THE STRESSES DEVELOPED DURING THE SIMPLE SHEAR OF A GRANULAR MATERIAL COMPRISED OF SMOOTH, UNIFORM, INELASTIC SPHERICAL PARTICLES

by

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ABSTRACT

From the approach of Maxwell transport theory in the context of dense gases, conservation laws and constitutive integrals for the flow of identical, smooth, inelastic, spherical granular materials are derived. The problem of rapid simple shear flow of such materials is considered specifically. The constitutive integrals are solved approximately by the use of asymptotic expansions and series transformations in terms of a non-dimensional parameter R, which is the ratio of the characteristic mean shear velocity to the r.m.s. of the particle fluctuation velocity and is found to depend upon the coefficient of restitution of the particles.

The predicted stresses are compared with the experiments of Savage and Sayed (1980) and yield the correct order of magnitude when the coefficient of restitution is given the values of around 0.8 to 0.9. Comparisons made with several previous theories exhibit similar trends of behaviour in the constitutive relationships. The present theory also shows fair agreement in comparison of stresses with the kinetic theory of dense gases using the hard sphere model in the case of simple shear.

RESUME

En appliquant la théorie de transport de Maxwell dans le contexte des gaz lourds, on obtient les lois de conservation et les intégrales constitutives pour un courant de milieux granulaire de grains à formes identiques, lisses, non-élastiques et sphériques. L'analyse actuelle est adoptée spécifiquement au problème de courant de cisaillement simple et rapide. Les intégrales constitutives sont solutiounées approximativement en utilisant les expansions asymptotiques et les transformations de suites en fonction d'un paramètre non-dimensionel R qui est le rapport de la vitesse charactéristique moyenne de cisaillement à la racine carrée moyenne de la vitesse de fluctuation des particules. On trouve que R dépend du coefficient de restitution des particules.

Les forces de tension prédites sont comparées aux expériences de Savage et Sayed (1980); elles donneut un ordre de grandeur exacte quand le coefficient de restitution a une valeur approximative de 0.8 à 0.9. Des comparaisons sont faites avec plusierurs théories précédentes; elles révèlent des comportement similaires concernant les relations constitutives. La théorie actuelle montre aussi une bonne correspondance en comparant les forces de tension avec la théorie cinétique de gaz lourds en utilisant le modèle de la sphère rigide dans le cas d'un simple cisaillement.

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CHAPTER 1 INTRODUCTION

The flow of granular materials, which is but one member of a vast family of two-phase flow systems, is a phenomenon that exists not only in nature but also occurs in numerous industrial processes. In nature, examples of granular flow include snow avalanches, drift of pack ice flow on the sea surface, landslides, submarine slides, debris flows and sediment transport in rivers. Such geophysical granular flow systems usually occur on large scales and in some cases they may be threats to the environment and human life. Information about the basic mechanisms responsible for these phenomena may contribute to the mastery and prevention of such catastrophic events. From the industrial and engineering point of view, ample applications of granular flow exist: the transportation of sand and gravel, grains, soil, ore, pills, oil sand, fluidized bed burning of coal, mineral and powder processing, slurry flows in pipelines, etc. A better understanding of the governing mechanisms of such processes may be beneficial to the design and improvement of the transport equipment and handling devices. In terms of industrial economics, such information about the basic granular behaviour may aid in the form of efficiency in performance of the processes. However, as is often the case, the subject is far from simple.

Bagnold (1954) classified the flows of granular materials into three categories: the macro-viscous, transitional and grain-inertia regimes. In the macro-viscous regime, the effects of fluid viscosity dominate over that of grain inertia. Conversely, in the grain-inertia regime, the effect of grain inertia dominate over that of fluid viscosity. In between these two limiting cases, there is the transitional regime where the system transits from inertia to viscous conditions and both effects are important. A consistent treatment and characterization of this dynamical problem of granular flow taking into account the effects of all three regimes is extremely difficult. So far not a single analytical theory which can describe satisfactorily the general flow behaviour of granular materials has emerged. Such slow development in the theoretical work is partially due to the complexity of the materials behaviour. As pointed out in a recent review by Savage (1982), a clear understanding of the mechanics underlying granular flows requires the utilization of ideas from fluid mechanics, plasticity theory, soil mechanics, rheology and kinetic theory of gases. Another hinderance to the theoretical developments is due to the scarcity of reliable experimental observations.

1.1 Review of Previous Work

Bagnold (1954) developed a rudimentary theoretical analysis for simple shear of granular materials and performed experiments on neutrally buoyant, identical, spherical particles made up of a mixture of paraffin wax and lead sterate suspended in Newtonian fluids (water and a glycerine-water-alcohol mixture). The mixture of beads was sheared in a coaxial rotating cylinder apparatus with a flexible rubber inner cylinder wall and a rotating rigid outer cylinder. In such a device, both shear and normal stresses were measured at various solids concentration and shear rates. In the macro-viscous regime, both measured shear and normal stresses indicated a linear depedence upon the shear rate. In the grain-inertia regime, both the shear and normal stresses were found to behave in a non-Newtonian way which depended upon the particle mass density, the square of the particle diameter and the square of the shear rate. The stresses increased rapidly with the increase of solids concentration, especially at high values.

Savage and Sayed (1980, 1982 and Sayed 1981) have carried out extensive viscometric experiments on dry granular materials, such as spherical glass and polystyrene beads, and angular particles of crushed walnut shells using a new model of annular shear cell. The device was designed to measure both the shear and normal stresses as functions of solids concentration and apparent shear rate. In their experiments of shearing single size spherical particles, both the shear and normal stresses indicated dependence upon the square of the shear rate at the lower concentrations and higher shear rates. However, at higher concentrations and lower shear rates, the stresses were found to be proportional to the shear rate of power less than two. This change in shear rate dependence was attributed to the increase of dry frictional effect between particles at high concentrations.

Tests with different sizes and mass densities of the particles indicated that the stresses depended upon particle mass density and the square of the particle diameter, supporting Bagnold's experimental results in the grain-inertia regime. Stresses also depended strongly upon solids concentration. The tests of angular crushed walnut shells shows similar trends in the results. When an initially well mixed binary size mixture of spherical particles was tested, particle segregation, having the small ones at the outer radii and large ones at the inner region of the shear cell, was reported to have occurred at the end of the test. This segregational effect of particle sizes under shear is by itself another distinct important phenomenon. As yet no theoretical explanation of this phenomenon from a dynamical point of view has been attempted.

The main concern of the present work deals specifically with the limiting case of granular flow in the grain-inertia regime, where the effect of fluid viscosity is negligible and the system of granular materials is subject to rapid deformation. The phenomenon of rapid granular flows has been investigated mainly along two lines of approach. The first one is based upon continuum theory analogous to the traditional continuum theory of hydrodynamics in which the molecular dynamics are not considered explicitly. The second approach is based upon microstructural theory analogous to the classical statistical mechanics in which the molecular dynamics are dealt with in detail and the macroscopic parameters are given by means of statistical averaging. The common goal is to establish the conservation and constitutive equations which govern the flow of granular materials under rapid deformation.

Goodman and Cowin (1971, 1972) had proposed a continuum theory for the flow of granular materials in the grain-inertia regime. The stress tensor was assumed to be made up of two parts, a rate-independent part and a rate-dependent part. The rate-independent part of the stress tensor was assumed to depend upon the solids fraction ν and the gradient of ν. The rate-dependent part was assumed to vary linearly with shear rate. Nunziato, Passman and Thomas (1980) modified the theory of Goodman and Cowin. The rate-independent part of the stress tensor was not changed, but the linear shear rate-dependent part of the stress tensor incorporated a variation of solid fraction based upon experiments. The choice of the dependence of grad ν and linear shear rate in the complete stress tensor is inappropriate due to certain inconsistences with physical arguments and experiments as pointed out by Jenkins and Cowin (1979) and Savage (1979).

Savage and Cowin (Savage 1979) attempted to improve the theory of Goodman and Cowin by incorporating variations of solids concentration and the square of the shear rate in the rate-dependent part of the stress tensor according to the viscometric experiments. However, the rate-independent, or quasi-static, part of the stress tensor was taken to be the same form as that of Goodman and Cowin. The proposed constitutive equations were applied to the problems of open channel flow down a rough inclined chute and the flow down a rough wall vertical channel. By choosing particular forms of the constitutive coefficients, the general traits of the predicted velocity profiles could be forced into agreement with the experiments.

McTigue (1982) employed the same method of stress decomposition. In his theory, the rate-independent part of the stress tensor satisfied the Mohr-Coulomb failure criterion and depended only upon the solids concentration ν. The rate-dependent stresses were found to depend upon the square of the shear rate by considering the collision frequency of each particle and the change of momentum in each elastic collision together with an empirical function of solids concentration deduced from experimental results. The theory was applied to the problem of gravity flow of granular materials down an inclined plane. General features of the velocity profile were demonstrated, however, the theory embodied at least more than one unknown parameter. Sayed (1981, Sayed and Savage 1982) had performed similar modifications to the continuum theory of Goodman and Cowin by using a slightly different form of rate-independent stresses based upon the quasi-static theory of Spencer (1964) which satisfied the Mohr-Coulomb yield criterion. The rate-dependent part of the stress tensor was represented by a Reiner-Rivlin isotropic fluid model which exhibited the dependence of the square of the shear rate. The functional forms of several constitutive coefficients in the theory were determined in accordance with the viscometric experimental results. The theory was then applied to the problem of two-dimensional inclined chute flow of granular materials. Reasonable predictions were made when compared to the experiments.

Bagnold (1954) formulated the stresses in the Couette flow of rigid and smooth granular materials from a simple microstructural point of view. The momentum transfer due to particle collisions between each layer was considered to be the dominant stress contribution. Thus, by multiplying the collision frequency with the number of grains in a unit area and the momentum change of each particle per collision, the shear and normal stresses were found to depend upon the square of the shear rate* and some unknown function of concentration and angle which were to be determined empirically.

Kanatani (1979) used a polar continuum model for the flow of rigid granular materials. Surface friction of each individual particle was considered to be the means of energy dissipation. Conservation laws were derived by using the couple-stress theory. The rotation of particles was regarded as an additional field quantity. By averaging the microscopic energy dissipation due to the friction of the particles, a macroscopic energy dissipation relation was deduced, from which the constitutive equations were inferred. Kanatani (1980)

*For the reason of dimensional homogeneity, when the stresses depend upon the square of the shear rate, they will also likely depend upon the particle mass density and the square of the particle diameter. Thus, in order to avoid repetition in the rest of the review, the dependence of the square of the shear rate will automatically imply the other dependencies, unless otherwise specified.

extended the theory to incorporate velocity and rotation fluctuation components into the mean flow field. An equation of state which took into account the effect of solids concentration was proposed. A condition of proportional partition of translation and rotational kinetic energy was imposed on each particle by introducing an unknown proportionality constant. Using the previous averaging method, the energy dissipation relation and the constitutive equations were obtained. However, the theory was not self-consistent in the sense that it depended on an indeterminate constant. The constitutive equations were applied to the problem of inclined gravity flow of granular particles and the stresses indicated dependence of the square of the shear rate.

Ogawa, Umemura and Oshima (1980) used a kinematic statistical model of particle fluctuations and collision dynamics to obtain the constitutive equations and the rate of energy dissipation for the flow of cohesive, rough and inelastic granular materials. The theory, which depended only upon material properties such as coefficient of friction and coefficient of restitution, was applied to the gravity flow of granular materials down a rough inclined plane.

Ackermann and Shen (1982) considered the case of simple shear of rough, inelastic granular particles in a Newtonian fluid. The stresses were formulated in a way similar to Bagnold's analysis, but in addition the effects of interstitial fluid, frictional and inelastic properties of the particles were considered. The collisional stresses were deduced from the statistical kinematic consideration of particle collisions. Although velocity fluctuations of the particles were considered in the model, the final form of the stresses for this case of simple shear had no explicit dependence on the assumed isotropic fluctuation component of the particle velocity. The stresses depended upon the square of the shear rate, material properties and certain consititutive constants which were chosen such that the predicted shear stress matched with the experimental results. Shen and Ackermann (1982, and Shen 1982) improved the previous theory and eliminated the unknown constitutive constants so that the theory was self-consistent. By a new estimation of the collisional frequency, the stresses depended upon the velocity fluctuation of the particles explicitly. Unfortunately, when the shear stress of the analysis was compared with the experiments of Bagnold (1954), Savage (1978) and Sayed (1981), the theoretical prediction was found to be about one order of magnitude low. An effective particle diameter correction factor was introduced, which was assumed to account for the effect of particle clustering during shear. The shear stress agreed well with experiments for a particular chosen value of this factor.

Savage and Jeffrey (1981) employed the approach of the kinetic theory of dense gases to consider the simple Couette flow of smooth and elastic particles. A plausible velocity distribution function was proposed, and the particle fluctuations and collision dynamics of the particles were examined carefully. The model involved no dissipation of energy and the theory depended upon an undetermined parameter R which was defined as the ratio of mean shear characteristic velocity to the r.m.s. of the fluctuation velocity of the particles. The collisional component of the stresses, which was assumed to be the dominant contribution, compared well with the experimental results of both shear and normal stresses when a particular value of R was chosen. The general characteristics of the model exhibited several interesting results. At small values of R much less than one, the shear stress depended linearly upon shear rate and the normal stress had no shear rate dependence. For moderate and high values of R, both predicted shear and normal shear were proportional to the square of the shear rate.

Jenkins and Savage (1982) extended the theory of Savage and Jeffrey to consider nearly elastic particles under general deformation. The governing conservation laws and the constitutive equations were derived in the context of kinetic theory of dense gases. The analysis involved an unknown coefficient in the collisional pair distribution function. The theory was applied to two problems; simple shearing flow between two horizontal plates and vertical gravity flow down a channel.

The above brief review shows that though the continuum approach may exhibit some gross features of the flow of granular materials, it requires additional information from experiments and particular insight in choosing the most appropriate form for the constitutive coefficients. All the above mentioned continuum theories did not consider the energy dissipation aspect of the granular system. The material properties associated with the collisional dynamics of the particles do not appear. In the microstructural approach, all the necessary properties of the system can be considered explicitly and the macroscopic variables are obtained by the method of statistical averaging. Different statistical methods have already indicated some degree of success in the formulation of the problem.

1.2 Plan of the Present Study

In the present study, the model employed is based upon the microstructural approach developed by Savage and Jeffrey (1981). The theory will be extended to deal with inelastic particles. In the following presentation, Chapter 2 contains the general formulation of the governing conservation laws and constitutive integrals essential for the flow of smooth, inelastic granular particles in the context of kinetic theory of gases, similar to what was done by Jenkins and Savage (1982). In Chapter 3, the present analysis will focus on the problem of simple shearing flow, called Couette flow, of granular materials analogous to what was done by Savage and Jeffrey (1981) but with the additional consideration of energy dissipation due to the inelastic property of the particles. The velocity pair distribution function proposed by Savage and Jeffrey will be adopted. The full analytical solutions of the integrals of the stresses and the rate of energy dissipation using series transformation will be presented in Chapter 4. In Chapter 5, comparisons will be made between the present theory, previous theoretical investigations and the appropriate experimental results. Conclusions of this study will be presented in Chapter 6.

CHAPTER 2 MAXWELL TRANSPORT EQUATION

From the classical transport theory of gases, the equation of change for the mean values of dynamical quantities associated with the individual molecules has been shown to generate identical hydrodynamic equations and the derivation can be found in numerous kinetic theory text books (Chapman & Cowling 1970, Jeans 1940, Present 1958, Reif 1965 ...). In this study, we attempt to make use of the transport theory for dense gases and make plausible modifications which are appropriate for the transport of identical, smooth, inelastic, spherical granular materials. In general, the theory of transport phenomena has been investigated mainly along two lines of approach which are known to give identical results. The first approach is based upon Boltzmann's integrodifferential equation for the velocity distribution function and the second one is based upon Maxwell's equation of change for dynamical quantities. Presently, we will follow closely Maxwell's formulation of the transport theory owing to its direct and conceptual simplicity over the Boltzmann's type of approach, and then we will proceed to derive the conservation laws which govern the flow of granular materials of the type mentioned above.

2.1 Elementary Kinetic Theory

In statistical mechanics, the state of a system may be defined by a set of generalized coordinates $\underline{r}_i$ and generalized velocity $\underline{c}_i$ for each of the individual particles of the system. For a system of N identical particles, each having 3 degrees of freedom, the total number of degrees of freedom for the whole system is 6N. Thus the microstate of this system is given by a set of 6N generalized coordinates and velocities, i.e. $(\underline{r}_i, \underline{c}_i)$, $i = 1,2,\ldots,N$*, and may be specified by a single point in the 6N dimensional space, usually called the phase space, having the mutually orthogonal axis, $\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N, \underline{c}_1, \underline{c}_2, \ldots, \underline{c}_N$. For a system of large N, it is practically impossible to know the exact microstate $(\underline{r}_i, \underline{c}_i)$ of the system and its evolution in time and space. Fortunately, in general, practical systems are defined by a set of macroscopic variables (η_j) where the range of j is much much smaller than that of i; for example, the η_j's can be average velocity, density, pressure, kinetic fluctuation energy, heat conductivity, viscosity, etc. The relationship between the microstate and the macrostate is that given a particular microstate $(\underline{r}_i, \underline{c}_i)$, there is a corresponding macrostate given by a set of macrovariables (η_j). However, given a particular macrostate, there is a continuum of microstates $(\underline{r}_i, \underline{c}_i)$. In other words, a set of macrovariables (η_j) specifies a region R in the phase space, while a set of microstates $(\underline{r}_i, \underline{c}_i)$ specifies a single point. As one may guess, the variables of the macrostate must correspond to some kind of mean values which are given by some form of averaging procedure of the microstates; namely the ensemble averaging method introduced by Gibbs (1960) which involves the principles

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* The set $(\underline{r}_i, \underline{c}_i)$, $i=1,2,\ldots,N$ is the short form of $(\underline{r}_1, \underline{r}_2, \ldots, \underline{r}_N, \underline{c}_1, \underline{c}_2, \ldots, \underline{c}_N)$ signifying a set of 6N generalized coordinates and velocities in the phase space, where $\underline{r}_1 = r_{x1}\underline{e}_x + r_{y1}\underline{e}_y + r_{z1}\underline{e}_z$ is the Cartesian coordinates of a particular particle and similarly $\underline{c}_1 = c_{x1}\underline{e}_x + c_{y1}\underline{e}_y + c_{z1}\underline{e}_z$ is the velocity of the particle and so on.

of probability. We define the normalized probability density function (or called the N-particle velocity distribution function) $f^{(N)}(\underline{r}_i,\underline{c}_i,t)$ such that $f^{(N)}(\underline{r}_i,\underline{c}_i,t)\, d\underline{r}_i d\underline{c}_i$* is the probability of finding the system in the microstate specified by the region $\underline{r}_i$, $\underline{r}_i+\underline{dr}_i$ and $\underline{c}_i$, $\underline{c}_i+\underline{dc}_i$ in the phase space. According to the theory of statistical mechanics (e.g. Harris, 1971) $f^{(N)}(\underline{r}_i,\underline{c}_i,t)$ satisfies the well known Liouville's equation which may be written as

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{i=1}^{N} \left| \frac{\partial f^{(N)}}{\partial \underline{r}_i}\cdot \underline{c}_i + \frac{\partial f^{(N)}}{\partial \underline{c}_i}\cdot \frac{\partial \underline{c}_i}{\partial t} \right| = 0 \qquad (2.1)$$

If $f^{(N)}(\underline{r}_i,\underline{c}_i,t)$ is known, we would be able to determine how each ensemble member or particle would evolve in the phase space and hence all the macrovariables could be found. However, due to the large number of degrees of freedom involved it becomes an impossible task to find a solution for such an equation even if all the necessary initial conditions are known.

Fortunately the macroscopic properties of interest in the system do not depend on the ensemble average taken with respect to $f^{(N)}$, but rather, on averages taken with respect to the first few so-called reduced distribution functions which are formally expressed as

$$f^{(1)}(\underline{r}_1,\underline{c}_1,t) = \int f^{(N)}(\underline{r}_1,\ldots,\underline{r}_N,\underline{c}_1,\ldots,\underline{c}_N,t)\,d\underline{r}_2\ldots d\underline{r}_N d\underline{c}_2\ldots d\underline{c}_N \qquad (2.2)$$

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*The symbol $d\underline{r}$ = dxdydz denotes a volume element at point $\underline{r}$ = (x,y,z) while $\underline{dr} = \Delta r_x \underline{e}_x + \Delta r_y \underline{e}_y + \Delta r_z \underline{e}_z$ denotes a small vector joining $\underline{r}$ to an adjacent point.

$$f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t) = \int f^{(N)}(\underline{r}_1,\ldots,\underline{r}_N,\underline{c}_1,\ldots,\underline{c}_N,t)\,d\underline{r}_3\ldots d\underline{r}_N d\underline{c}_3\ldots d\underline{c}_N$$

etc., (2.3)

where $f^{(1)}$ is called the single particle velocity distribution function, $f^{(2)}$ the two-particle or pair velocity distribution function, etc.; integrations are taken for all values of positions and velocities respectively.

