for both species is between 0 and 1 anywhere in the channel. The total solid fractions $\bar{v}$ are chosen between 0.3 and 0.45. Three different cases are studied, which result in three very different profiles of the solid fraction distributions and the granular temperature distributions. The three typical cases are explained as follows.

Figure 9 shows the granular temperature and solid fraction distribution for $\Upsilon_L^* = 10$, $\overline{v_\alpha} = 0.03$, $\overline{v_\beta} = 0.28$, and $R_1 = 2.9$. The second derivative of granular temperature is always positive in the channel indicating that the fluctuating energy is added to the system everywhere, and the energy dissipation is greater than the shear work done to the system. The ratio of v_β/v_α is increasing with the granular temperature resulting from the granular thermal diffusion similar to the oscillatory no-flow system. Note that the first derivative of granular temperature at $Y = 0$ is positive.

Figure 10 presents the distributions of granular temperature and solid fraction for $\Upsilon_L^* = 15$, $\overline{v_\alpha} = 0.08$, $\overline{v_\beta} = 0.25$, and $R_1 = 2.5$. The second derivative of granular temperature is positive, similar to the last case, indicating that the energy dissipation is larger than the shear work so that the fluctuating energy has to be conducted into the system. The first derivative at $Y = 0$ is negative causing the granular temperature to decrease until a certain position ($Y = 0.068$ in this case) where the first derivative of granular temperature starts to change sign. The corresponding

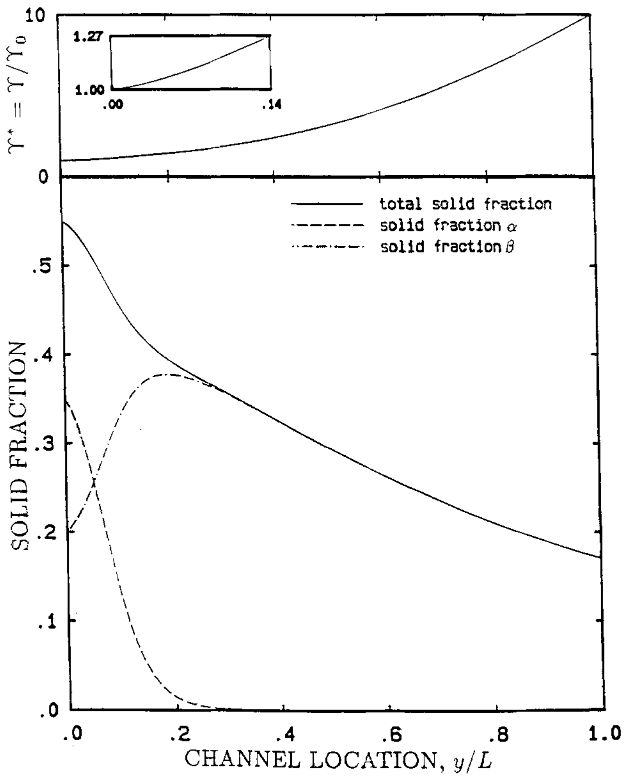

Fig. 9. Granular temperature and solid fraction distributions in a shear flow for $T_L{}^* = 10$, $\overline{\nu_\alpha} = 0.03$, $\overline{\nu_\beta} = 0.28$, and $R_1 = 2.9$

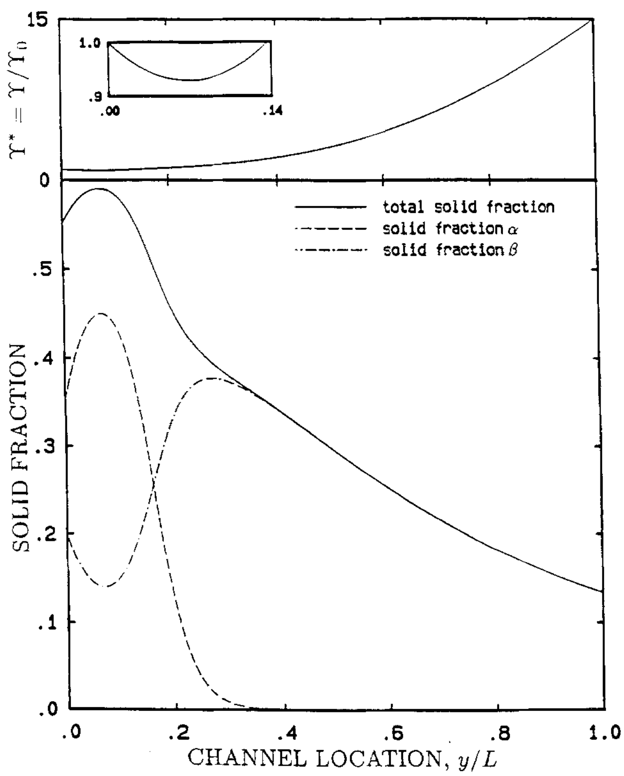

Fig. 10. Granular temperature and solid fraction distributions in a shear flow for $T_L{}^* = 15$, $\overline{\nu_\alpha} = 0.08$, $\overline{\nu_\beta} = 0.25$, and $R_1 = 2.5$

solid fraction of the smaller particles shows the same trend as the granular temperature before $Y = 0.272$. Since after this position the solid fraction of the larger particles is relatively small, the smaller particle solid fraction decreases with the increase of granular temperature to maintain a constant pressure.