As usual, the single particle distribution function $f^{(1)}(\underline{r},\underline{c},t)$ is defined such that $f^{(1)}(\underline{r},\underline{c},t)d\underline{r}d\underline{c}$ is the probability of finding a particle which at time t is located in the volume element between $\underline{r}$ and $\underline{r}+d\underline{r}$, having velocities lying in the range $\underline{c}$ and $\underline{c}+d\underline{c}$. Similarly, the pair distribution function $f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ is defined such that $f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ $d\underline{r}_1 d\underline{r}_2 d\underline{c}_1 d\underline{c}_2$ is the probability of finding a pair of particles which at time t are located in the volume elements $d\underline{r}_1$ and $d\underline{r}_2$ centred at the points $\underline{r}_1$, $\underline{r}_2$ and having the velocities within the ranges $\underline{c}_1$ and $\underline{c}_1+d\underline{c}_1$, and $\underline{c}_2$ and $\underline{c}_2+d\underline{c}_2$. The single particle distribution function $f^{(1)}(\underline{r},\underline{c},t)$ provides a description of the macroscopic state of the system and permits the determinations of the macroscopic quantities of physical interest. Let us define the local number density $n(\underline{r},t)$ at $\underline{r}$ such that $n(\underline{r},t)d\underline{r}$ is the number of particles located in the volume element $d\underline{r}$ at time t and is given by definition

$$n(\underline{r},t) = \int f(\underline{r},\underline{c},t)\,d\underline{c} \qquad (2.4)$$

where integration is over all possible velocities. Let $\phi(\underline{r},\underline{c},t)$ be any function that denotes a physical property of a particle located at $\underline{r}$ with velocity $\underline{c}$ at time t. The mean value of ϕ which corresponds to a specific macroscopic variable may be determined by taking the ensemble average with respect to $f^{(1)}$

and by definition is given as

$$\langle\phi(\underline{r},t)\rangle = \bar{\phi}(\underline{r},t) = \frac{1}{n(\underline{r},t)}\int \phi(\underline{r},\underline{c},t)f(\underline{r},\underline{c},t)d\underline{c} \qquad (2.5)$$

Furthermore, we proceed to consider the fluxes of various properties of the particles which are of important interest in the transport theory. Consider a surface element of area dS moving with the mean velocity $\underline{u}$. Take $\hat{n}$ to be a unit vector drawn normal to the element in the direction from the negative to the positive side (Figure 1). Due to the random fluctuations of the particles, they may pass in and out of dS and thus create a flux of particle properties across the surface element. For particles of velocity $\underline{v}$ relative to dS, the number of such particles which pass through the surface element is just the number contained in the cylinder of volume $|\hat{n}\cdot\underline{v}|dt\ dS$ and is therefore given by $f^{(1)}(\underline{r},\underline{c},t)d\underline{c}$ $|\hat{n}\cdot\underline{v}|dt\ dS$ (see Reif 1965). The net amount of ϕ which is transported per unit time per unit area across the surface element dS in its positive normal direction is just the difference of the amount of ϕ carried in from that carried out. Since each particle carries the property ϕ $(\underline{r},\underline{c},t)$, the total amount of ϕ carried by the particles out of dS, $\underline{H}_{out}(\underline{r},t)$, in the positive $\hat{n}$ direction in time dt is given by

$$\hat{n}\cdot\underline{H}_{out}(\underline{r},t)dtdS = \int_{\hat{n}\cdot\underline{v}>0} f^{(1)}(\underline{r},\underline{c},t)d\underline{c}|\hat{n}\cdot\underline{v}|dtdS\phi(\underline{r},\underline{c},t) \qquad (2.6)$$

Similarly the total amount of ϕ carried in, $\underline{H}_{in}(\underline{r},t)$, in time dt is given by

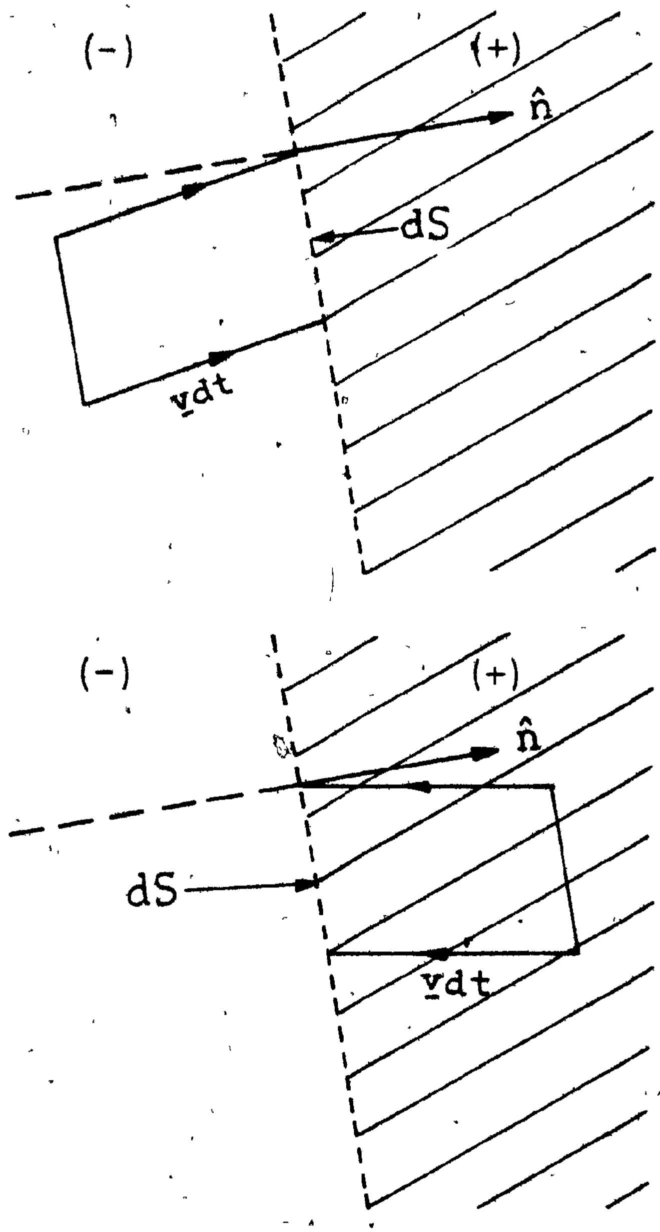

Fig. 1 The element of area of dS with unit normal $\hat{n}$ moving with mean velocity $\underline{u}$ divides the medium into (+) and (-) region. The figures illustrate particles passing in (from +ve to -ve side) and out (from -ve, to +ve side) of the element of area dS in time dt (Reif 1965)

$$\hat{n}\cdot\underline{H}_{in}(\underline{r},t)dtdS = \int_{\hat{n}\cdot\underline{v}<0} f^{(1)}(\underline{r},\underline{c},t)d\underline{c}|\hat{n}\cdot\underline{v}|dtdS\phi(\underline{r},\underline{c},t) \tag{2.7}$$

By noting that in integral (2.6) $\hat{n}\cdot\underline{v} = |\hat{n}\cdot\underline{v}|$ and in integral (2.7) $\hat{n}\cdot\underline{v} = -|\hat{n}\cdot\underline{v}|$, the net flux of ϕ per unit time per unit area, $\underline{H}(\underline{r},t)$, in the positive $\hat{n}$ direction is found by dividing the difference of (2.7) from (2.6) by dtdS, and it becomes

$$\hat{n}\cdot\underline{H}(\underline{r},t) = \int f^{(1)}(\underline{r},\underline{c},t)d\underline{c}\ \hat{n}\cdot\underline{v}\phi \tag{2.8}$$

Thus, the flux vector $\underline{H}(\underline{r},t)$ may be expressed as

$$\underline{H}(\underline{r},t) = \int f^{(1)}(\underline{r},\underline{c},t)\underline{v}\phi dc = n\langle\underline{v}\phi\rangle \tag{2.9}$$

2.2 Formulation of Transport Theory

Following the treatment of Reif (1965) we attempt to derive the equation of change for the mean value of dynamical quantities $\langle\phi(\underline{r},\underline{c},t)\rangle$ for the flow of granular materials. Consider a fixed volume element between $\underline{r}$ and $\underline{r}+\underline{dr}$ which contains $n(\underline{r},t)d\underline{r}$ particles in motion. The total mean value $\langle n\phi\rangle d\underline{r}$ of the dynamical quantity ϕ for all particles in the volume element $d\underline{r}$ increases in the time interval between t and t+dt by an amount

$$\frac{\partial}{\partial t}\langle n\phi\rangle\, d\underline{r}dt = \psi_{int} + \psi_{kF} + \psi_{col} \tag{2.10}$$

where the quantities ψ represent various contributions from different means of interactions.

Firstly, ψ_{int} is an intrinsic increase in the total mean value of ϕ in $d\underline{r}$ because of the change of the quantity $\phi(\underline{r},\underline{c},t)$ of each particle with respect to its position and velocity perhaps due to an external force field. For each particle of velocity $\underline{c}$, it changes position by an amount $\underline{dr} = \underline{c}dt$ and velocity by $\underline{dc} = (\underline{F}/m)dt$; so the corresponding change in ϕ is given by

$$(D\phi)dt = \frac{\partial\phi}{\partial t}dt + \frac{\partial\phi}{\partial \underline{r}}\cdot\underline{v}dt + \frac{\partial\phi}{\partial \underline{c}}\cdot\frac{\underline{F}}{m}dt \qquad (2.11)$$

where $\underline{F}$ is the external force acting on the particles with mass m. Thus the intrinsic increase in the mean value of ϕ in the volume element is

$$\psi_{int} = n\langle D\phi\rangle d\underline{r}dt \qquad (2.12)$$

Secondly, ψ_{kF} is a kinetic flux increase in the total mean value of ϕ because of the net kinetic flux of particles which enter and leave the volume element $d\underline{r}$ in time dt. The increase in the mean value of ϕ caused by particles entering $d\underline{r}$ at $\underline{r}$ in time dt is

$$\langle n\phi\underline{c}\rangle\, d\underline{r}dt \qquad (2.13)$$

by using similar arguments from determining the flux of dynamical quantities. Correspondingly the decrease caused by particles leaving the volume element $d\underline{r}$ at a new location $\underline{r}+\underline{dr}$ is given by

$$\langle n\phi\underline{c}\rangle d\underline{r}dt + \frac{\partial}{\partial\underline{r}}\cdot\langle n\phi\underline{c}\rangle d\underline{r}dt \qquad (2.14)$$

Subtracting (2.14) from (2.13), the kinetic flux increase ψ_{kF} is given as

$$\psi_{kF} = -\frac{\partial}{\partial\underline{r}}\cdot\langle n\phi\underline{c}\rangle d\underline{r}dt \qquad (2.15)$$

Thirdly, ψ_{col} is a collisional increase in the total mean value of ϕ in $d\underline{r}$ because of the random interparticle collisions in such volume element. To obtain ψ_{col}, we follow a treatment analogous to Enskog's analysis of the collisional transfer of molecular properties in dense gases using the hard spheres model as described by Chapman & Cowling (1970). Consider two identical particles 1 and 2 of diameter σ centered at 0_1 and 0_2 colliding with a relative velocity $\underline{q} = \underline{c}_1 - \underline{c}_2$ as shown in Figure 2. In time dt prior to the collision, particle 2 moved through a distance of $\underline{q}dt$ relative to particle 1. At collision, center 0_2 of particle 2 must lie within an area of $\sigma^2 d\underline{k}$ which is a surface element on a sphere of radius σ and centre 0_1. Hence, for a collision to occur within time dt then 0_2 must lie inside the volume $\sigma^2 d\underline{k}(\underline{k}\cdot\underline{q})dt$, where $\underline{k}$ is a unit vector along the centre line from particle 1 to 2 and $d\underline{k}$ is the solid angle. Thus the probable number of collisions per unit time such that 0_1 lies within the volume $d\underline{r}$ and in which $\underline{c}_1, \underline{c}_2$ and $\underline{k}$ lie within the ranges, $d\underline{c}_1$, $d\underline{c}_2$ and $d\underline{k}$ is

$$f^{(2)}(\underline{r},\ \underline{c}_1, \underline{r}+\sigma\underline{k}, \underline{c}_2, t)\ \sigma^2 \underline{k}(\underline{k}\cdot\underline{q})\ d\underline{k}d\underline{c}_1 d\underline{c}_2 d\underline{r} \qquad (2.16)$$

During a collision particle 1 at $\underline{r}$ gains a quantity $(\phi_1' - \phi_1)$ of the property ϕ at the expense of particle 2, where primed quantity denotes that after the collision. The total gain for all collisions inside the volume element $d\underline{r}$ in time dt is therefore

$$\psi_{col} = d\underline{r}dt\sigma^2 \iiint_{\underline{k}\cdot\underline{q}>0} (\underline{k}\cdot\underline{q})\, f^{(2)}(\underline{r}, \underline{c}_1, \underline{r}+\sigma\underline{k}, \underline{c}_2, t)\, d\underline{k}d\underline{c}_1 d\underline{c}_2 (\phi_1' - \phi_1) \qquad (2.17)$$

where $\underline{k}\cdot\underline{q}>0$ is the integration limits accounting for all those particles that are about to collide. Interchanging the roles of particle 1 and 2 or correspondingly the subscript 1 and 2

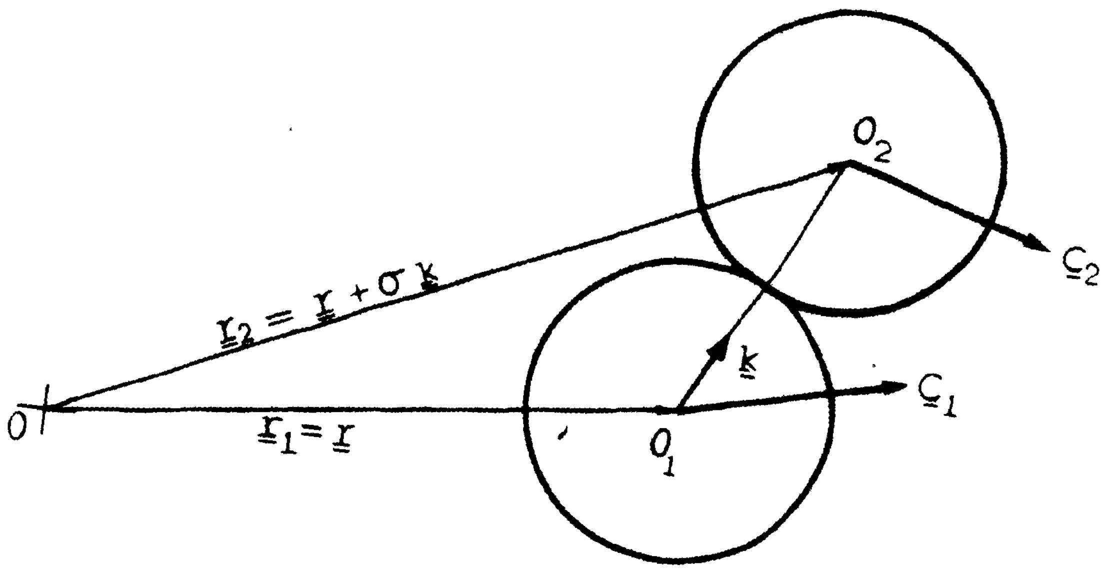

Fig. 2 Binary collision of particles

in equation (2.17) and noting that $\underline{q}\to-\underline{q}$ and $\underline{k}\to-\underline{k}$ we obtained a similar expression of the form

$$\psi_{col}=d\underline{r}dt\sigma^2 \iiint_{\underline{k}\cdot\underline{g}>0} (\underline{k}\cdot\underline{g})\, f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\,d\underline{k}d\underline{c}_1d\underline{c}_2(\phi_2'-\phi_2) \tag{2.18}$$

Expanding $f^{(2)}(\underline{r},\underline{c}_1,\underline{r}+\sigma\underline{k},\underline{c}_2,t)$ in (2.17) into Taylor series, it gives

$$f^{(2)}(\underline{r},\underline{c}_1,\underline{r}+\sigma\underline{k},\underline{c}_2,t)=(1+\sigma\underline{k}\cdot\nabla+\frac{1}{2!}(\sigma\underline{k}\cdot\nabla)^2+\ldots)f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t) \tag{2.19}$$

By taking half the sum of (2.17) and (2.18) and using (2.19) the collisional increase can be expressed in the form

$$\psi_{col} = [-\nabla\cdot\theta(\phi) + \chi(\phi)]\, d\underline{r}dt \tag{2.20}$$

where $$\theta(\phi) = -\frac{1}{2}\sigma^3 \int_{\underline{k}\cdot\underline{g}>0} (\phi_1'-\phi_1)(\underline{k}\cdot\underline{g})\underline{k}\,[1+\frac{1}{2!}\sigma\underline{k}\cdot\nabla+\frac{1}{3!}(\sigma k\cdot\nabla)^2 + \ldots]\, f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\, d\underline{k}d\underline{c}_1d\underline{c}_2 \tag{2.21}$$

and $$\chi(\phi) = \frac{\sigma^2}{2}\int_{\underline{k}\cdot\underline{g}>0} (\phi_1'+\phi_2'-\phi_1-\phi_2)(\underline{k}\cdot\underline{g})\, f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\, d\underline{k}d\underline{c}_1d\underline{c}_2 \tag{2.22}$$

The collisional transfer contribution $\theta(\phi)$ may be interpreted as a flux vector term of property ϕ while $\chi(\phi)$ may be seen as analogous to a source or sink term (more discussion in Appendix A).

With the use of equations (2.12), (2.15) and (2.20) the equation of change for the mean value of dynamical quantity (2.10) can be written as

$$\frac{\partial}{\partial t}\langle n\phi\rangle = n\langle D\phi\rangle - \nabla\cdot\langle n\underline{c}\phi\rangle - \nabla\cdot\theta(\phi) + \chi(\phi) \tag{2.23}$$

Subsequently, we may use the above equation to obtain the conservation equations that govern the flow of identical, smooth, inelastic, spherical granular materials. By letting ϕ be the mass of a particle m in (2.22), it gives the equation of conservation of mass

$$\frac{\partial \rho}{\partial t} = -\nabla\cdot(\rho \underline{u}) \tag{2.24}$$

where $\rho = mn$ is the bulk mass density and $\underline{u}$ is the mean velocity. Letting ϕ be $m\underline{c}$ the linear momentum of a particle with fluctuation velocity defined as $\underline{v} = \underline{c}-\underline{u}$ in (2.23), it gives the equation of conservation of linear momentum

$$\rho \frac{d\underline{u}}{dt} = \rho \underline{b} - \nabla\cdot\underset{\sim}{P} \tag{2.25}$$

with

$$\underset{\sim}{P} = \underset{\sim}{P}_k + \underset{\sim}{P}_c \tag{2.26}$$

and

$$\underset{\sim}{P}_k = \rho\langle \underline{v}\ \underline{v}\rangle \tag{2.27}$$

$$\underset{\sim}{P}_c = \theta(m\underline{c}) \tag{2.28}$$

where $\underset{\sim}{P}$ is the pressure tensor made up of a kinetic or diffusional part $\underset{\sim}{P}_k$ and a collisional part $\underset{\sim}{P}_c$, and $\underline{b}$ is the external force per unit mass. Letting ϕ be $1/2\ mc^2$ the kinetic translational energy of a particle in (2.23), it gives the equation of conservation of the translational fluctuation kinetic energy

$$\frac{3}{2}\rho \frac{dT}{dt} = -\underset{\sim}{P}:\nabla\underline{u} - \nabla\cdot\underline{Q} - \gamma \tag{2.29}$$

with

$$\frac{3}{2}T \doteq \frac{\langle v^2\rangle}{2} \tag{2.30}$$

$$\underline{Q} = \underline{Q}_k + \underline{Q}_c \tag{2.31}$$

and

$$\underline{Q}_k = \frac{\rho}{2}\langle \underline{v}\ v^2\rangle \tag{2.32}$$

$$Q_c = \theta(1/2\, mv^2) \qquad (2.33)$$

$$\gamma = -\chi(1/2\, mc^2) \qquad (2.34)$$

where 3T/2 is the fluctuation specific kinetic energy, Q is the flux of fluctuation energy consisting of a kinetic part Q_k and a collisional part Q_c, γ is the collisional rate of energy dissipation per unit volume due to the inelasticity of the particles.

CHAPTER 3

GENERAL INTEGRAL FORM FOR THE STRESS TENSOR AND ENERGY DISSIPATION FOR THE CASE OF SIMPLE SHEAR

Consider an assembly of identical, smooth, inelastic, spherical particles of diameter σ which is subjected to motion consisting of simple shear with mean velocity $\underline{u} = u(z)\underline{e}_y$, where $\underline{e}_y$ is the unit vector in the y-direction as shown in Figure 3. The instantaneous velocity $\underline{c}(\underline{r},t)$ of a particle in a volume element $d\underline{r}$ differs from its local mean translational velocity $\underline{u}(\underline{r})$ by a random fluctuating part $\underline{v}(\underline{r},t)$ due to interparticle collisions, i.e.,

$$\underline{c}(\underline{r},t) = \underline{u}(\underline{r}) + \underline{v}(\underline{r},t) \tag{3.1}$$

The effect of the interstitial fluid is assumed to be negligible and for simplicity the surface friction of the particles is also neglected.

In this analysis, we are concerned with situations where granular materials are being sheared at moderately high solids concentration and mean shear rate such that the effect of interparticle collisions dominates over that of free particle diffusion between layers. In other words, the mean free path is likely to be smaller than the diameter of the particles, hence the probability of particles transfering momentum by going from one layer to another is small. Thus, the major stress contribution comes from the collisional transfer of momentum between particles. Furthermore; we assume that the collisions are almost instantaneous and the probability of multiple interparticle collisions is negligibly small so that only binary collisions need to be treated.

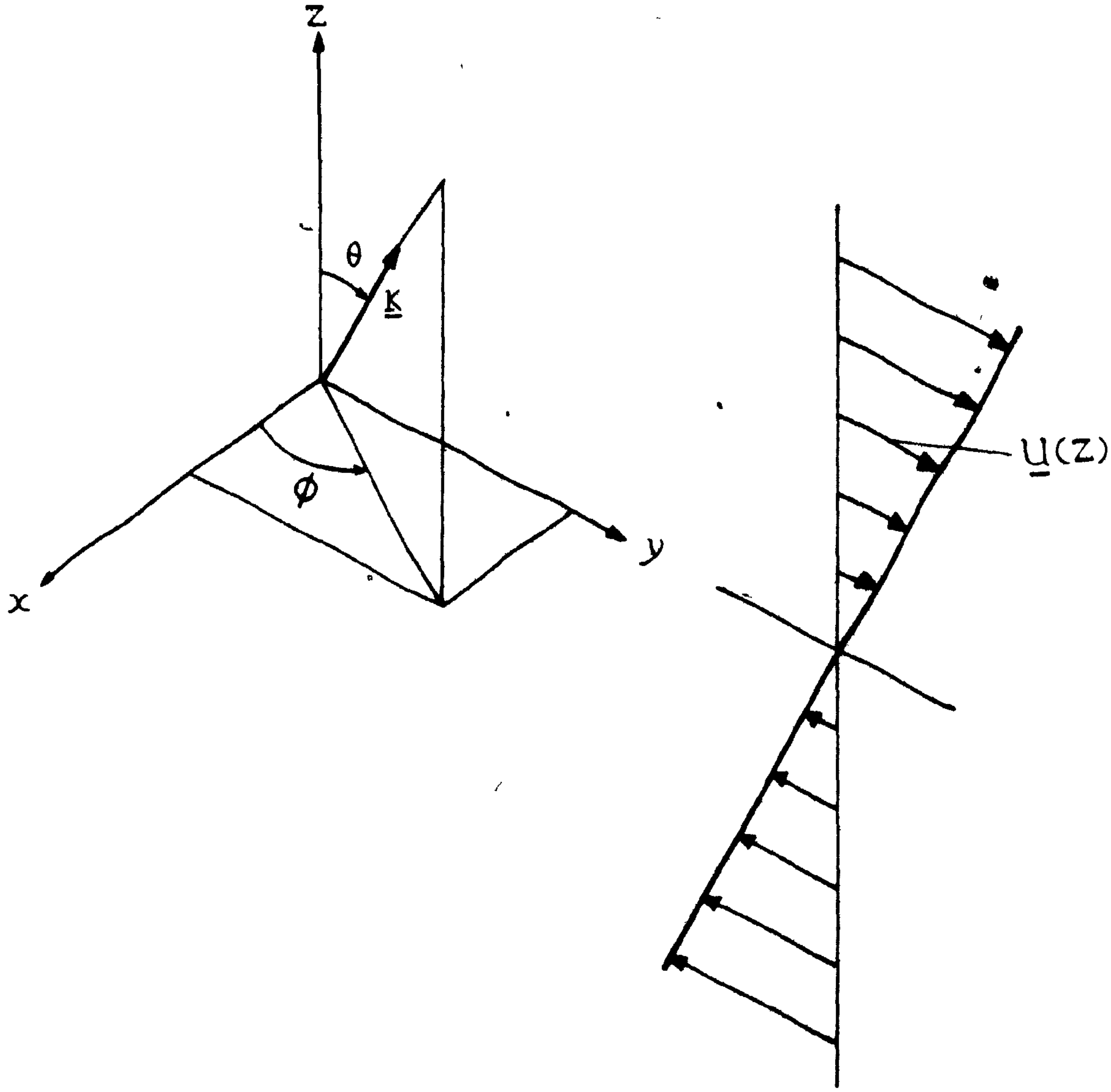

Fig. 3 Definition of simple shear flow and coordinate system

At very high concentration, this assumption is expected to break down critically due to the clustering and prolonged contacts of particles.

Since dry friction is ignored, the inelasticity of the particles which damps out and converts the fluctuation kinetic energy into heat acts as the only dissipative mechanism. Particles are assumed to have no rotational energy but translational energy only. The inelastic collisions of particles are characterized by the coefficient of restitution e of the particles which varies from zero to one depending on the material. For perfectly elastic collisions, e has the value of one which corresponds to no energy dissipation in the system. For e less than one, the rate of energy dissipation is a function of the coefficient of restitution and the impact velocities which depend upon the shear rates and velocity fluctuation. However, if e equals zero, the particles no longer rebound after a collision. Multiple collisions would therefore be frequent contrary to the assumption of binary collision. Hence we restrict ourselves to consider only particles with a moderately high value of e such that the impact duration during a collision is small compared to the average time interval between collisions and that negligible permanent deformation of particles occurs. Furthermore, we assume that the coefficient of restitution is constant, though experiments have shown that e actually depends on the impact velocity (Goldsmith 1960). Such phenomenon of impact would no doubt present another degree of difficulty, nevertheless, we are content at the present to the first order of approximation to take e as a mean value.

As suggested by Savage and Jeffrey (1981) we follow the approach of kinetic theory of dense gases and use a pre-collisional description of both positions and velocities of the particles. This enables us to calculate the stress components and the rate of energy dissipation in the system by the use of the statistical mechanics method as presented in Chapter Two.

3.1 The Non-Equilibrium Configurational and Collisional Pair Distribution Function

Since only binary collisions for identical, smooth, inelastic, spherical particles are considered, we require the form of the complete pair distribution function $f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ as defined previously. Following almost exactly what Savage and Jeffrey (1981) had proposed, we assume that the complete pair distribution function can be expressed as the product of the pair correlation function $g(\underline{r}_1,\underline{r}_2)$ and the single particle velocity distribution function $f^{(1)}$ for each particle,

$$f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t) = g(\underline{r}_1,\underline{r}_2)f^{(1)}(\underline{r}_1,\underline{c}_1,t)f^{(1)}(\underline{r}_2,\underline{c}_2,t) \quad (3.2)$$

where subscripts 1 and 2 denote the positions and velocities of particles 1 and 2 respectively.

In the kinetic theory of dense gases, the pair-correlation function $g(\underline{r}_1,\underline{r}_2)$ accounts for the correlation of position between molecules due to the influence of the potential energy associated with each molecule. To be more rigorous, $g(\underline{r}_1,\underline{r}_2)$

should be replaced by $g(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ which takes into account not only the precollision correlation of positions but also the velocities of the molecules (see Reed and Gubbin 1973). The main difficulty in the kinetic theory lies in finding such unknown correlation function $g(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ for the cases of dense gases. Enskog studied the case where the molecules were taken to be hard spheres (Chapman and Cowling 1970). This greatly simplifies the correlation function since hard sphere molecules no longer have either long range or short range potential influence on each other, therefore the correlation of velocities for the molecules need not be specified. With the assumptions of binary collision and molecular chaos, the pair correlation function $g(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ is replaced by $g(\underline{r}_1,\underline{r}_2)$. Enskog made a further assumption that $g(\underline{r}_1,\underline{r}_2)$ may be approximated by the local equilibrium pair correlation function $g(\underline{r})$ and a number of collisional transfer of molecular propertes may then be expressed in terms of $g(\underline{r})$.

Analogous to what was done by Enskog, Savage and Jeffrey (1981) applied the theory of hard spheres dense gases to the analysis of smooth, hard, elastic and spherical granular materials. In principle, the hard sphere theory may be expected to work better in the case of granular particles than that of molecules in the sense of the absence of repulsive and attractive forces between the grains (except when electrostatic forces build up to an extent that they would play a significant role in grain flow).

Savage and Jeffrey (1981) made no attempt to solve the Boltzmann equation by a perturbation method to obtain the complete pair distribution function as Enskog did but rather they proposed the plausible form of $f^{(2)}(\underline{r}_1, \underline{c}_1, \underline{r}_2, \underline{c}_2, t)$ appropriate for granular flow by using physical arguments, which we will adopt also.

Let us suppose with Savage and Jeffrey (1981) that the single velocity distribution is locally Maxwellian about the mean transport velocity. In the case of fluidized beds, the experiments of Carlos and Richardson (1968) show some justification for this assumption. In more recent work dealing with numerical modelling of 2 dimensional granular flow, Campbell (1982) investigated the form of the single particle velocity and the spatial pair distribution. The velocity distribution was found to be quite close to the Maxwellian form. Thus we also adopt the form of Maxwellian velocity distribution function for $f^{(1)}$ and further make the assumption that there is no fluctuation gradient in the system, hence

$$f^{(1)}(\underline{r}, \underline{c}, \underline{u}(\underline{r})) = n\left(\frac{1}{2\pi T}\right)^{3/2} \exp\left(-\frac{(\underline{c}-\underline{u})^2}{2T}\right) \tag{3.3}$$

where $3T/2 = \langle v^2\rangle/2$ is defined as before the specific kinetic energy of fluctuation, $\langle v^2\rangle$ is the mean square of velocity fluctuation assumed to be constant, and n is the number density at $\underline{r}$. The assumption of $\langle v^2\rangle$ being independent of position implies that the system is 'isothermal' due to the kinetic fluctuation energy being the same everywhere. In general this assumption is not true, but it is possible for the simple shear flow case to be examined here.

Savage and Jeffrey (1981) have also proposed the form of the pair correlation function. The way that they determine such a function is by making a kinematic argument. Due to the presence of the mean shear $\underline{u}$, the pair correlation function $g(\underline{r}_1,\underline{r}_2)$ differs from the equilibrium isotropic pair correlation function (or better known as the equilibrium radial distribution function) $g_o(\sigma)$ which is evaluated at contact $|\underline{r}_1-\underline{r}_2| = \sigma$. Consider a particle moving along with the local mean transport velocity, it would likely experience more collisions with particles on its 'upstream' quadrants than its 'downstream' ones (Figure 4). This effect gives rise to a bias in the distribution of collisions. Essentially, Savage and Jeffrey (1981) argued that the ratio of the non-equilibrium pair correlation function $g(\underline{r}_1,\underline{r}_2)$ to the corresponding equilibrium one $g_o(\sigma)$ may be given by the ratio of the probability of collision of a pair of particles at $\underline{r}_1$ and $\underline{r}_2$ having velocities in the ranges of $\underline{c}_1$ and $\underline{dc}_1$, $\underline{c}_2$ and $\underline{dc}_2$ respectively in the non-equilibrium state to the probability of collision of such particles in the equilibrium state in the sense that $\nabla u=0$, giving

$$\frac{g(\underline{r}_1,\underline{r}_2)}{g_o(\sigma)} = \mathrm{erfc}\left(\frac{\sigma \underline{kk}:\nabla \underline{u}}{2T^{1/2}}\right) \tag{3.4}$$

where erfc(x) is the complementary error function

$$\mathrm{erfc}(x) = \frac{2}{\pi^{1/2}} \int_x^\infty e^{-t^2}\, dt \tag{3.5}$$

Since $g(\underline{r}_1,\underline{r}_2)$ describes the distribution of collisions for a particular configuration of a particle, Savage and Jeffrey (1981) choose to call $g(\underline{r}_1,\underline{r}_2)$ the collisional pair distribution

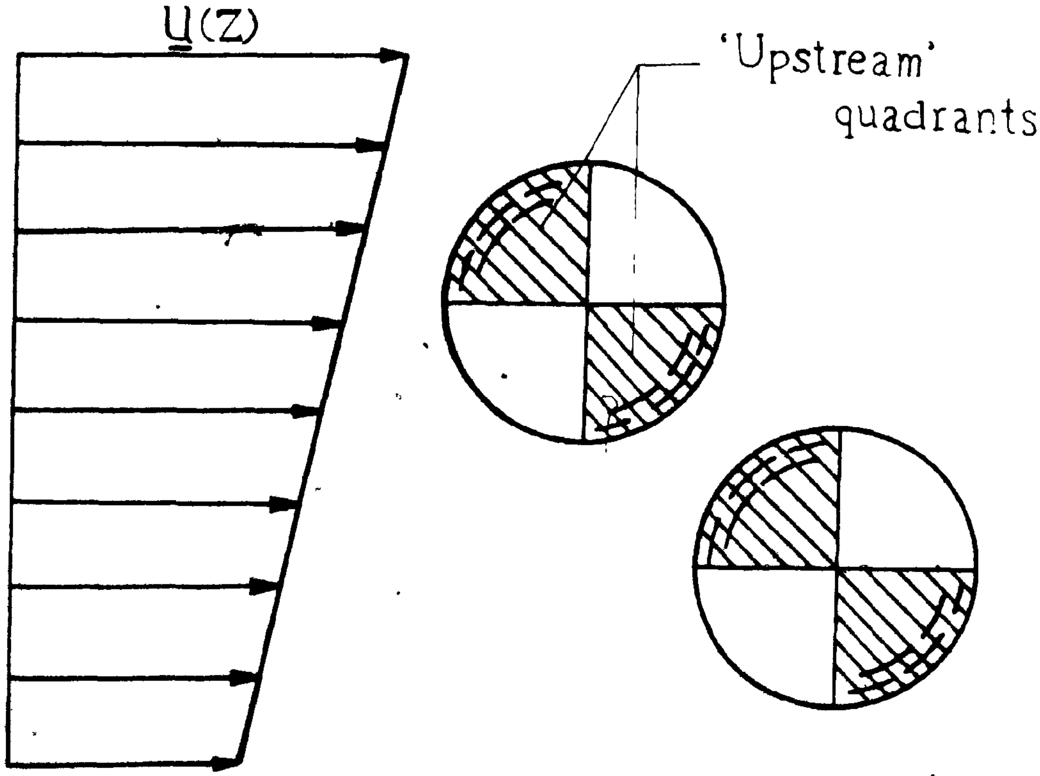

Fig. 4 Anisotropic collision distribution of each particle arises due to the mean shear motion. Shaded 'upstream' quadrants receive more collisions than the 'downstream' ones (Savage and Jeffrey 1981)

function instead of the pair correlation function. The above form of the collisional pair distribution function is cast in a slightly different form than that of Savage and Jeffrey. The tensor product $\underline{\underline{k}}\underline{\underline{k}}:\nabla\underline{u} = (\underline{k}\cdot\nabla\underline{u})\cdot\underline{k}$ may be expressed in terms of the spherical coordinates θ and ϕ (Figure 3) as

$$\underline{\underline{k}}\underline{\underline{k}}:\nabla\underline{u} = \frac{du}{dz} \sin\theta \cos\theta \sin\phi \tag{3.6}$$

hence

$$g(\underline{r}_1,\underline{r}_2)/g_o(\sigma) = \operatorname{erfc}\left(\frac{\sqrt{3}}{2}\left(\sigma \frac{du}{dz}/\langle v^2\rangle^{\frac{1}{2}}\right)\sin\theta\cos\theta\sin\phi\right) \tag{3.7}$$

The variations of $g(\underline{r}_1,\underline{r}_2)/g_o(\sigma)$ with θ for various values of $\sqrt{3}/2\ R \sin\phi$, where

$$R = \frac{\sigma \frac{du}{dz}}{\langle v^2\rangle^{1/2}} \tag{3.8}$$

is the ratio of mean shear characteristic velocity to the r.m.s. precollision velocity fluctuation, is shown in Figure 5*. For small values of R $g(\underline{r}_1,\underline{r}_2)/g_o(\sigma)$ is ellipsoidal, and for large R the variations in $g(\underline{r}_1,\underline{r}_2)/g_o(\sigma)$ are step-like. Recent computer experiments done by Campbell (1982) show similar forms of anisotropy in the collisional distribution at low concentration, however, at high concentrations spikes appear in the distribution function.

For the equilibrium radial distribution function, we adopt the semi-empirical equation by Carnahan and Starling (1969) as suggested by Savage and Jeffrey (1981), which for a system of identical hard spheres can be expressed in terms of the solids fraction ν as

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* The single particle distribution function and the collisional pair distribution function given by Savage and Jeffrey (1981) need to be corrected by replacing $\langle v^2\rangle$ with $2\langle v^2\rangle/3$.

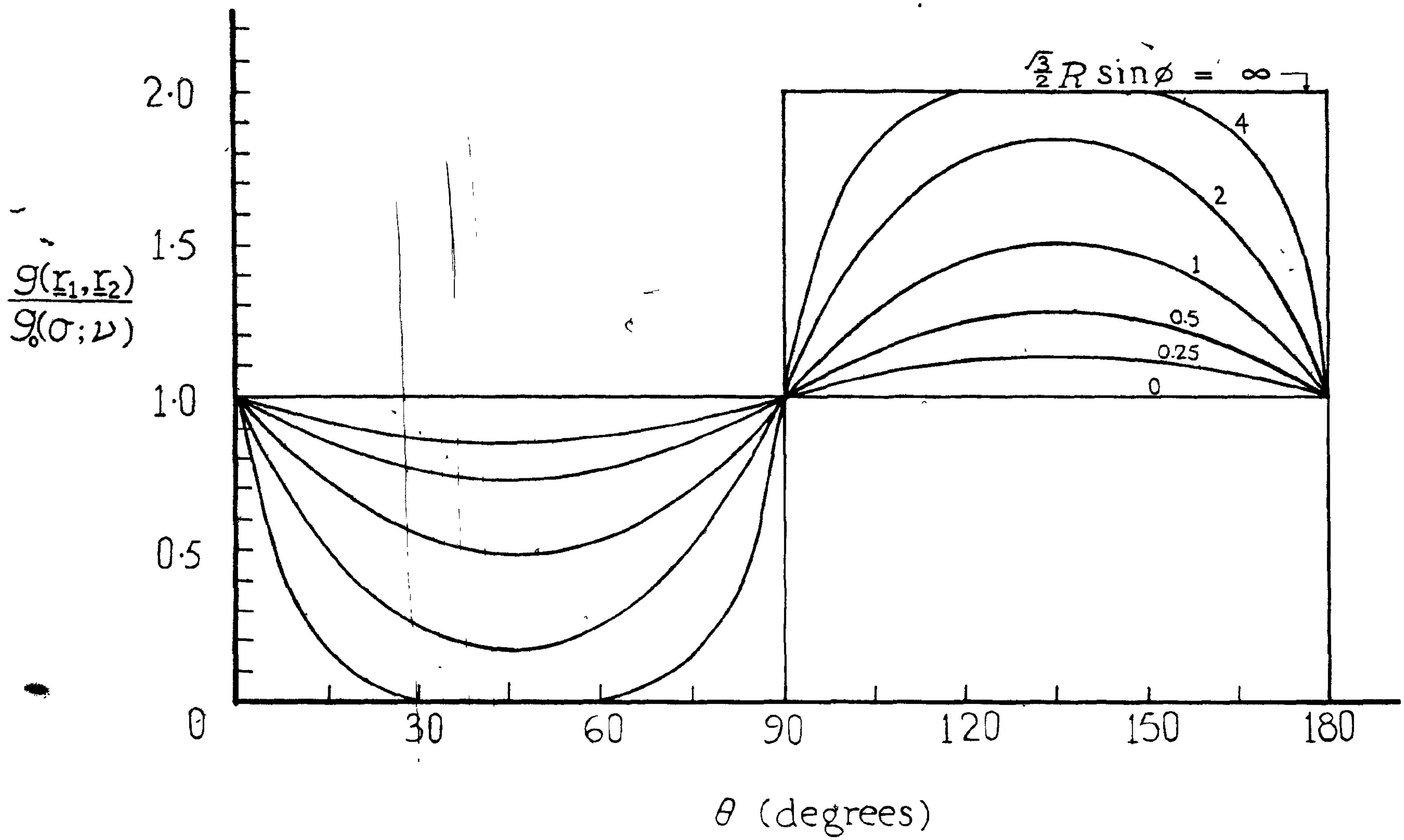

Fig. 5 Collisional pair distribution function (Savage and Jeffrey 1981)

$$g_o(\sigma;\nu) = \frac{1}{(1-\nu)} + \frac{3\nu}{2(1-\nu)^2} + \frac{\nu^2}{2(1-\nu)^3} \quad (3.9)$$

This equation is evaluated at contact $r=\sigma$ and agrees well with computer similations of molecular dynamics for values of ν up to 0.5. Combining equations (3.3) and (3.4) with the use of (3.9), the complete pair distribution function $f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)$ given by (3.2) is

$$f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t) = \frac{n^2}{(2\pi T)^3} g_o(\nu)\ \mathrm{erfc}\left(\frac{\sigma \underline{k}\underline{k}:\nabla \underline{u}}{2T^{1/2}}\right)\exp\left(-\frac{(\underline{c}_1-\underline{u}_1)^2+(\underline{c}_2-\underline{u}_2)^2}{2T}\right) \quad (3.10)$$

By using the above equation, we can determine the stress tensor and the rate of energy dissipation as discussed in Chapter Two once the collisional properties are known.

3.2 Stress Tensor and the Rate of Energy Dissipation

In a collision between two identical, smooth, inelastic, spherical particles of diameter σ with mass m, the total linear momentum is conserved. The momentum of both particles may be expressed in the following ways

$$m\underline{c}_1' = m\underline{c}_1 - \underline{J} \quad (3.11)$$

$$m\underline{c}_2' = m\underline{c}_2 + \underline{J} \quad (3.12)$$

where primed quantities denote the values after the collision and $\underline{J}$ is the impulse of force associated with the change of momentum due to the inelastic collision. The precollision relative velocity $\underline{g} = \underline{c}_1-\underline{c}_2$ is related to the post-collision one $\underline{g}' = \underline{c}_1' - \underline{c}_2'$ in the component normal to the plane of contact as

$$\underline{k}\cdot\underline{g}' = -e(\underline{k}\cdot\underline{g}) \qquad (3.13)$$

where $\underline{k}$ is the unit vector along the centre line from particle 1 to 2 as defined before. Hence, the impulse $\underline{J}$ may be written in terms of the precollision relative velocity as

$$\underline{J} = \frac{m}{2}(1+e)(\underline{k}\cdot\underline{g})\underline{k} \qquad (3.14)$$

From this we may relate the particle velocities before and after the collision as

$$\underline{c}_1' = \underline{c}_1 - \frac{(1+e)}{2}(\underline{k}\cdot\underline{g})\underline{k} \qquad (3.15)$$

$$\underline{c}_2' = \underline{c}_2 + \frac{(1+e)}{2}(\underline{k}\cdot\underline{g})\underline{k} \qquad (3.16)$$

These enable us to proceed to formulate the expression for the stress (or called pressure) tensor and the rate of energy dissipation.

As mentioned previously, the dominant stress generation is assumed to come from the rate of collisional transfer of momentum of inelastic particles. Thus, we may take the total stress tensor to be approximately equal to the rate of collisional transfer of momentum, i.e. $\underset{\sim}{P} \doteq \underset{\sim}{P}_c$ which is given by equation (2.28) with the dynamical quantity $\phi = m\underline{c}$. Using equation (3.15) and substituting into (2.28) neglecting higher order terms, the stress tensor is

$$\underset{\sim}{P} = \frac{(1+e)}{4} m\sigma^3 \int_{\underline{k}\cdot\underline{g}>0} (\underline{k}\cdot\underline{g})^2 \underline{k}\underline{k} f^{(2)}(\underline{r}_1, \underline{c}_1, \underline{r}_2, \underline{c}_2, t)\, d\underline{k}\, d\underline{c}_1\, d\underline{c}_2 \qquad (3.17)$$

If the particles were elastic, i.e. e=1, we essentially obtain the same integral form given by Savage and Jeffrey (1981).

To obtain the rate of energy dissipation per unit volume we consider the energy lost $\Delta\varepsilon$ during each collision which may be expressed as

$$\Delta\varepsilon = \phi_1 + \phi_2 - \phi_1' - \phi_2' \qquad (3.18)$$

and by letting $\phi = \frac{1}{2} mc^2$ it becomes

$$\Delta\varepsilon = \frac{m}{4} (1-e^2)(\underline{k}\cdot\underline{g})^2 \qquad (3.19)$$

Hence, by noting that $\gamma = -\chi(\frac{1}{2} mc^2)$ being the energy sink term in equation (2.34) the integral expression for the rate of energy dissipation per unit volume is

$$\gamma = \frac{(1-e^2)}{8} m\sigma^2 \int_{\underline{k}\cdot\underline{g}>0} (\underline{k}\cdot\underline{g})^3 f^{(2)}(\underline{r}_1,\underline{c}_1,\underline{r}_2,\underline{c}_2,t)\,d\underline{k}\; d\underline{c}_1\; d\underline{c}_2 \qquad (3.20)$$

As can be seen immediately if the particles were elastic, i.e. e=1, there would be no energy dissipation because γ is zero.