The third case is presented in Fig. 11 for $\Upsilon_L{}^* = 1.15$, $\overline{\nu_\alpha} = 0.07$, $\overline{\nu_\beta} = 0.35$, and $R_1 = 2.2$. The second derivative of granular temperature is negative in the channel indicating that the energy dissipation is smaller than the shear work done to the system. Hence, the fluctuating energy is conducted from the system. The solid fractions and the granular temperature are relatively flat in the center of the channel.

Note that in the first two cases the granular thermal diffusion causes segregation of the two species of particles. By contrast, in the last case, there is not a complete segregation of the particles.

Figure 12 shows the velocity distributions for these three shear flow cases. The shear rate in the beginning of the channel for the third case is the largest and the granular temperature in this case is relatively small ($\Upsilon_L{}^* = 1.15$). Hence the shear work is higher than the energy dissipation resulting in the negative second derivative of the granular temperature.

In the literature, a shear flow with constant granular temperature, constant solid fractions and constant shear rate is called a simple shear flow. Since no granular temperature gradient exists in these flows, there is no granular thermal diffusion. Most binary mixtures studies only discuss simple shear flows. Jenkins and Mancini [9] assumed a simple shear flow to predict the shear stress for a binary particle mixture. They compared with the numerical results from Farrell et al. [6] and the computer simulation results from Walton [31]. The current numerical integration is checked with Jenkins and Mancini's result using the same assumptions; no difference is found between the two calculations.

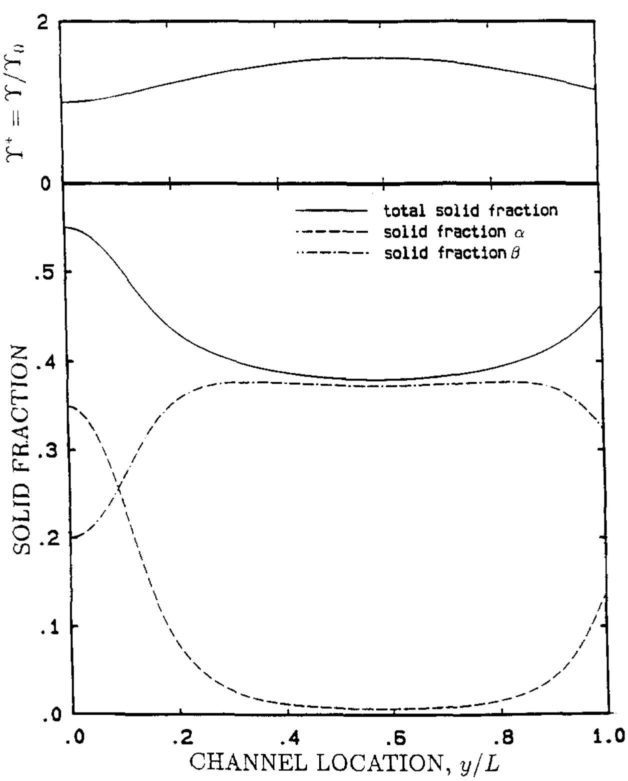

Fig. 11. Granular temperature and solid fraction distributions in a shear flow for $T_L{}^* = 1.15$, $\overline{\nu_\alpha} = 0.07$, $\overline{\nu_\beta} = 0.35$, and $R_1 = 2.2$

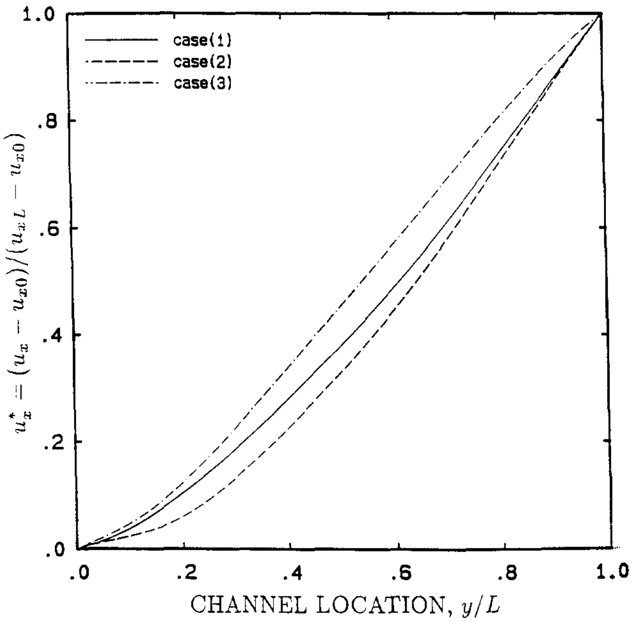

Fig. 12. Velocity distributions for the cases in Figs. 9–11

5 Conclusions

Jenkins and Mancini [9] extended the revised Enskog theory to binary mixtures of smooth, nearly elastic granular material. The transport equations and constitutive relations are used to examine granular thermal diffusion in an oscillatory no-flow system and in a sheared flow. Due to the granular thermal diffusion, the lighter (smaller) particles tend to move to the place with higher granular temperature, and the heavier (larger) particles tend to move in the opposite direction. The granular thermal diffusion is more significant when the difference in sizes or masses of the two species is increased or the granular temperature gradient is increased. Although the boundary conditions used to integrate the governing equations may not be physically realistic, the results indicate that the two different types of particles may be completely segregated due to this effect. Future work should focus on the experimental measurements of the relation between granular thermal diffusion and particle segregation.

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