CHAPTER 4

SOLUTIONS FOR THE STRESS TENSOR AND THE RATE OF ENERGY DISSIPATION PER UNIT VOLUME

The stress tensor $\underset{\sim}{P}$ and the rate of energy dissipation per unit volume γ given by equations (3.17) and (3.20) respectively may be evaluated by using the proposed complete pair distribution function $f^{(2)}$ in (3.9) and they may be written as

$$\underset{\sim}{P} = \frac{(1+e)}{4} \frac{n^2 m \sigma^3}{(2\pi T)^3} \int_{\underline{k}\cdot\underline{g}>0} (\underline{k}\cdot\underline{g})^2 \underline{k}\underline{k} g_o(\nu) \operatorname{erfc}\left(\frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right) \exp\left(-\frac{(\underline{c}_1-\underline{u}_1)^2+(\underline{c}_2-\underline{u}_2)^2}{2T}\right) d\underline{k}\,d\underline{c}_1 d\underline{c}_2 \qquad (4.1)$$

and

$$\gamma = \frac{(1-e^2)}{8} \frac{n^2 m \sigma^2}{(2\pi T)^3} \int_{\underline{k}\cdot\underline{g}>0} (\underline{k}\cdot\underline{g})^3 g_o(\nu) \operatorname{erfc}\left(\frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right) \exp\left(-\frac{(\underline{c}_1-\underline{u}_1)^2+(\underline{c}_2-\underline{u}_2)^2}{2T}\right) d\underline{k}\,d\underline{c}_1 d\underline{c}_2 \qquad (4.2)$$

The velocities $\underline{c}_1$ and $\underline{c}_2$ can be expressed in terms of the variables $\underline{w}$, the center of mass velocity, and $\underline{g}$, the relative velocity

$$\underline{c}_1 = \underline{w} + \tfrac{1}{2}\,\underline{g} \qquad (4.3a)$$

$$\underline{c}_2 = \underline{w} - \tfrac{1}{2}\,\underline{g} \qquad (4.3b)$$

with the modulus of the Jacobian being unity, i.e., $d\underline{c}_1 d\underline{c}_2 = d\underline{w}d\underline{g}$. Also the mean velocities of the particles $\underline{u}_1$ and $\underline{u}_2$ may be expressed in the following ways:

$$\underline{u}_1(\underline{r}_1) = \underline{u}(\underline{r}) - \frac{\sigma}{2}\,\underline{k}\cdot\nabla\underline{u} \tag{4.4a}$$

$$\underline{u}_2(\underline{r}_2) = \underline{u}(\underline{r}) + \frac{\sigma}{2}\,\underline{k}\cdot\nabla\underline{u} \tag{4.4b}$$

where $\underline{r}$ is the position of the point of contact of the particles. Using equations (4.3a,b) and (4.4a,b), the stress tensor and the rate of energy dissipation per unit volume may be written as

$$\underset{\sim}{P} = \frac{(1+e)}{4}\,\frac{n^2 m\sigma^3}{(2\pi T)^3}\int_{\underline{k}\cdot\underline{g}>0}(\underline{k}\cdot\underline{g})^2\,\underline{k}\underline{k}g_o(\nu)\ \mathrm{erfc}\left(\frac{\sigma\underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$
$$\exp\left(-\frac{4\underline{w}_o^2 + (\underline{g} + \sigma\underline{k}\cdot\nabla\underline{u})^2}{4T}\right)d\underline{k}\,d\underline{w}_o\,d\underline{g} \tag{4.5}$$

and

$$\gamma = \frac{(1-e^2)}{8}\,\frac{n^2 m\sigma^2}{(2\pi T)^3}\int_{\underline{k}\cdot\underline{g}>0}(\underline{k}\cdot\underline{g})^3\,g_o(\nu)\ \mathrm{erfc}\left(\frac{\sigma\underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$
$$\exp\left(-\frac{4\underline{w}_o^2 + (\underline{g} + \sigma\underline{k}\cdot\nabla\underline{u})^2}{4T}\right)d\underline{k}\,d\underline{w}_o\,d\underline{g} \tag{4.6}$$

with $\underline{w}_o = \underline{w}-\underline{u}$. Several integrations may then be performed (Appendix B) to yield

$$\underset{\sim}{P} = \frac{(1+e)}{8}\,\frac{n^2 m\sigma^3}{(\pi T)^{\frac{1}{2}}}\int_{\underline{k}\cdot\underline{g}>0}(\underline{k}\cdot\underline{g})^2\,\underline{k}\underline{k}g_o(\nu)\ \mathrm{erfc}\left(\frac{\sigma\underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$
$$\exp\left(-\frac{(\underline{k}\cdot\underline{g} + \sigma\underline{k}\underline{k}:\nabla\underline{u})^2}{4T}\right)d\underline{k}\,d(\underline{k}\cdot\underline{g}) \tag{4.7}$$

and

$$\gamma = \frac{(1-e^2)}{16}\,\frac{n^2 m\sigma^2}{(\pi T)^{\frac{1}{2}}}\int_{\underline{k}\cdot\underline{g}>0}(\underline{k}\cdot\underline{g})^3 g_o(\nu)\ \mathrm{erfc}\left(\frac{\sigma\underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$
$$\exp\left(-\frac{(\underline{k}\cdot\underline{g} + \sigma\underline{k}\underline{k}:\nabla\underline{u})^2}{4T}\right)d\underline{k}\,d(\underline{k}\cdot\underline{g}) \tag{4.8}$$

Letting $\zeta = \underline{k}\cdot\underline{g}/(4T)^{\frac{1}{2}}$, the above equations may be rewritten as

$$\underset{\sim}{P} = \frac{(1+e)n^2 m\sigma^3 T}{\pi^{\frac{1}{2}}} \int_{\zeta>0} \zeta^2 \underline{k}\underline{k} g_o(\nu) \; \mathrm{erfc}\left(\frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$

$$\exp\left(-\left(\zeta + \frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)^2\right) d\underline{k}d\zeta \qquad (4.9)$$

and

$$\gamma = \frac{(1-e^2)n^2 m\sigma^2 T^{2/3}}{\pi^{\frac{1}{2}}} \int_{\zeta>0} \zeta^3 g_o(\nu) \; \mathrm{erfc}\left(\frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)$$

$$\exp\left(-\left(\zeta + \frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}}\right)^2\right) d\underline{k}d\zeta \qquad (4.10)$$

By noting that the bulk solid density ρ_b = nm, solid fraction $\nu = n\pi\sigma^3/6$ and the mean shear velocity to r.m.s. velocity fluctuation ratio $R = \frac{\sigma(du/dz)}{<v^2>^{\frac{1}{2}}}$ as defined previously, the stress tensor and the rate of energy dissipation may be non-dimensionalized to become

$$\underset{\sim}{P}^* = \frac{\underset{\sim}{P}}{\rho_b \nu g_o(\nu)\left(\sigma\frac{du}{dz}\right)^2\left(\frac{1+e}{2}\right)} = \frac{4}{\pi^{3/2}\sqrt{3}R^3} \int_{\zeta>0} \zeta^2 \underline{k}\underline{k} \; \mathrm{erfc}(\Phi)$$

$$\exp\left(-(\zeta+\Phi)^2\right) d\underline{k}d\zeta \qquad (4.11)$$

and

$$\gamma^* = \frac{\gamma}{\rho_b \nu g_o(\nu)\sigma^2\left(\frac{du}{dz}\right)^3(1-e^2)} = \frac{2}{\pi^{3/2}\sqrt{3}R^3} \int_{\zeta>0} \zeta^3 \; \mathrm{erfc}(\Phi)$$

$$\exp\left(-(\zeta+\Phi)^2\right) d\underline{k}d\zeta \qquad (4.12)$$

where the parameter Φ is defined according to equations (3.6) and (3.7) to be

$$\Phi = \frac{\sigma \underline{k}\underline{k}:\nabla\underline{u}}{2T^{\frac{1}{2}}} = \frac{\sqrt{3}}{2} R \sin\theta\cos\theta\sin\phi \qquad (4.13)$$

Furthermore, from Figure 3 the unit vector $\underset{\sim}{k}$ may be defined to be

$$\underset{\sim}{k} = \sin\theta \cos\phi \, \underset{\sim}{e}_x + \sin\theta \sin\phi \, \underset{\sim}{e}_y + \cos\theta \, \underset{\sim}{e}_z \tag{4.14}$$

and the solid angle

$$d\underset{\sim}{k} = \sin\theta \, d\theta d\phi \tag{4.15}$$

Thus by making use of equations (4.14) and (4.15), the non-dimensional stress tensor and rate of energy dissipation per unit volume can be expressed as

$$\underset{\sim}{P}^* = \frac{4}{\pi^{3/2}R^2} \int_{\zeta=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \zeta^2 \underset{\sim}{k}\underset{\sim}{k} \, \mathrm{erfc}\,(\Phi) \exp\left(-(\zeta+\Phi)^2\right) \sin\theta \, d\theta \, d\phi \, d\zeta \tag{4.16}$$

and

$$\gamma^* = \frac{2}{\pi^{3/2}\sqrt{3}\,R^3} \int_{\zeta=0}^{\infty} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \zeta^3 \, \mathrm{erfc}\,(\Phi) \exp\left(-(\zeta+\Phi)^2\right) \sin\theta \, d\theta \, d\phi \, d\zeta \tag{4.17}$$

with

$$\underset{\sim}{k}\underset{\sim}{k} = \begin{pmatrix} \sin^2\theta\cos^2\phi & \sin^2\theta\cos\phi\sin\phi & \sin\theta\cos\theta\cos\phi \\ \sin^2\theta\cos\phi\sin\phi & \sin^2\theta\sin^2\phi & \sin\theta\cos\theta\sin\phi \\ \sin\theta\cos\theta\cos\phi & \sin\theta\cos\theta\sin\phi & \cos^2\theta \end{pmatrix} \tag{4.18}$$

Unfortunately the integrations of (4.16) and (4.17) cannot be performed analytically and numerical integration seems to be a sensible alternative. However, analytical solutions of such integrals are desirable even though the solutions might be approximate ones. Hence in order to by-pass the numerical integration and see some important features of the solutions, we will use the method of asymptotic expansion and series transformation to obtain the approximate forms of the stresses and the rate of energy dissipation per unit volume.

Savage and Jeffrey (1981) had considered the collisional stress tensor for the case of simple shear of smooth, hard, elastic and spherical granular materials and found essentially the same integral form as given by equation (4.1) with e=1. In order to obtain the solution of the integral, they performed numerical integrations as well as asymptotic expansions both for small and large values of the parameter R in the integrand and discussed the physical significance involved. The parameter R, being the ratio of mean shear characteristic velocity to the r.m.s. fluctuation velocity, depends on the material properties of the particles. When a mass of granular material is subjected to simple shear by external means, the velocity fluctuations of the particles will increase in magnitude until the energy dissipation inside the bulk solid is balanced with the mechanical work input. Energy may be dissipated in the form of thermal heat caused by the inelastic collisions and the frictional rubbing of particles. Thus R may obtain values depending upon the coefficient of restitution and the dry frictional coefficient of the particles. The case considered by Savage and Jeffrey (1981) was a system of no energy dissipation. As a result, the parameter R could not be determined directly from the material properties. However, the present analysis takes into account the inelasticity though ignores the dry friction of the particles, R will be known once the balance of work done and energy dissipation is established.

Following the treatment of Savage and Jeffrey (1981), the integrands of the non-dimensional stress tensor and rate of energy dissipation per unit volume given by (4.16) and (4.17) respectively will be expanded in terms of the parameter R asymptotically for small and large values and the expansions will be matched by means of series transformation to obtain the form of approximate solutions valid for general values of R. The rate of work done by shear will then be equated with the rate of energy dissipation per unit volume to obtain a relationship between the parameter R and the coefficient of restitution e of the particles.

4.1 Solution for small R expansion

Consider R to be small, then correspondingly the magnitude of Φ given by equation (4.13) will also be small, i.e. limit $\Phi \to 0$. Hence, the complementary error function and the exponential function in the integrands of the integrals (4.16) and (4.17) may be expanded as follows:

$$\operatorname{erfc}(\Phi) = 1 - \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{\Phi^{2n+1}}{n!\,(2n+1)}$$

$$= 1 - \frac{2\Phi}{\sqrt{\pi}} + \frac{2\,\Phi^3}{3\sqrt{\pi}} - \frac{\Phi^5}{5\sqrt{\pi}} + \frac{\Phi^7}{21\sqrt{\pi}} - \ldots \qquad (4.19)$$

and

$$\exp\left(-(\zeta+\Phi)^2\right) = e^{-\zeta^2}\left(1-2\zeta\Phi + 2\zeta^2\Phi^2 - \frac{4}{3}\zeta^3\Phi^3+\ldots\right)$$
$$\left(1 - \Phi^2 + \frac{\Phi^4}{2} - \frac{\Phi^6}{6} + \ldots\right) \tag{4.20}$$

With the above expansions, the integration of $d\zeta$ in both integrals may be performed term by term to yield

$$\underset{\sim}{P}^* = \frac{4}{\pi^{3/2}R^2} \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \underline{\underline{kk}}\, F(\Phi)\, \sin\theta\, d\theta d\phi \tag{4.21}$$

and

$$\gamma^* = \frac{2}{\pi^{3/2}\sqrt{3}\, R^3} \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} G(\Phi)\, \sin\theta\, d\theta d\phi \tag{4.22}$$

where

$$\begin{aligned} F(\Phi) = {} & \frac{\sqrt{\pi}}{4} - \frac{3}{2}\Phi + \left(\frac{\sqrt{\pi}}{2} + \frac{2}{\sqrt{\pi}}\right)\Phi^2 - \frac{7}{6}\Phi^3 + 0 \times \Phi^4 + \frac{19}{60}\Phi^5 \\ & - \frac{4}{45\sqrt{\pi}}\Phi^6 - \frac{13}{140}\Phi^7 + \frac{16}{315\sqrt{\pi}}\Phi^8 + \frac{67}{3024}\Phi^9 - \frac{4}{225\sqrt{\pi}}\Phi^{10} \\ & - \frac{103}{23760}\Phi^{11} + \frac{736}{155925\sqrt{\pi}}\Phi^{12} + 0\,(\Phi^{13}) \end{aligned} \tag{4.23}$$

and

$$\begin{aligned} G(\Phi) = {} & \frac{1}{2} - \left(\frac{3\sqrt{\pi}}{4} + \frac{1}{\sqrt{\pi}}\right)\Phi + 3\,\Phi^2 - \left(\frac{\sqrt{\pi}}{2} + \frac{8}{3\sqrt{\pi}}\right)\Phi^3 + \frac{3}{4}\Phi^4 \\ & + \frac{2}{5\sqrt{\pi}}\Phi^5 - \frac{1}{5}\Phi^6 - \frac{8}{105\sqrt{\pi}}\Phi^7 + \frac{1}{16}\Phi^8 + \frac{17}{540\sqrt{\pi}}\Phi^9 \\ & + \frac{43}{2520}\Phi^{10} + \frac{64}{17325\sqrt{\pi}}\Phi^{11} + \frac{167}{47520}\Phi^{12} + 0\,(\Phi^{13}) \end{aligned} \tag{4.24}$$

Using the definition of Φ in (4.13) and also the dyadic product $\underline{\underline{kk}}$ given by (4.18), the components of the non-dimensional stresses and the rate of energy dissipation per unit volume may be integrated and expressed in terms of the ratio R as

$$P^*_{xx} = \frac{4}{3R^2} + \left(\frac{\sqrt{\pi}}{2} + \frac{2}{\sqrt{\pi}}\right)\frac{4}{35\sqrt{\pi}} - \frac{R^4}{15015\pi} + \frac{R^6}{230945\pi} - \frac{81R^8}{424938800\pi}$$

$$+ \frac{R^{10}}{146965000\pi} - O(R^{12}) \qquad (4.25)$$

$$P^*_{yy} = P^*_{zz} = \frac{4}{3R^2} + \left(\frac{\sqrt{\pi}}{2} + \frac{2}{\sqrt{\pi}}\right)\frac{12}{35\sqrt{\pi}} - \frac{R^4}{2145\pi} + \frac{9R^6}{230945\pi} - \frac{81R^8}{38630800\pi}$$

$$+ \frac{R^{10}}{11305000\pi} - O(R^{12}) \qquad (4.26)$$

$$P^*_{yz} = P^*_{zy} = -\frac{12}{5\sqrt{3\pi}\,R} - \frac{R}{5\sqrt{3\pi}} + \frac{57R^3}{8008\sqrt{3\pi}} - \frac{9R^5}{29920\sqrt{3\pi}}$$

$$+ \frac{1809R^7}{165541376\sqrt{3\pi}} - \frac{8343R^9}{24723712000\sqrt{3\pi}} + O(R^{11}) \qquad (4.27)$$

$$\gamma^* = \frac{4}{\sqrt{3\pi}\,R^3} + \frac{6}{5\sqrt{3\pi}\,R} + \frac{9R}{280\sqrt{3\pi}} - \frac{9R^3}{8008\sqrt{3\pi}} + \frac{63R^5}{1244672\sqrt{3\pi}}$$

$$- \frac{10449R^7}{4966241280\sqrt{3\pi}} + \frac{13527R^9}{197789696000\sqrt{3\pi}} + O(R^{11}) \qquad (4.28)$$

The non-dimensional normal stress P^*_{yy} is found to be the same as P^*_{zz} while P^*_{xx} differs from both in the second term onward. The series given by (4.25) and (4.26) shows that these stresses have even powers of R dependence. Truncating after the first terms of the series, we find the corresponding dimensional normal stresses are isotropic and have no dependence of particle diameter and shear rate. The second term gives rise to anisotropy between P_{xx} and $P_{yy} = P_{zz}$ which depends upon the square of the particle diameter and shear rate similar to the results of Bagnold's stress model (1954) in his grain-inertia regime. Higher order terms of the normal stresses consist of coefficients of rapidly decreasing magnitude and alternating signs and increasing even powers of particle diameter and shear rate dependence. Similarly, the non-dimensional shear stress $P^*_{yz} = P^*_{zy}$ and the rate of energy dissipation per unit volume γ^* given by (4.27) and (4.28) have odd powers of R dependence. Considering just the first term of both series, the corresponding dimensional shear stress depends linearly upon the particle diameter and shear rate while γ depends inversely on the particle diameter and has no dependence of shear rate. Higher order terms give results analogous to those of the normal stresses. All of the above mentioned quantities depend on the velocity fluctuations associated with the interparticle collisions which cause the behaviour of the flow of granular materials to be different from that of liquid flow.

4.2 Solution for large R

Consider R to be large, i.e., limit $R \to \infty$. The complementary error function in the integrands of both integrals (4.16) and (4.17) obeys

$$\lim_{R \to \infty} \operatorname{erfc}\left(\frac{\sqrt{3}}{2} R \sin\theta\cos\theta\sin\phi\right) \begin{cases} = 2 & \text{for } (\sin\theta\cos\theta\sin\phi) < 0 \\ = 0 & \text{for } (\sin\theta\cos\theta\sin\phi) > 0 \end{cases} \tag{4.29}$$

Thus the ranges of integration will be taken over the face of the sphere where $0 \leq \theta \leq \frac{\pi}{2}$ for $\pi \leq \phi \leq 2\pi$ and $\pi \leq \theta \leq \frac{3\pi}{2}$ for $0 \leq \phi \leq \pi$. For large R, the integrals may be evaluated asymptotically by the method of steepest descent to yield

$$\underset{\sim}{P}^* = \frac{4}{35}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 8/\pi \\ 0 & 8/\pi & 3 \end{pmatrix} \tag{4.30}$$

and

$$\gamma^* = \frac{8}{35\pi} \tag{4.31}$$

In these first order large R solutions, the stress tensor $\underset{\sim}{P}$ is proportional to the square of particle diameter and shear rate while the rate of energy dissipation per unit volume γ is proportional to the square of particle diameter and cube of the shear rate. The ratio of shear to normal stress, $|P_{yz}/P_{zz}| = 8/3\pi = \tan 40.3^{\circ}$.

4.3 General solution for R

The expansions for small R and the asymptotic values for large R of the non-dimensional stress tensor and rate of energy dissipation per unit volume may be forced to join to give series that are valid for all R by the method of series transformation, namely the 'quasi-Euler' transformation. The traditional Euler transformation appropriate for the above series takes the form (Van Dyke 1964)

$$\varepsilon = \frac{R^2}{R^2+d} \tag{4.32}$$

where d is an arbitrary constant. By putting the series of $\underset{\sim}{P}^*$ and γ^* in terms of ε and d in the small R expansion* from (4.25) to (4.28), the transformed expressions are

$$P^*_{xx} = \left(\frac{1-\varepsilon}{\varepsilon d}\right)\left(\frac{4}{3} + \frac{4}{35\sqrt{\pi}}\left(\frac{\sqrt{\pi}}{2} + \frac{2}{\sqrt{\pi}}\right)\left(\frac{\varepsilon d}{1-\varepsilon}\right) - \frac{1}{15015\pi}\left(\frac{\varepsilon d}{1-\varepsilon}\right)^3\right) \quad (4.33)$$

$$P^*_{yy} = P^*_{zz} = \left(\frac{1-\varepsilon}{\varepsilon d}\right)\left(\frac{4}{3} + \frac{12}{35\sqrt{\pi}}\left(\frac{\sqrt{\pi}}{2} + \frac{2}{\sqrt{\pi}}\right)\left(\frac{\varepsilon d}{1-\varepsilon}\right) - \frac{1}{2145\pi}\left(\frac{\varepsilon d}{1-\varepsilon}\right)^3\right) \quad (4.34)$$

$$P^*_{yz} = P^*_{zy} = -\left(\frac{1-\varepsilon}{\varepsilon d}\right)^{1/2}\left(\frac{12}{5\sqrt{3\pi}} + \frac{1}{5\sqrt{3\pi}}\left(\frac{\varepsilon d}{1-\varepsilon}\right) - \frac{57}{8008\sqrt{3\pi}}\left(\frac{\varepsilon d}{1-\varepsilon}\right)^3\right) \quad (4.35)$$

$$\gamma^* = \left(\frac{1-\varepsilon}{\varepsilon d}\right)^{3/2}\left(\frac{4}{\sqrt{3\pi}} + \frac{6}{5\sqrt{3\pi}}\left(\frac{\varepsilon d}{1-\varepsilon}\right) + \frac{9}{280\sqrt{3\pi}}\left(\frac{\varepsilon d}{1-\varepsilon}\right)^2 - \frac{9}{8008\sqrt{3\pi}}\left(\frac{\varepsilon d}{1-\varepsilon}\right)^3\right) \quad (4.36)$$

We may further expand the factors $(1-\varepsilon)^{1/2}$, $(1-\varepsilon)^{3/2}$, $(1-\varepsilon)^{-1}$, $(1-\varepsilon)^{-2}$ and $(1-\varepsilon)^{-3}$ into power series up to the degree corresponding to that of the parameter R in the original series, the expansions become

$$P^*_{xx} = \frac{4}{3}(\varepsilon d)^{-1} + \left(0.1298994 - \frac{4}{3}d^{-1}\right) - 2.119946\mathrm{x}10^{-5}(\varepsilon d)^2 \quad (4.37)$$

$$P^*_{yy} = P^*_{zz} = \frac{4}{3}(\varepsilon d)^{-1} + \left(0.3896982 - \frac{4}{3}d^{-1}\right) - 1.4839622\mathrm{x}10^{-4}(\varepsilon d)^2 \quad (4.38)$$

$$P^*_{yz} = P^*_{zy} = -(\varepsilon d)^{-1/2}(0.781764 - (0.390882 - 0.065147\, d)\varepsilon - (0.0977205 - 0.0325735\, d + 2.3185434 \times 10^{-3} d^2)\varepsilon^2) \quad (4.39)$$

---

*The number of terms used in the series are only up to the power of 4 or less of the parameter R because additional terms show little improvement in the transformed series.

$$\gamma^* = (\varepsilon d)^{-3/2}\,(1.30294 + (1.95441 - 0.390882\,d)\varepsilon$$
$$+ (0.4886025 - 0.195441d + 0.01040054d^2)\varepsilon^2$$
$$+ (0.0814338 - 0.0488603d + 5.235027\times10^{-3}d^2$$
$$- 3.660858\times10^{-4}d^3)\varepsilon^3) \tag{4.40}$$

The advantage of using the Euler transformation is that the magnitude of R can be taken out to infinity while the transformed variable $\varepsilon \to 1$, hence the validity of the transformed series may be extended for all values of R. Let us take ε to be one in the transformed expansions of $\underset{\sim}{P}^*$ and γ^* given by eq. (4.37) to (4.40), the series now depends only on the arbitrary constant d. Each of these series may be fitted to give identical asymptotic results corresponding to those given in (4.30) and (4.31) simply by solving the appropriate value of d in each case. Thus, the final forms of the series valid for general R are

$$P^*_{xx} = 0.049130173504\left(\frac{R^2}{R^2+27.1387873936}\right)^{-1} + 0.0807692290523$$
$$- 0.0156136882706\left(\frac{R^2}{R^2+27.1387873936}\right)^2 \tag{4.41}$$

$$P^*_{yy} = P^*_{zz} = 0.07504766006422\left(\frac{R^2}{R^2+17.7665018192}\right)^{-1} + 0.314650599358$$
$$- 0.0468410571429\left(\frac{R^2}{R^2+17.7665018192}\right)^2 \tag{4.42}$$

$$P^*_{yz} = P^*_{zy} = -\left(\frac{R^2}{R^2+20.6473941193}\right)^{-\frac{1}{2}} (0.172045391382$$

$$+ 0.210001387831 \left(\frac{R^2}{R^2+20.6473941193}\right)$$

$$- 0.0910205975593 \left(\frac{R^2}{R^2+20.6473941193}\right)^2) \qquad (4.43)$$

$$\gamma^* = \left(\frac{R^2}{R^2+0.888348036208}\right)^{-3/2} (1.55614373166$$

$$- 1.91949649499 \left(\frac{R^2}{R^2+0.888348036208}\right)$$

$$+ 0.386063604215 \left(\frac{R^2}{R^2+0.888348036208}\right)^2$$

$$+ 0.0500467045239 \left(\frac{R^2}{R^2+0.888348036208}\right)^3) \qquad (4.44)$$

These results are shown in Figures 6 to 9 together with the successive partial sums of the original series given by (4.25) to (4.28). The transformed series of the stress tensor gives values which are identical on graph with the numerical integration performed by Savage and Jeffrey (1981)*. Thus we may have confidence that the transformed series of the rate of energy dissipation per unit volume γ^* is indeed valid also.**

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*The present ratio R is multiplied by a conversion factor of $\sqrt{2/3}$ in order to confirm the results of Savage and Jeffrey (1981) due to the error in their $f^{(1)}$ as noted previously.

**Later comparison of numerical computation done by Dr. Jeffrey and the present transformed series of rate of energy dissipation has shown that both calculations agree in average to 3 significant figures.

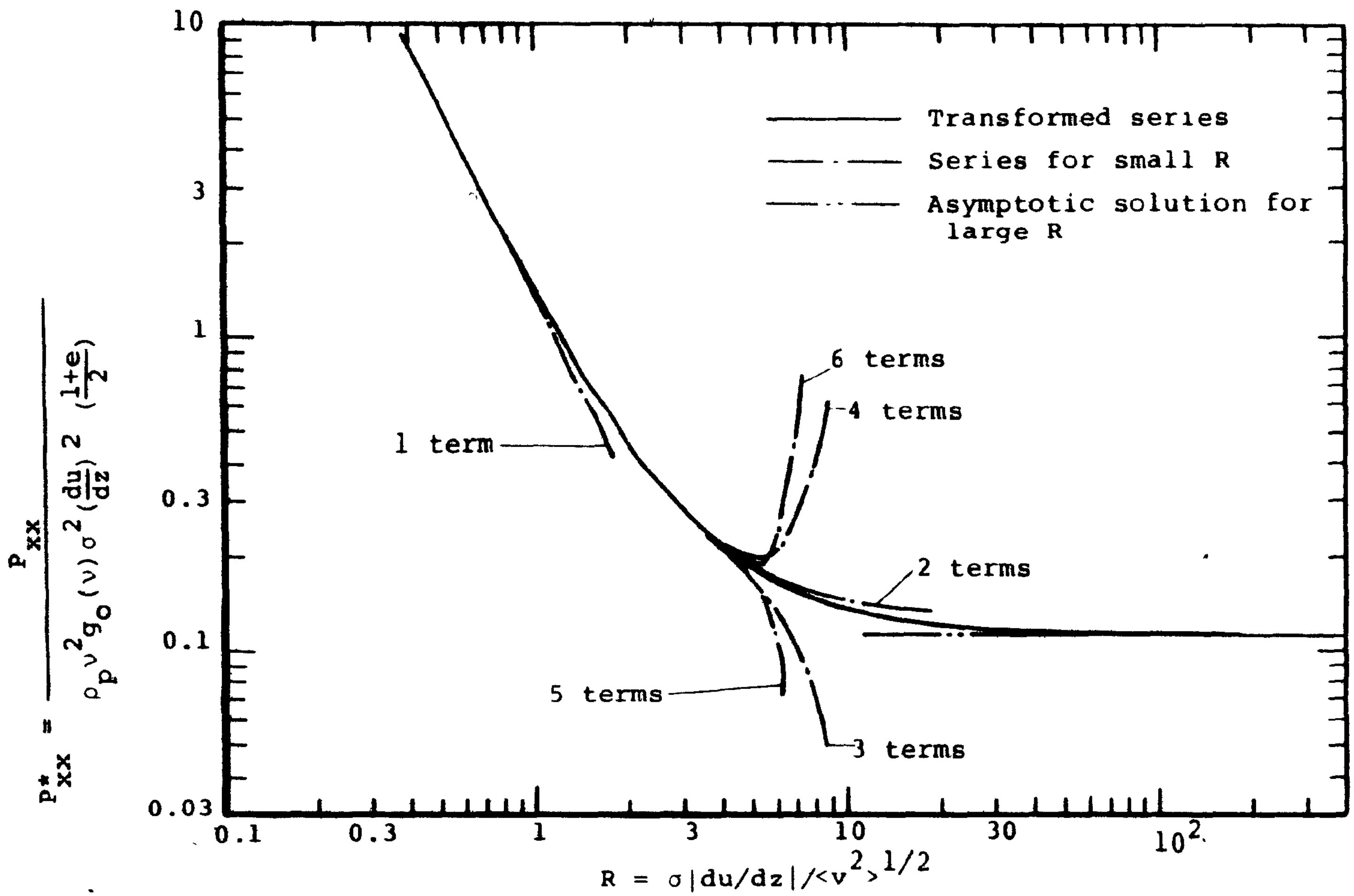

Fig. 6 Variation of non-dimensional normal stress component P^*_{xx} with ratio of characteristic mean shear velocity to fluctuation velocity R for the case of simple shear

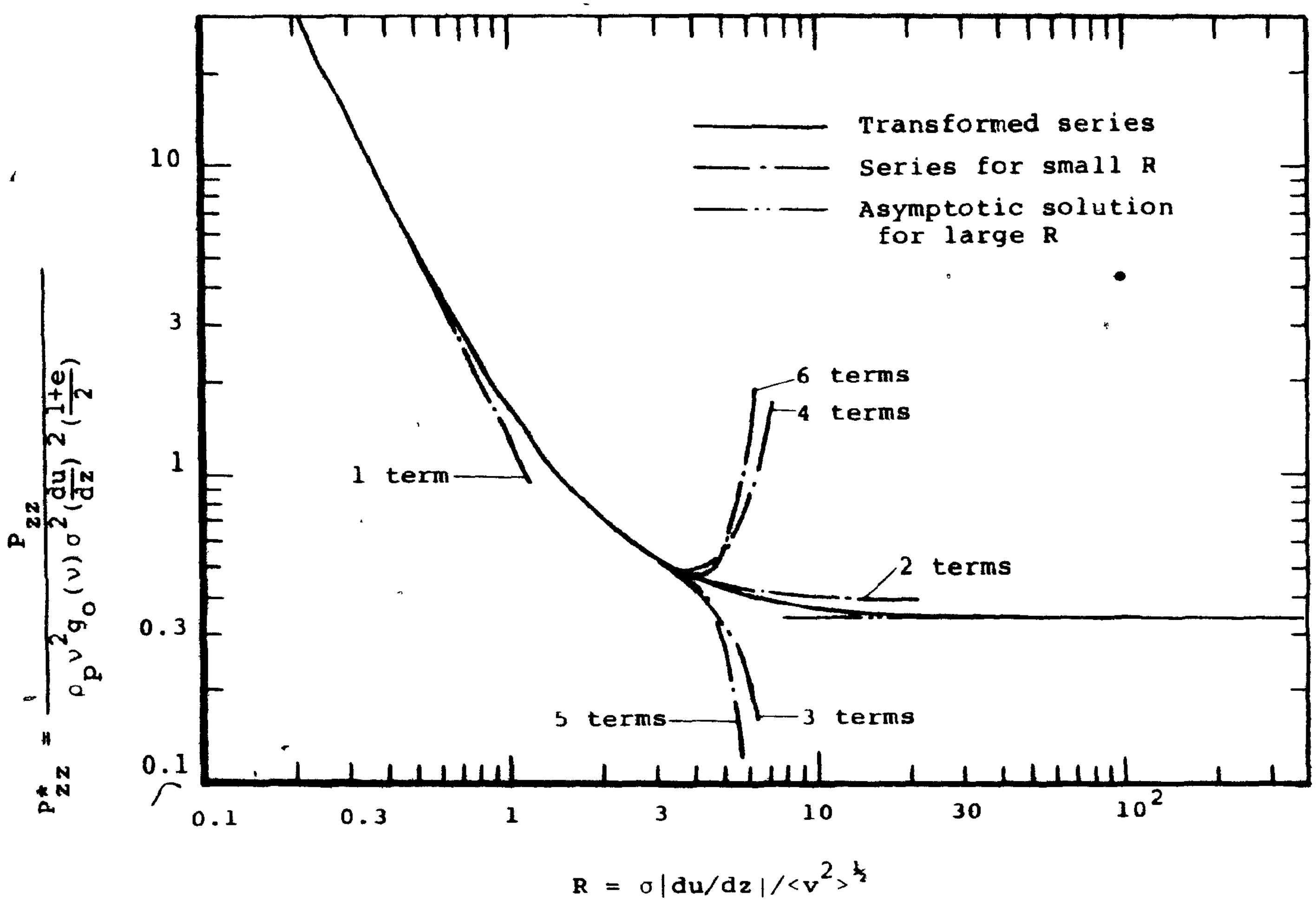

Fig. 7 Variation of non-dimensional normal stress component $P^*_{yy} = P^*_{zz}$ with ratio of characteristic mean shear velocity to fluctuation velocity R for the case of simple shear

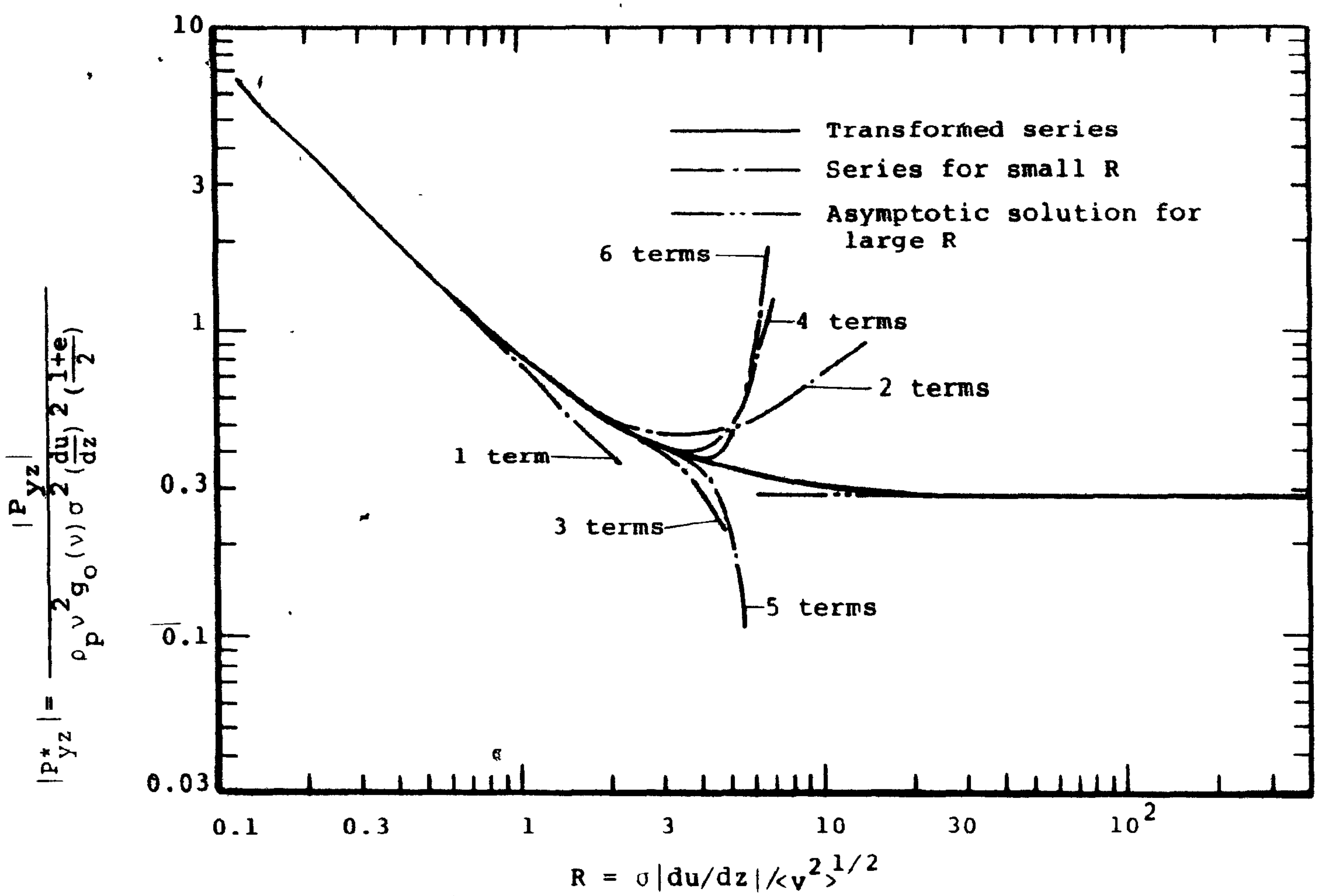

Fig. 8 Variation of non-dimensional shear stress component $P^*_{yz} = P^*_{zy}$ with the ratio of characteristic mean shear velocity to fluctuation velocity R for the case of simple shear

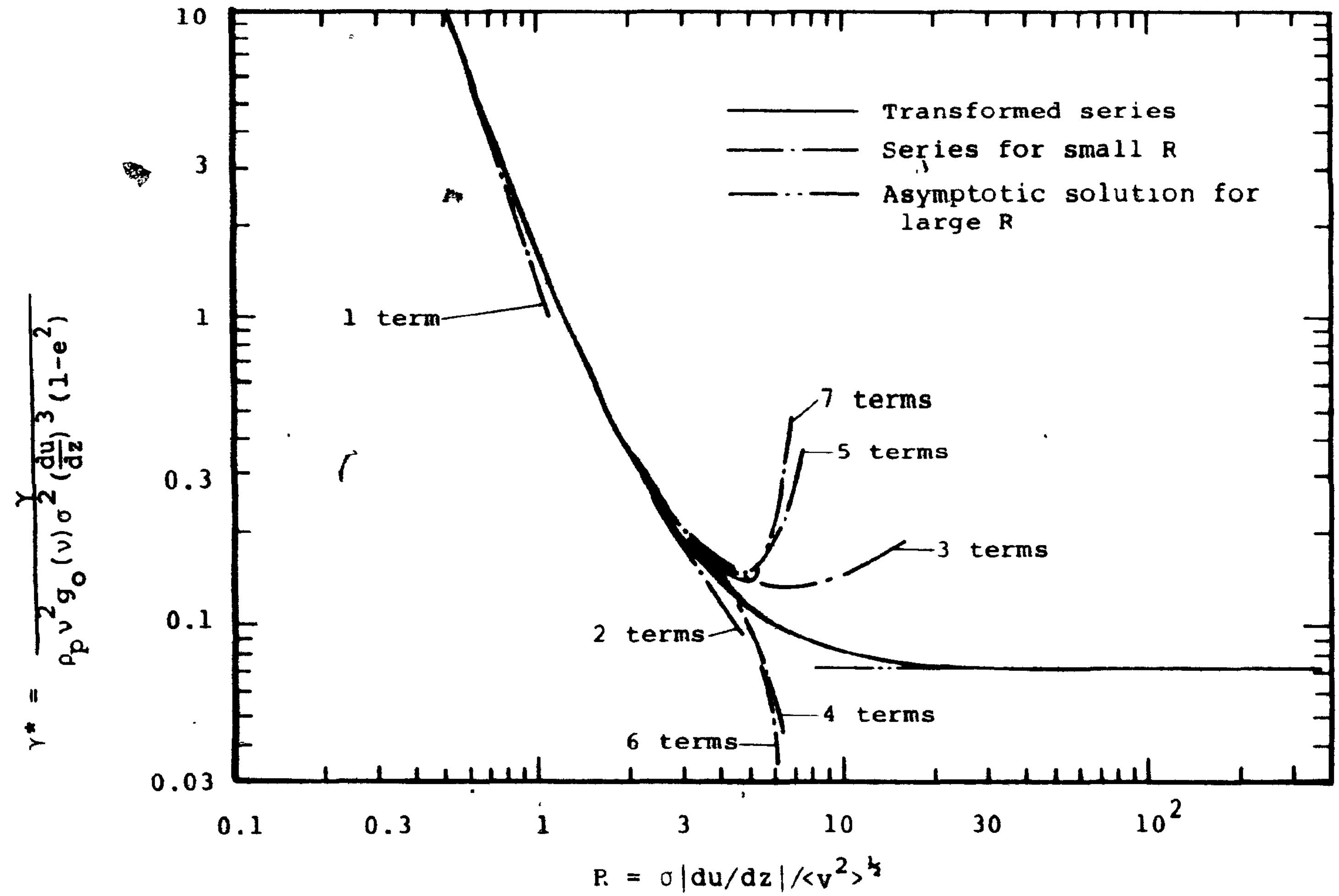

Fig. 9 Variation of non-dimensional rate of energy dissipation per unit volume γ^* with ratio of characteristics mean shear velocity to fluctuation velocity R for the case of simple shear

4.4 Relationship between R and e

The energy balance equation for the equilibrium state of steady kinetic fluctuation energy with no energy flux derived from the energy conservation law given by (2.29) takes the form

$$- \underset{\sim}{P}:\nabla \underline{u} - \gamma = 0 \tag{4.45}$$

From this, we may determine the relationship between the coefficient of restitution e and the mean shear velocity to r.m.s. fluctuation velocity ratio R for the case of simple shear by noting that

$$- P_{yz} \frac{du}{dz} = \gamma \tag{4.46}$$

Using equations (4.43) and (4.44) together with the non-dimensional parameters given in (4.11) and (4.12), equation (4.46) yields

$$e = 1 - \frac{P^*_{yz}}{2\gamma^*} \tag{4.47}$$

If the coefficient of restitution of a certain granular material were given, we could solve the corresponding value of R simply by using (4.43) and (4.44), hence the values of stresses and energy dissipation could be calculated. This relationship between e and R is plotted in Figure 10 which indicates a range of values of e between 1 and -1. When e equals zero, R has the value of upper bound about 2.73. Physically the coefficient of restitution e has its usual range from zero to one as the parameter R goes from zero to infinity. An interpretation of the negative values of e which correspond to large R is not obvious. One possible clue is that the present analysis is incomplete in the sense that we have ignored frictional energy dissipation which undoubtedly plays an important role. In other words, if we were to consider also frictional losses, the lower value of e might be brought back to zero. The negative value of e may be regarded simply as a fictitious value which has no physical meaning. In all the existing theories (Ogawa, et al. 1980, Shen 1982, Jenkins and Savage 1982) including the present one, all the relationships of e vs. R behave in a similar manner and can yield negative e for large R as shown in Figure 10. Detailed discussions of each of these theoretical formulations are reserved for Chapter 5.

CHAPTER 5 THEORY VERIFICATION

In recent years, a number of microstructural theories involving statistical averaging methods of obtaining the constitutive equations for rapid granular flow were proposed. The most pertinent ones are the theories put forward by Ogawa, Umemura and Oshima (1980), Shen (1982), Jenkins and Savage (1982). The common characteristics of these theories and the present one is that the constitutive relationships are calculated explicitly and do not rely upon any empirical phenomenological coefficients which are determined from viscometric experiments or by other means. Instead, in all these formulations the constitutive relations are expressed in terms of material properties such as adhesive coefficient, coefficient of kinetic friction and coefficient of restitution, etc. for the individual particle. Once these coefficients are known, the macroscopic continuum properties of granular flow can be determined explicitly. In this chapter, previous theories will be compared with the present analysis and the appropriate experimental results. When necessary, the algebraic form of the previous theories will be recast to correspond to the present analysis in order to make direct comparisons.

5.1 Comparison Between the Present Theory and Previous Theoretical Works

5.1.1 Ogawa, Umemura and Oshima (1980)

Ogawa, et al. (1980) determined the stress tensor and the rate of energy dissipation for the flow of adhesive, rough, inelastic spherical granular particles by employing a simple statistical kinematic model of particle collision. In their model the friction of the particles was considered but particle rotation was ignored. Furthermore, the fluctuations were assumed to be random and isotropic, and no kinetic energy flux is involved in the analysis. The constitutive equations of stresses and rate of energy dissipation were determined by averaging the rate of transfer of kinetic fluctuation energy of the particles over all possible collisions.

Each particle is considered to be inside an imaginary collision sphere of radius b which represents the 'wall' being set up by the neighbouring particles. In each collision, a fraction of α' of the particle is assumed to adhere to the surface of the sphere and the rest $(1-\alpha')$ rebound from it with a loss of kinetic energy. The fraction α', or called adhesive coefficient here, is assumed to be constant. Multiplying the number density of particles by the change in kinetic energy per collision and the estimated collision frequency of magnitude $\langle v^2\rangle^{1/2}/(2b-\sigma)$ gives the total rate of change of fluctuation energy per unit volume which is then equated to the rate of work done by stresses and the rate of energy dissipation per unit volume. By comparing the forms of both sides, Ogawa, et al. proposed the following constitutive equations of stress tensor and the rate of energy dissipation γ_o:

$$\underset{\sim}{P} = \frac{\rho_b}{4(1-(\nu/\nu^*)^{1/3})} (K_1\langle v^2\rangle\delta_{ij}+b\langle v^2\rangle^{1/2}(K_2D_{ij}+K_3D_{\ell\ell}\delta_{ij})) \qquad (5.1)$$

$$\gamma_o = -K_o \frac{\rho_b}{4(1-(\nu/\nu^*)^{1/3})} \frac{\langle v^2\rangle^{3/2}}{b} \qquad (5.2)$$

where ν^* is said to correspond to the 'packed state' of granular materials, $D_{ij} = (u_{i,j}+u_{j,i})/2$ is the rate of strain tensor, δ_{ij} is the unit tensor and for the case of cohesionless and smooth particles, the K's are given as

$$K_o = -\frac{(1-e^2)}{3} \tag{5.3}$$

$$K_1 = -\frac{2}{9}e(3+e) \tag{5.4}$$

$$K_2 = \frac{(1+e)^2}{9} \tag{5.5}$$

with $K_3 = 0$.

Consider the case of simple shear flow of granular materials. We may non-dimensionalize and express $\underset{\sim}{P}$ and γ_o in terms of the parameter R as

$$P_{xx} = P_{yy} = P_{zz} \quad \text{and} \quad P_{yz} = P_{zy} \tag{5.6a,b}$$

$$\frac{P_{zz}}{\rho_p\ \sigma^2(\frac{\partial u}{\partial z})^2} = \Psi_1(\nu)\ \frac{4e(3+e)}{9R^2} \tag{5.7}$$

$$\frac{P_{yz}}{\rho_p\ \sigma^2(\frac{\partial u}{\partial z})^2} = -\Psi_2(\nu)\ \frac{(1+e)^2}{18R} \tag{5.8}$$

and

$$\frac{\gamma_o}{\rho_p\ \sigma^2(\frac{\partial u}{\partial y})^3} = \Psi_3(\nu)\ \frac{4(1-e^2)}{3R^3} \tag{5.9}$$

where

$$\Psi_1(\nu) = \frac{1}{8}\ \frac{\nu}{(1-(\nu/\nu^*)^{1/3})} \tag{5.10}$$

$$\Psi_2(\nu) = \Psi_1(\frac{\nu^*}{\nu})^{1/3} \tag{5.11}$$

$$\Psi_3(\nu) = \Psi_1\ (\frac{\nu}{\nu^*})^{1/3} \tag{5.12}$$

and ρ_p is the mass density of the solid particle.

The dependence of R in the stresses $\underset{\sim}{P}$ and γ_o resembles the first term small R solution of $\underset{\sim}{P}$ and γ of the present theory given by equations (4.25) to (4.28). Unfortunately, the stresses of both theories depend differently on the coefficient of restitution e, we cannot compare them directly until a relationship of e and R is established for the theory of Ogawa, et al. However, we may compare the non-dimensional rate of energy dissipation by dividing equation (5.9) by a normalizing concentration function defined as

$$\Psi(\nu) = \nu^2 g_o(\nu) \tag{5.13}$$

Taking the solid fractions ν to be 0.5 and $\nu^* = 0.64$ for a randomly packed state, the first term small R solution of the present theory gives $\gamma^* = 1.3029\ R^{-3}$ from (4.28) and the one of Ogawa et al. $\gamma_o^* = \dfrac{\gamma_o}{\rho_p \nu^2 g_o \sigma^2 (\frac{du}{dz})^3 (1-e^2)} = 0.6477\ R^{-3}$ (note $\rho_b = \nu\rho_p$). If we take ν^* to be 0.74 corresponding to an array of closest packed spheres, γ_o^* is lowered giving $\gamma_o^* = 0.3980\ R^{-3}$. This shows that the rate of energy dissipation of Ogawa et al.(1980) is about 2 or 3 times lower than that of the present theory depending on what the packed state is meant to be. In order to compare the theories with no ambiguity, both values of ν^* will be considered in each calculation.

Using the balance equation of rate of work done by stresses and the rate of energy dissipation per unit volume, i.e. $P_{ij}D_{ij} = \gamma_o$ assuming under a steady state, we may obtain a relationship between R and e in their model which is

$$R^2 = 24\left(\frac{\nu}{\nu^*}\right)^{2/3}\left(\frac{1-e}{1+e}\right) \tag{5.14}$$

Interestingly, the variation of R with e behaves in a similar manner as equation (4.47) of the present theory that the coefficient of restitution has a range of values between 1 and -1 as R goes from zero to infinity as shown in Figure 10. The value of e being zero corresponds to the upper bound of $R = 4.512$, $\nu^* = 0.64$ or $R = 4.2988$ with $\nu^* = 0.74$. In general the values of e correspond to higher values of R than those of the present theory.

Now we may compare the stresses* by dividing equations (5.7) and (5.8) by (5.13) giving

$$\frac{P_{zz}}{\rho_p \nu^2 g_o \sigma^2 \left(\frac{\partial u}{\partial z}\right)^2} = C_1(\nu)\ \frac{4e(3+e)}{9R^2} \tag{5.15}$$

$$\frac{P_{yz}}{\rho_p \nu^2 g_o \sigma^2 \left(\frac{\partial u}{\partial z}\right)^2} = -C_2(\nu)\ \frac{(1+e)^2}{18R} \tag{5.16}$$

where $C_1(\nu) = \Psi_1(\nu)/\Psi(\nu)$ (5.17)

and $C_2(\nu) = \Psi_2(\nu)/\Psi(\nu)$ (5.18)

The concentration functions Ψ_1, Ψ_2 and Ψ_3 given by (5.10) to (5.12) associated with the normal stresses, shear stresses and the rate of energy dissipation per unit volume respectively are shown in Fig. 11 together with $\Psi(\nu)$ of the present

*Sign convention of the stresses of Ogawa, et al.(1980) is changed in accordance with those used in the present analysis.

theory given by (5.13). Both theories show quite a different variation with concentration ν. Using the R and e relationship in (5.14), we may determine the stresses. The variations of the normal and shear stresses in terms of R and e are shown in Figs. 12 to 15 together with those of the present theory. The stresses of Ogawa, et al. are much lower than the present ones. For example, when $e = 0.9$ with $\nu^* = 0.74$, the normal stresses of Ogawa, et al. are about 16 times lower and the shear stresses are about 7 times lower as shown in the Figs. 14,15. These differences in stresses amplify further with the decrease of e. The reason for such large quantitative differences in the stresses is not clear, but is possibly due to the number of assumptions made involving the averaging process in their theory.

In all of the above calculations of stresses for comparison, the solid fraction ν is taken to be 0.5 as the reference value. We may set up modification factors for the stresses shown in each of these graphs to be

$$C_{oN}(\nu) = C_1(\nu)/C_1(0.5) \tag{5.19}$$

for the normal stresses and

$$C_{oS}(\nu) = C_2(\nu)/C_2(0.5) \tag{5.20}$$

for the shear stresses. These relations are shown in Figure 16. For a given value of ν other than 0.5, one may take the corresponding correction values from these figures and multiply them with the respective stresses obtained from

Figs. 12 to 15 to give the correct values of stresses of Ogawa, et al.

5.1.2 Shen (1982)

Shen (1982) had used a similar statistical model and derived her constitutive equations for rough, inelastic spherical particles including interstitial fluid drag effects. The case a simple shear of granular materials was considered and assumptions similar to those of Ogawa, et al.(1980) were made. The fluctuation velocity was assumed to be isotropic and rotary inertia effects were neglected. The stresses were determined by letting

$$P_{ij} = p_i \cdot \Delta M_j \cdot f \tag{5.21}$$

where p_i is the average number of particles per unit area which is normal to the i-th coordinate direction, ΔM_j is the average j-th component of the momentum transfer per collision and f is the collisional frequency of a particle inside that unit area. A similar formulation for the stresses was originally used by Bagnold(1954). The rate of energy dissipation per unit volume was given by

$$\gamma = n \cdot F \cdot E \tag{5.22}$$

where n is the number of particles per unit volume, F is the collisional frequency of a particle and E is the energy lose of each particle per collision. The magnitude of the collision frequency F was estimated in a manner similar to that of Ogawa, et al. (1980) by writing

$$F = 2f = \langle v^2 \rangle^{\frac{1}{2}}/S \tag{5.23}$$

where S is the mean separation distance of the particles.

In order to simplify the analysis of the dynamics of particle collisions, a number of approximations were made. The main one is that $R(1+ 1/\lambda) << 1$ where $\lambda = \sigma/S$ is defined as the linear concentration of the particles. This eliminates the consideration of the effect of anisotropic collisions. Another important assumption is that $\tan^{-1} \mu(1+e) \to 0$ and μ is the coefficient of friction. Hence the friction cone* effect is excluded. For the purpose of comparison in the case of negligible interstitial fluid effect and smooth particle, the stresses and the rate of energy dissipation may be written in terms of the parameter R as

$$P_{xx} = P_{yy} = P_{zz} \text{ and } P_{yz} = P_{zy} \tag{5.24a,b}$$

$$\frac{P_{zz}}{\rho_p \nu^2 g_o \sigma^2 (\frac{\partial u}{\partial z})^2} = C_3(\nu) \frac{8\sqrt{2}\ (1+e)}{\pi^2\ R^2} \tag{5.25}$$

$$\frac{P_{yz}}{\rho_p \nu^2 g_o \sigma^2 (\frac{\partial u}{\partial z})^2} = - C_1(\nu) \frac{0.212(1+e)}{R} \tag{5.26}$$

$$\gamma_S^* = \frac{\gamma_S}{\rho_p \nu^2 g_o \sigma^2 (\frac{\partial u}{\partial z})^2 (1-e^2)} = C_3(\nu) \frac{5}{4R^3} \tag{5.27}$$

where $C_3(\nu) = \Psi_3(\nu)/\Psi(\nu)$ (5.28)

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* When two particles collide, the post-collisional velocity components parallel to the plane of contact are restricted by the effect of friction and inelasticity of the particles. The effect of particle rotation due to the frictional forces is neglected. Hence, a 'friction cone' of an interior angle of $\tan^{-1}\mu(1+e)$ may be found such that for collisions occuring within the friction cone, the component of total relative momentum along the plane of contact will vanish.

Interestingly, the above stresses and rate of energy dissipation per unit volume have the same form of R dependence as those of Ogawa, et al. (1980) and the first term small R solution of $\underset{\sim}{P}$ and γ of the present theory. However, the concentration functions associated with the stresses differ from those of Ogawa, et al. (1980). A formula for R and e may be established easily by using the balance law of rate of shear work and energy dissipation which gives

$$R^2 = \left(\frac{\nu}{\nu^*}\right)^{1/3} \frac{(1-e)}{0.2120} \tag{5.29}$$

The plot of this equation is given together with the previous ones in Figure 10 which shows that R has an upper limit of about 2 when e = 0. Its behaviour is different from the previous two in the sense that the range of e starts from one and extends to negative infinity as R takes on values from zero to infinity.

Computations for the stresses in terms of R and e are performed in a manner similar to those of Ogawa, et al. (1980) and are shown in Figs. 12 to 15. The magnitude of Shen's stresses are higher than those of Ogawa, et al. (1980); however, they are still considerably lower than those of the present theory. For example, when e = 0.9 with ν^* = 0.74 and ν = 0.5, the normal stresses of Shen are about 6 times lower and the shear stresses are about 2.5 times lower as shown in Figs. 14 & 15. With a decrease of e, these differences are enlarged further. The variations of stresses with ν may be described by the factors similar to those used in the discussion of the theory of Ogawa, et al. (1980). For the theory of Shen (1982), they may be defined as

$$C_{SN}(\nu) = C_3(\nu)/C_3(0.5) \tag{5.30}$$

for the normal stresses and

$$C_{SS}(\nu) = C_1(\nu)/C_1(0.5) \tag{5.31}$$

for the shear stresses. They are shown in Figure 17.

We may also compare the rate of energy dissipation. Consider the case of $\nu^* = 0.64$ and $\nu = 0.5$. The non-dimensional rate of energy dissipation per unit volume of Shen (1982) is found to be $\gamma_S^* = 0.4858\ R^{-3}$ from (5.27) which is about 2.5 times lower than the first term small R solution of the present theory which is $\gamma^* = 1.3029\ R^{-3}$. In the case of $\nu^* = 0.74$ and $\nu = 0.5$, $\gamma_S^* = 0.2985\ R^{-3}$ which is about 4 times lower than γ^*.

5.1.3 Jenkins and Savage (1982)

Jenkins and Savage (1982) have dealt with the problem of general deformation of smooth, nearly elastic spherical granular materials. Following an approach similar to the kinetic theory of dense gases outlined in Chapman and Cowling (1970), they determinated the general collisional constitutive equations for the stresses, kinetic energy flux and rate of energy dissipation per unit volume. Essentially, their theory is applicable to general deformations but is an asymptotic analysis for small R. Their pair distribution function $f^{(2)}$ and single particle distribution function $f^{(1)}$ were taken to have the same forms used in the present theory as given by equation (3.2) and (3.3) with similar assumptions made. A general collisional pair distribution function $g(\underline{r}_1,\underline{r}_2)$ was assumed on the basis of dimensional arguments to be

$$g(\underline{r}_1,\underline{r}_2) = g_o(\nu)\ (1 - \frac{\alpha\sigma \underline{k}\underline{k}:\nabla \underline{u}}{\sqrt{\pi}T}) \tag{5.32}$$

where α is a constant. If $\alpha = 1$, $g(\underline{r}_1,\underline{r}_2)$ is essentially the first order expansion for small R of the $g(\underline{r}_1,\underline{r}_2)$ of the present theory given by equation (3.4) which is the same one used by Savage and Jeffrey (1981). By using this linearized $f^{(2)}$, the integrals for the collisional flux of fluctuation energy $\underline{Q}_c$ in (2.33), the collisional stress tensor $\underset{\sim}{P}$ in (2.28) and the rate of energy dissipation per unit volume in (2.34) may be evaluated to yield

$$\underline{Q}_c = -\kappa\nabla T \tag{5.33}$$

$$\underset{\sim}{P}_c = (\kappa\sigma^{-1}(\pi T)^{\frac{1}{2}} - \frac{\kappa}{5}\ (2+\alpha)\ \mathrm{tr}\underset{\sim}{D})\underset{\sim}{I} - \frac{2\kappa}{5}\ (2+\alpha)\underset{\sim}{D} \tag{5.34}$$

$$\gamma = 6(1-e)\kappa(T+(\pi/4-\alpha/3)\sigma(T/\pi)^{\frac{1}{2}}\ \mathrm{tr}\underset{\sim}{D})/\sigma^2 \tag{5.35}$$

where $\kappa = 2\nu g_o(\nu)(1+e)\rho\sigma(T/\pi)^{\frac{1}{2}}$ (5.36)

$$\underset{\sim}{D} = (u_{i,j}+u_{j,i})/2 \tag{5.37}$$

and $\underset{\sim}{I}$ is the unit tensor.

Consider the case of simple shear $\underline{u} = u(z)\ \underline{e}_y$ with no fluctuation gradients, i.e., $\underline{Q}_c = 0$, and taking the collisional stresses to be the dominant contributions, the constitutive equations with $\alpha = 1$ become

$$P^*_{xx} = P^*_{yy} = P^*_{zz} = \frac{4}{3R^2} \tag{5.38}$$

$$P^*_{yz} = P^*_{zy} = -\frac{12}{5\sqrt{3\pi}\ R} \tag{5.39}$$

$$\gamma^* = \frac{4}{\sqrt{3\pi}\ R^3} \tag{5.40}$$

which are exactly the first term solutions of the present theory. The parameter R and the coefficient of restitution e relation may be found readily to be

$$R^2 = \frac{10}{3}\,(1-e) \tag{5.41}$$

This equation of R is plotted along with the others in Fig. 10 It shows the same functional behaviour as that of Shen (1982) with the upper bound of R = 1.8257 being the lowest. The stresses given by (5.38) and (5.39) are plotted non-dimensionally against both R and e in Figs. 12 to 15. In the graphs of stresses vs. R, obvious deviations in magnitudes between the stresses of Jenkins and Savage and those of the present theory can be noted in the figures. In the plot of stresses vs. e, the magnitudes of the shear stress of Jenkins and Savage and that of the present theory are too close to be distinguished on the graph, while the difference in the normal stress is more noticeable.

All four of the microstructural theories, including the present theory, basically show the same form and trend of behaviour in the constitutive equations at least for the case of identical, smooth, inelastic granular materials. Quantitatively the magnitudes of the macroscopic properties modelled by analogs to the kinetic theory of dense gases are considerably higher than those considered from the kinematic particle collision models. In order to verify all these theories, we shall make use of the appropriate experimental data available.

5.2 Comparison Between Theories and Experiments

Savage and Sayed (1980) have performed a number of tests of dry granular materials under high shear rate in their annular shear cell in which the interstitial fluid is air. In these experiments, both shear and normal stresses were obtained when various mean concentrations of granular particles were sheared. The range of concentrations ν tested is between 0.45 and 0.53 which is considered to be high and probably most appropriate for the comparison of the present analysis. The materials used were 1.0 mm diameter polystyrene spheres of specific gravity 1.095 and 1.8 mm diameter Ballotini spherical glass beads of specific gravity 2.97. These experimental data, firstly used by Savage and Jeffrey (1981) to verify their stresses, are shown in Figs. 18 and 19 . Stresses increase rapidly upon increasing high concentration.

Unfortunately, the material properties such as the coefficient of restitution of each material are not given or known, therefore we have to choose a value for e in order to calculate the stresses in each of the four theories. For the stresses of Ogawa, et al. (1980) and Shen (1982) with the coefficient of friction taken to be zero, only computations of e = 0.9 are shown, whereas for the stresses of Jenkins and Savage (1982) and the present theory, calculations of e = 0.95, 0.9 and 0.8 are shown in Figs. 18 & 19. These values of e from 0.95 to 0.8 are probably in the range for the glass beads (see

Goldsmith 1960), however, little information about the value of e for the polystyrene beads is available except that it should be lower than that of the glass beads. Since stresses increase with increasing values of e as predicted by the present model, the stresses associated with glass beads should be higher than those with the polystyrene beads. However, the experimental data show the opposite trend. The stresses for the polystyrene beads are slightly higher. The differences between the theoretical prediction and the experimental evidence are probably due to the incompleteness of the present theory in the sense that surface friction of the granular materials is ignored. Glass beads are brittle materials, so when they are sheared under high shear rate and loads, the beads are roughened and surface friction would no doubt become an important energy dissipative mechanism. According to the theories of Ogawa, et al. (1980) and Shen (1982), stresses decrease with increasing values of coefficient of friction. Thus, it is possible for the stresses associated with the glass beads to be lower than those of the polystyrene beads since the coefficient of friction of the glass beads is probably higher in this case.

At $e = 0.9$, the shear stress of the present theory and that of Jenkins and Savage (1982) pass right through the experimental results, but the normal stress predicted is a bit high in magnitude. This shows not only that these two theories predict the right order of magnitude of stresses but also that the small R linearization is quite sufficient especially for high values of e. At the same value of $e = 0.9$, the normal stress of Shen (1982) is very close to the experimental data especially when $\nu^* = 0.64$, but the shear stress is off considerably; for example, when $\nu = 0.5$ and $\nu^* = 0.64$ Shen's shear stress is about 4 times lower in magnitude and 6 times lower if $\nu^* = 0.74$. Both shear and normal stresses predicted by Ogawa, et al.(1980) have the lowest magnitudes and fall short by a large amount; for example, when $\nu = 0.5$ and $\nu^* = 0.64$, their shear stress is about 12 times too low while their normal stress is about 4 times lower than the data. If $\nu^* = 0.74$, their shear stress is about 16 times too low while their normal stress is about 5 times lower than the tests.

As complementary information, we may plot the shear to normal stress ratio against solid concentration ν as in Figure 20. The stress ratio for the present theory may be found readily by dividing equation (4.43) by (4.44) giving

$$\left|\frac{P_{yz}}{P_{zz}}\right| = \left|\frac{P^*_{yz}}{P^*_{zz}}\right| \tag{5.42}$$

Similarly by taking the quotient of equations (5.38) and (5.39) the stress ratio for Jenkins and Savage (1982) is

$$\left|\frac{P_{yz}}{P_{zz}}\right| = \frac{3\sqrt{2}}{\sqrt{5\pi}}(1-e)^{\frac{1}{2}} \tag{5.43}$$

and from equations (5.7), (5.8) and (5.14) the stress ratio for Ogawa, et al. (1980) is

$$\left|\frac{P_{yz}}{P_{zz}}\right| = \frac{(1+e)^2}{e(3+e)} \left(\frac{3(1-e)}{8(1+e)}\right)^{\frac{1}{2}} \tag{5.44}$$

Also from equations (5.25) and (5.26) the stress ratio for Shen (1982) is

$$\left|\frac{P_{yz}}{P_{zz}}\right| = \frac{0.1151\ \pi^2}{2\sqrt{2}} \left(\frac{\nu^*}{\nu}\right)^{1/6} (1-e)^{\frac{1}{2}} \tag{5.45}$$

As shown in the figure, all the above theoretical predictions fall below the experimental values. Comparatively the present theory and the one of Jenkins and Savage represent predictions closest to the test results. The shear to normal stress ratio of Ogawa, et al. (1980) and Shen (1982) are both about 4 times too low when e = 0.9. One obvious characteristic shown in Fig. 20 is that the stress ratio of each of the theories, except Shen's, does not depend upon concentration. From the experimental results, the stress ratio of the glass beads indicates a slight dependence on concentration, while the stress ratio of the polystyrene beads indicates a stronger dependence.

So far, the present theory has fair agreement with the experiments on granular materials. Apparently, this theory is not limited in the consideration of granular particles only. Since the theory follows the same line of approach as the kinetic theory of dense gases, we may draw a comparison between the two readily.

5.3 Comparison Between the Present Theory and the Kinetic Theory of Dense Gases

The hard sphere molecular model for dense gases used by Enskog as presented in Chapman and Cowling (1970) is the most appropriate theory for comparison. We require only the part of stresses that arise from the collisional transfer of momentum in correspondance to the present analysis, which are given as

$$\underset{\sim}{P} = \left(\frac{4}{5} \langle v^2\rangle - \frac{5.09}{6} \sqrt{\frac{\pi}{3}} \langle v^2\rangle^{\frac{1}{2}} \sigma \nabla \cdot \underline{u}\right) \rho_b \nu \chi_o(\nu) \underset{\sim}{I}$$

$$- \frac{1.016}{\sqrt{3\pi}} \left(\nu + \frac{38.06}{5} \nu^2 \chi_o(\nu)\right) \frac{m\langle v^2\rangle^{\frac{1}{2}}}{\sigma^2} \left(\underset{\sim}{D} - \frac{1}{3} \nabla \cdot \underline{u}\underset{\sim}{I}\right) \qquad (5.46)$$

and $\chi_o(\nu) = 1 + \frac{5}{2} \nu + 4.5904 \ \nu^2$ (5.47)

where the factor $\chi_o(\nu)$ is analogous to the radial distribution function at contact in uniform gas.

In the case of simple shear, $\nabla \cdot \underline{u} = 0$, the normal and shear stresses become

$$P_{xx} = P_{yy} = P_{zz} = \frac{4}{5} \rho_b \nu \chi_o(\nu) \langle v^2\rangle \qquad (5.48)$$

$$P_{yz} = P_{zy} = - \frac{1.016}{2\sqrt{3\pi}} \left(\nu + \frac{38.06}{5} \nu^2 \chi_o(\nu)\right) \frac{m\langle v^2\rangle^{\frac{1}{2}}}{\sigma^2} \frac{\partial u}{\partial z} \qquad (5.49)$$

We may again non-dimensionalize these stresses in terms of the parameter R to be

$$\frac{P_{zz}}{\rho_p (\sigma \frac{\partial u}{\partial z})^2} = \frac{4\nu^2 \chi_o(\nu)}{5R^2} \qquad (5.50)$$

and

$$\frac{P_{yz}}{\rho_p (\sigma \frac{\partial u}{\partial z})^2} = - \frac{1.016}{12} \sqrt{\frac{\pi}{3}} \left(\nu + \frac{38.06}{5} \nu^2 \chi_o(\nu)\right) \frac{1}{R} \qquad (5.51)$$

Consider the stresses of the present theory, the first term small R solutions are sufficient since we are dealing with elastic hard spheres, i.e. e = 1. Note that when e = 1, there will be no energy dissipation in the system, hence the parameter R remains indeterminate but not zero. From equations (4.25) and (4.26), the normal and shear stresses are

$$\frac{P_{zz}}{\rho_p(\sigma\frac{\partial u}{\partial z})^2} = \frac{4\nu^2 g_o(\nu)}{3R^2} \tag{5.52}$$

$$\frac{P_{yz}}{\rho_p(\sigma\frac{\partial u}{\partial z})^2} = - \frac{12\nu^2 g_o(\nu)}{5\sqrt{3\pi}\ R} \tag{5.53}$$

Comparing the expressions of stresses between the two theories, the functional difference is between $\chi_o(\nu)$ and $g_o(\nu)$ These two functions are plotted in Figure 21 which shows that they differ by a large amount at high concentration. Since $g_o(\nu)$ is derived semi-empirically from computer similations of molecular dynamics, one would presumably take $g_o(\nu)$ to be more accurate than $\chi_o(\nu)$ especially at higher concentration. For the purpose of comparison we not only use the formula of $\chi_o(\nu)$ as given by Chapman and Cowling to calculate their stresses but also we replace $\chi_o(\nu)$ by $g_o(\nu)$. These two calculations of stresses are both shown in Figures 22 and 23 together with the stresses of the present theory as in (5.52) and (5.53). By using their $\chi_o(\nu)$, both of their shear and normal stresses are low compared to those of the present theory. But when we let $\chi_o(\nu) \equiv g_o(\nu)$, their shear stress is quite close to the present one especially at high concentration of $\nu = 0.2$ onward. However, their normal stress differs from the present one by a factor of 5/3. This shows that the present theory is compatible with the formal analysis of dense gases of hard sphere model at least in the case of simple shear.

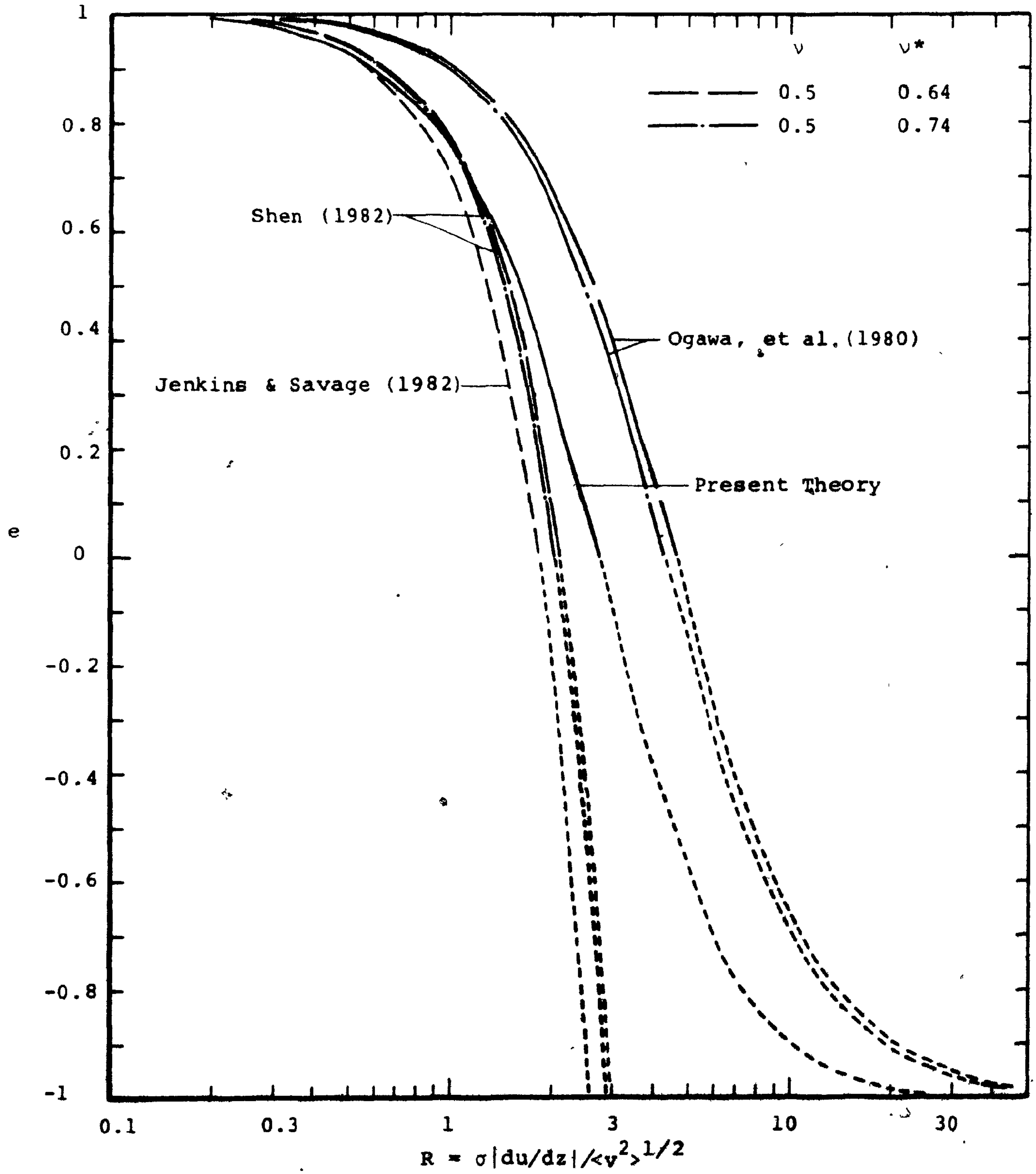


Fig. 10 Variation of characteristic mean shear to fluctuation velocity ratio R with coefficient of restitution e as predicted by various theories for the case of simple shear

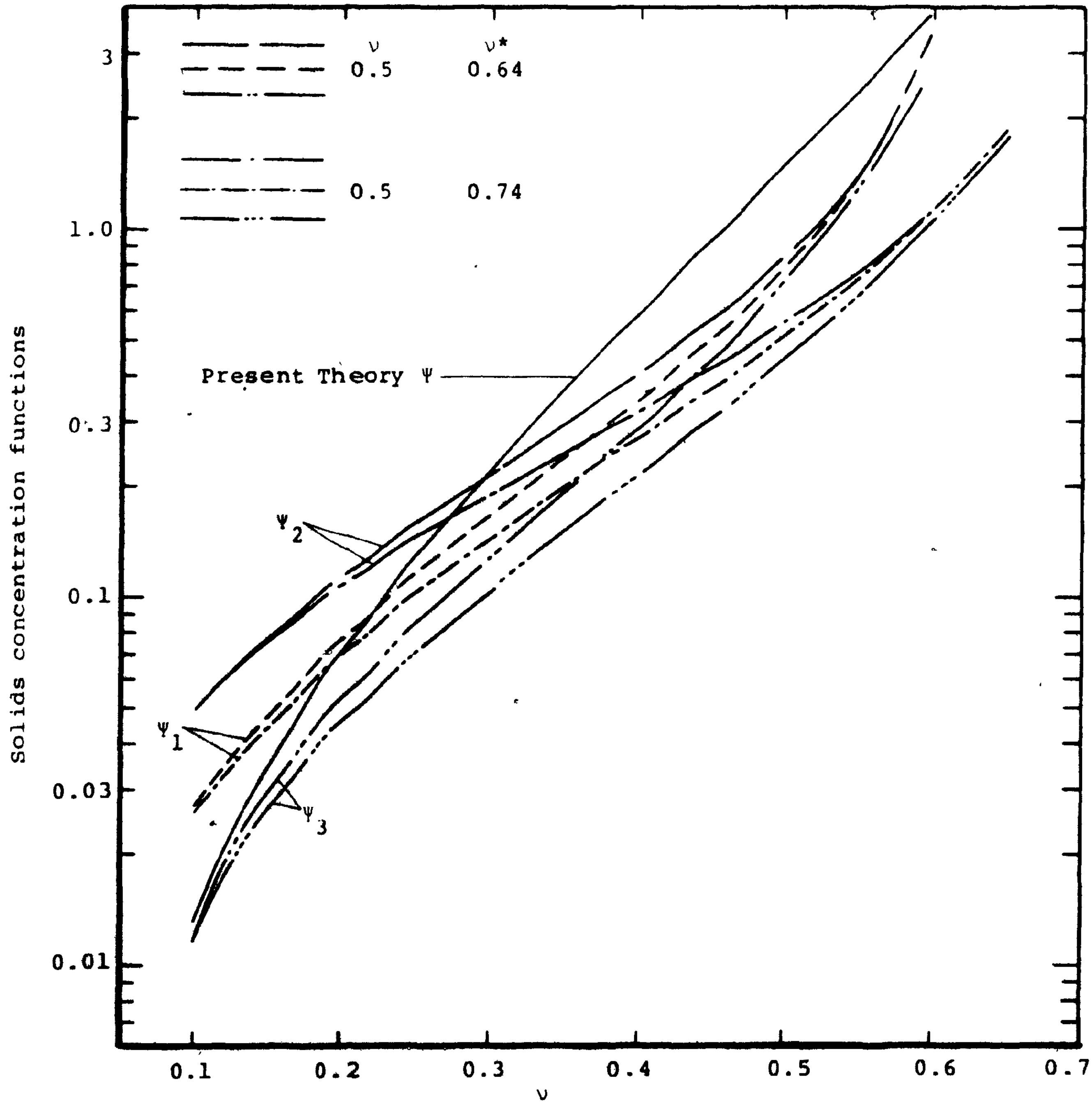


Fig. 11 Solids concentration functions of various theories in terms of solids fraction ν

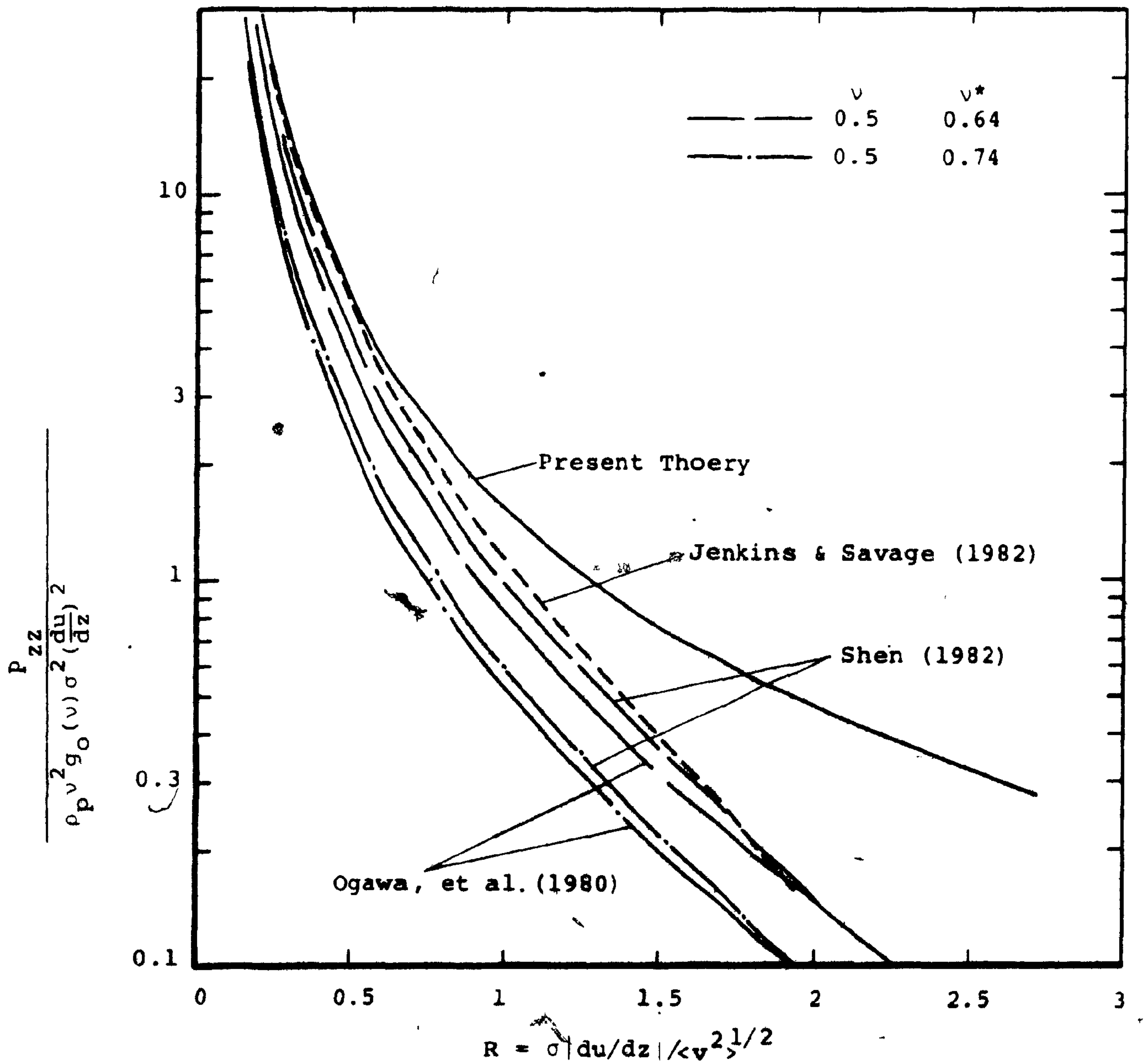


Fig. 12 Variation of non-dimensional normal stress component P^*_{zz} of various theories with the ratio of characteristic mean shear velocity to fluctuation velocity R for the case of simple shear

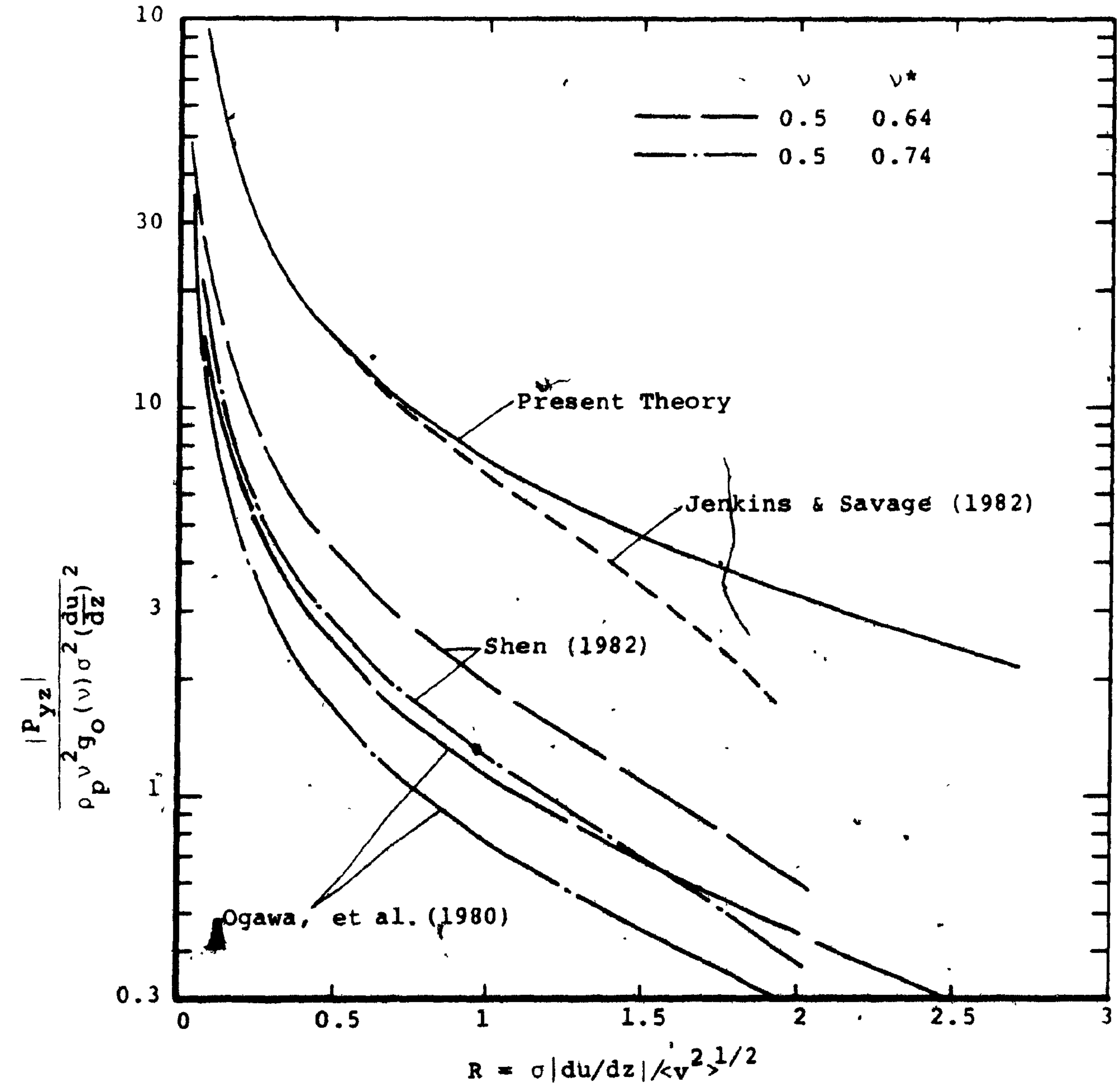


Fig. 13 Variation of non-dimensional shear stress component P^*_{yz} of various theories with the ratio of characteristic mean shear velocity to fluctuation velocity R for the case of simple shear.

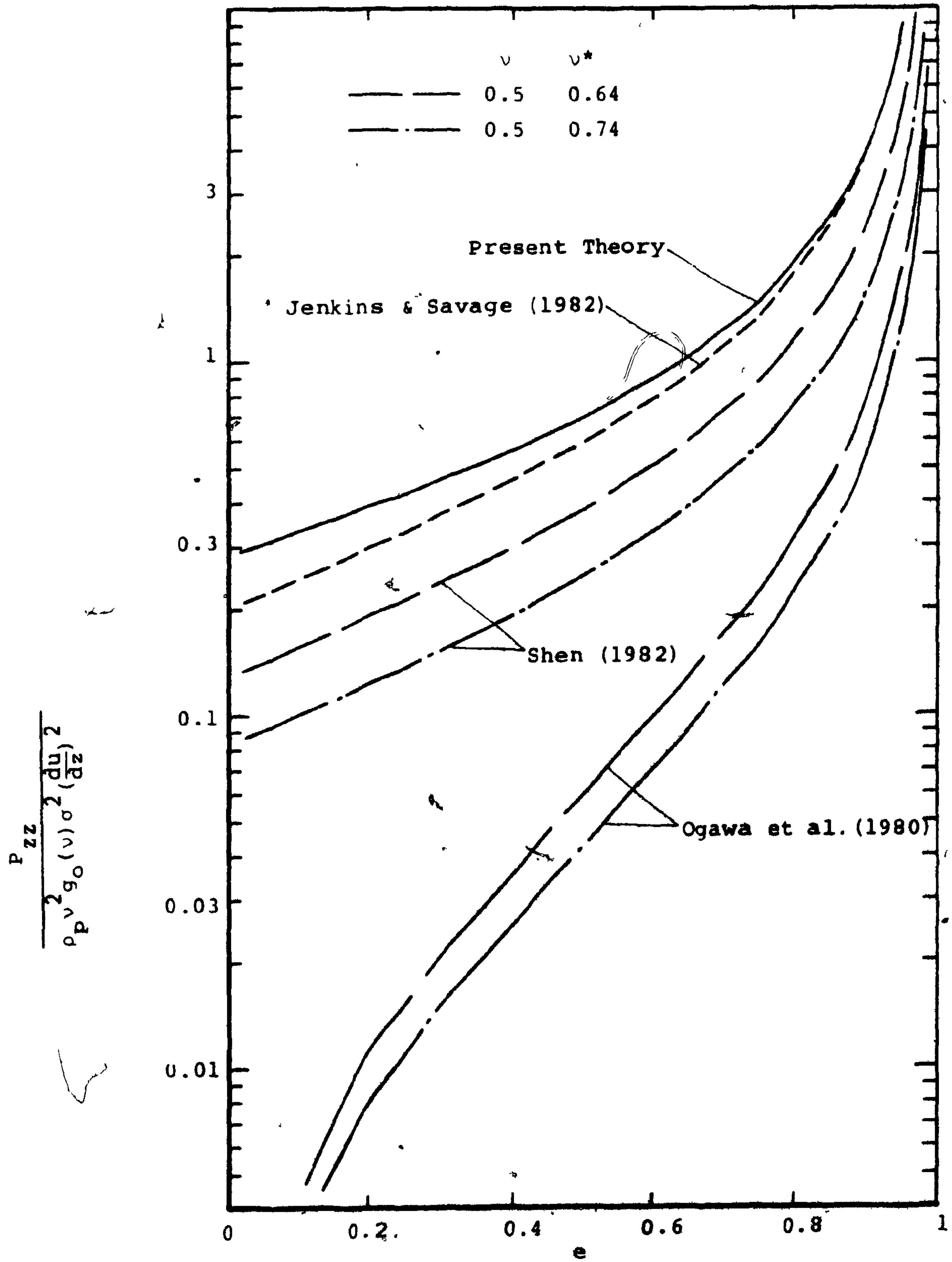


Fig. 14 Variation of non-dimensional normal stress component P^*_{zz} of various theories with the coefficient of restitution e for the case of simple shear

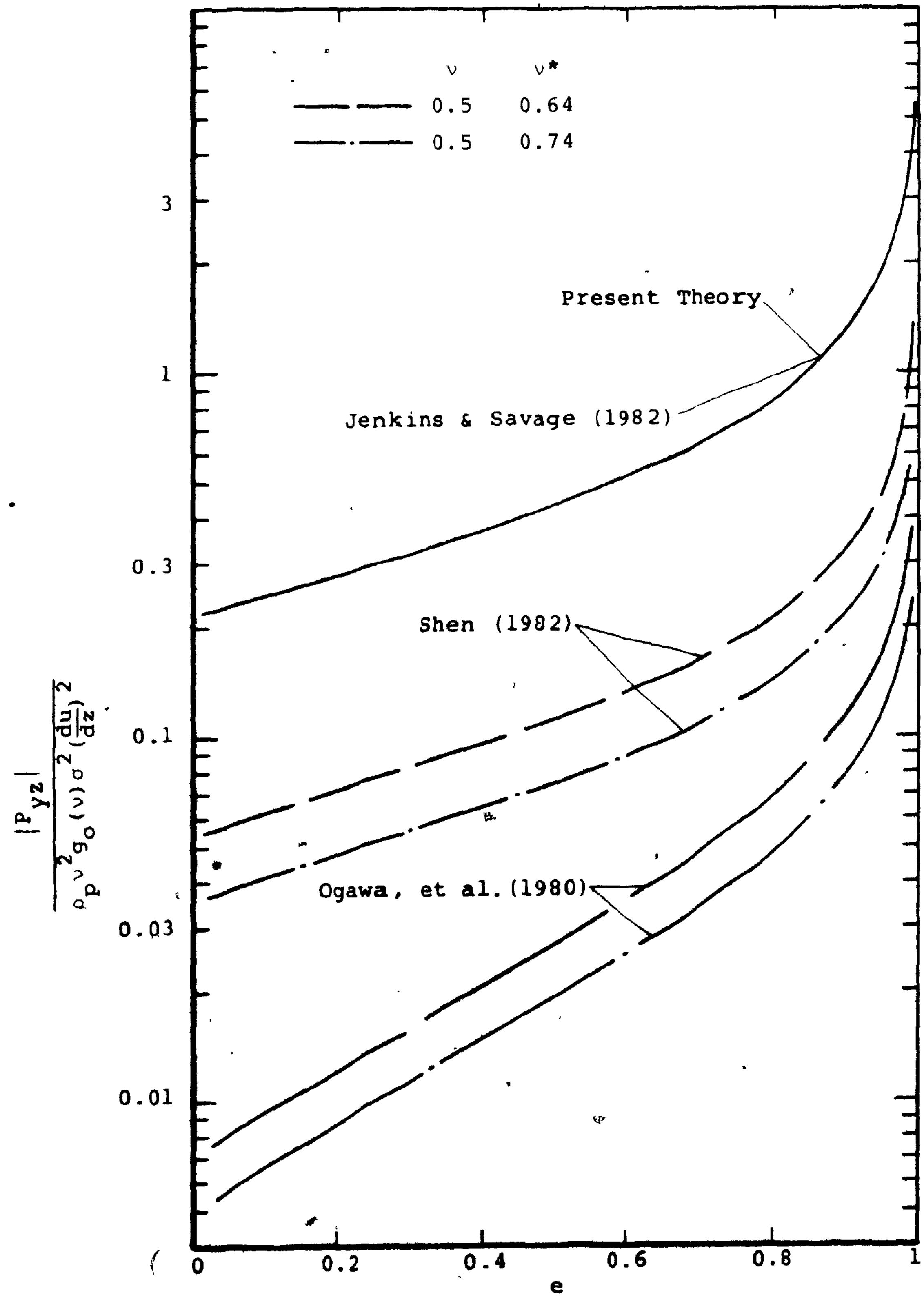
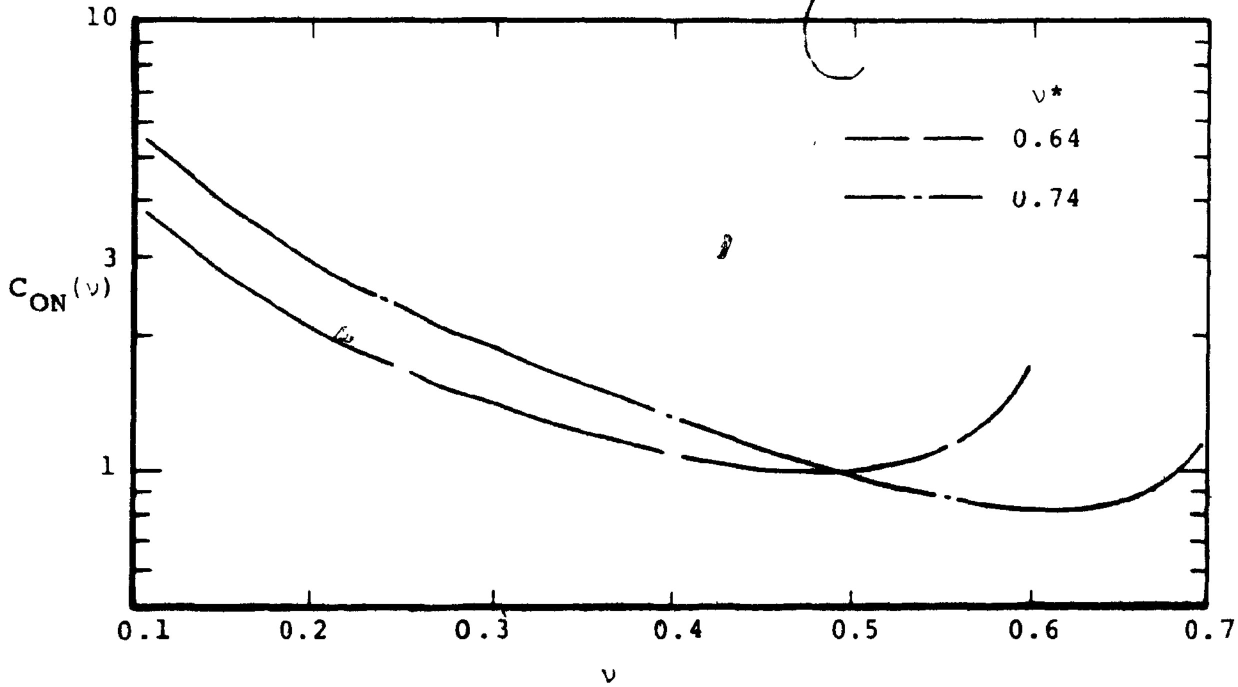
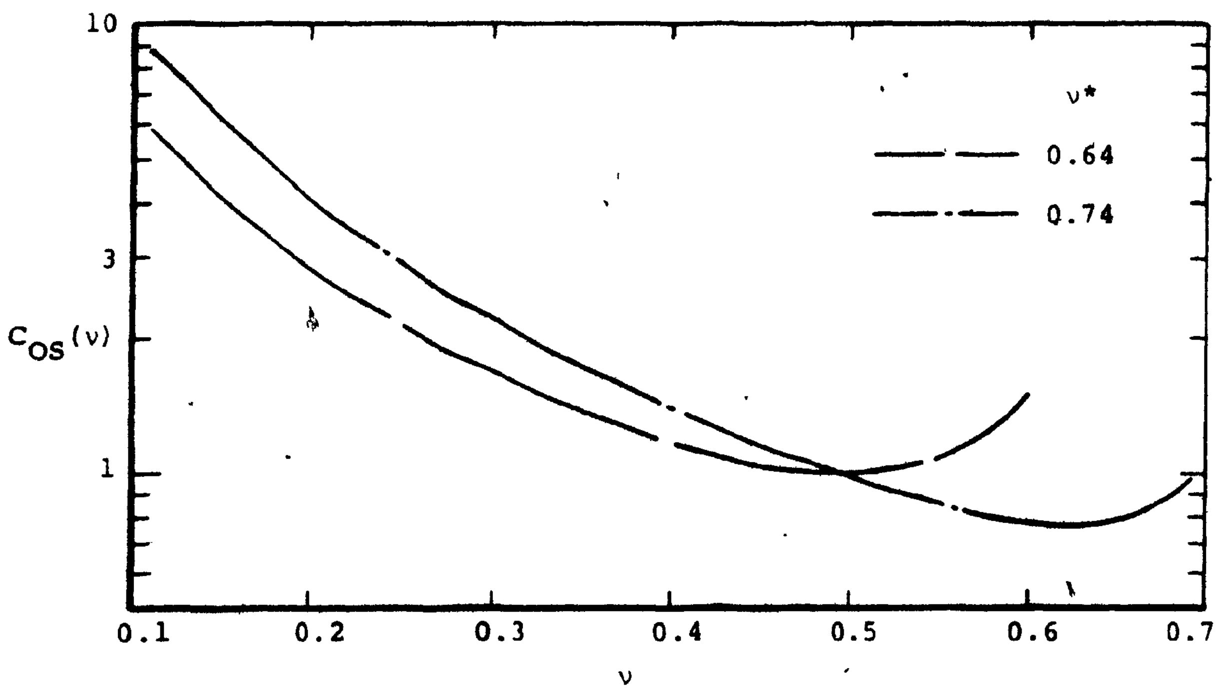


Fig. 15 Variation of non-dimensional shear stress component P^*_{yz} of various theories with the coefficient of restitution e for the case of simple shear



(a)



(b)

Fig. 16 Ratio of concentration functions for the (a) normal stress, (b) shear stress of the theory of Ogawa, et al. (1980)

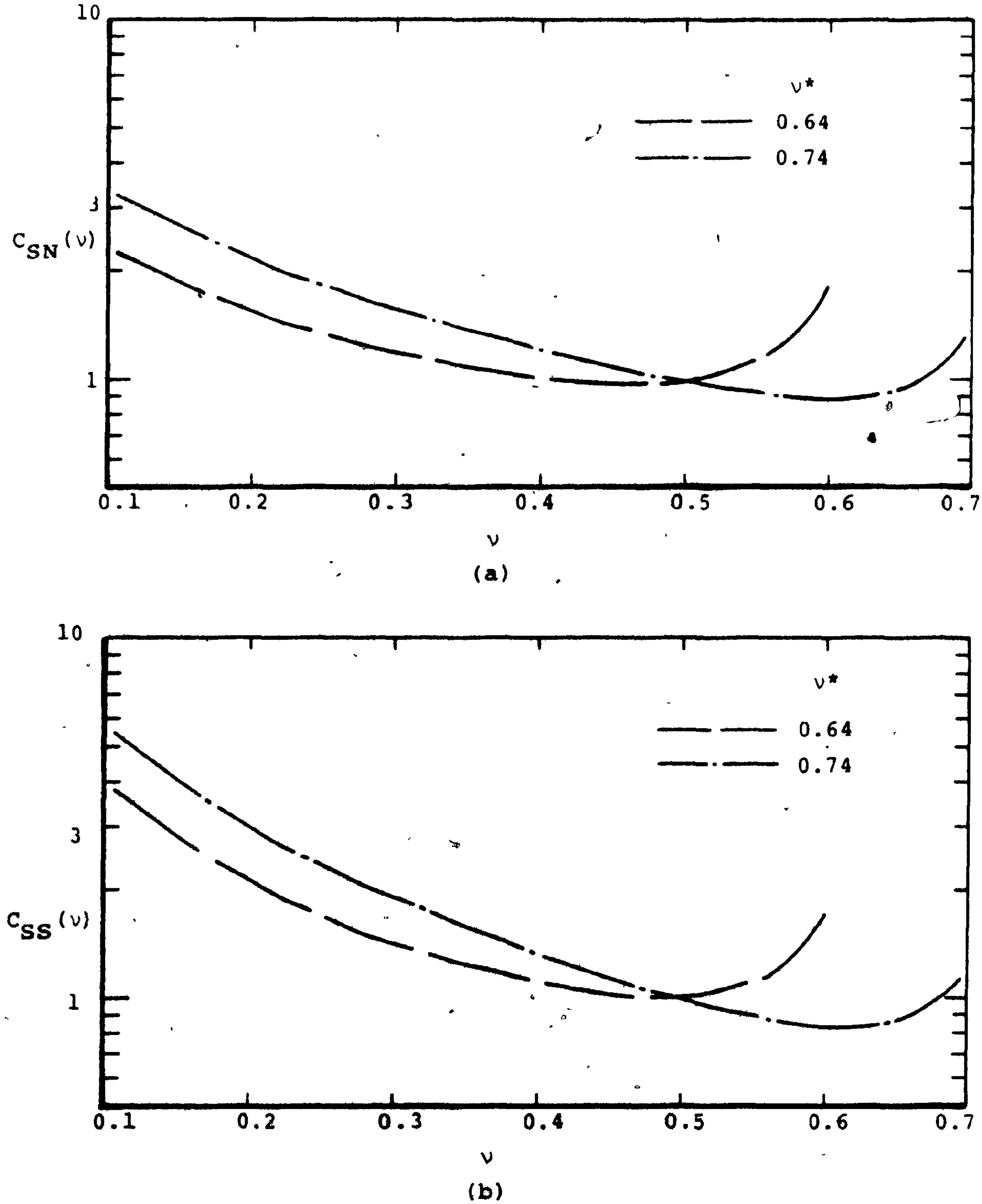


Fig. 17 Ratio of concentration functions for the (a) normal stress, (b) shear stress of the theory of Shen (1982)

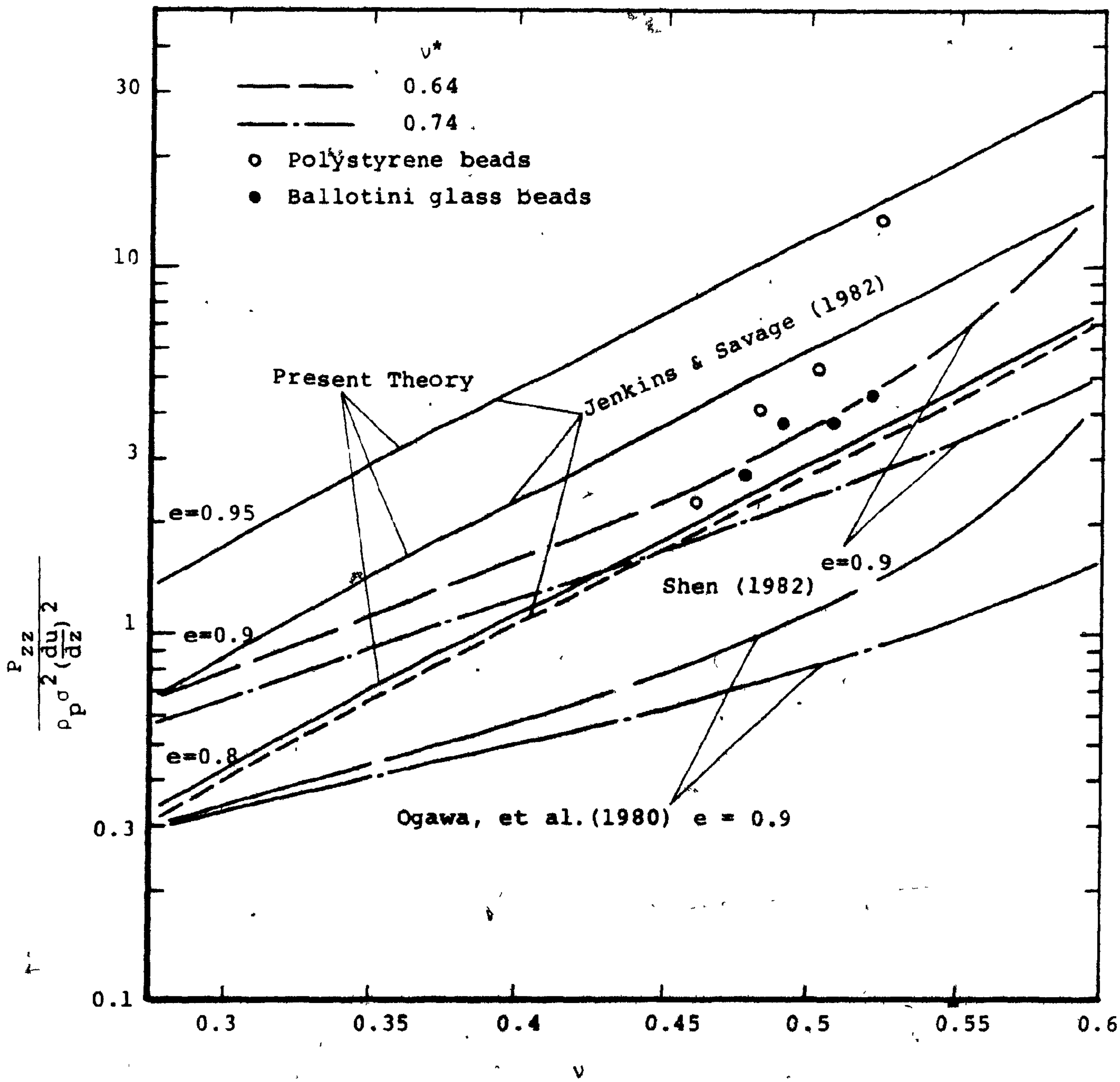


Fig. 18 Variation of non-dimensional normal stress with solids fraction ν for the case of simple shear. Comparison of various theories with experiments of Savage and Sayed (1980)

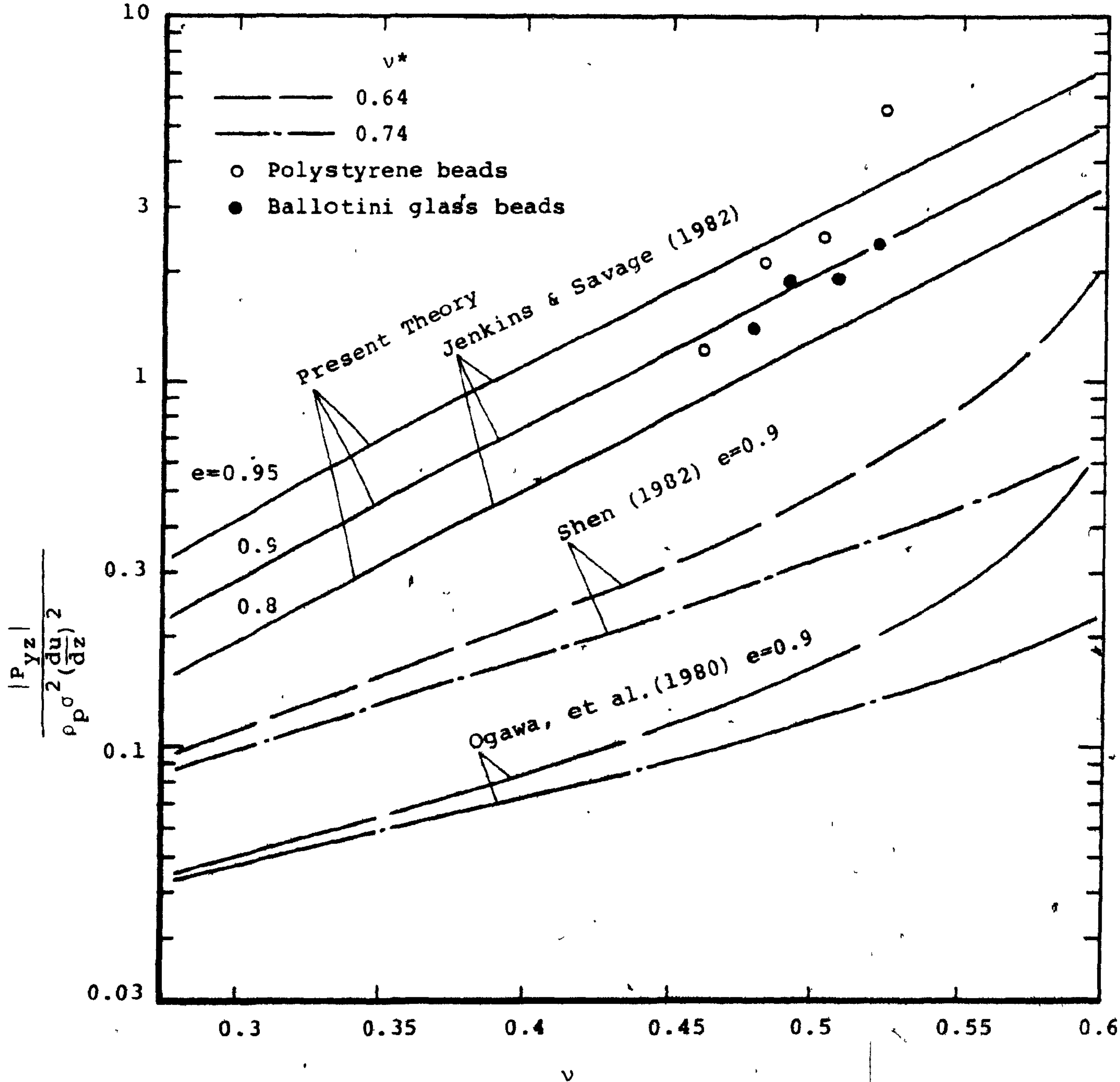


Fig. 19 Variation of non-dimensional shear stress with solids fraction ν for the case of simple shear. Comparison of various theories with experiments of Savage and Sayed (1980)

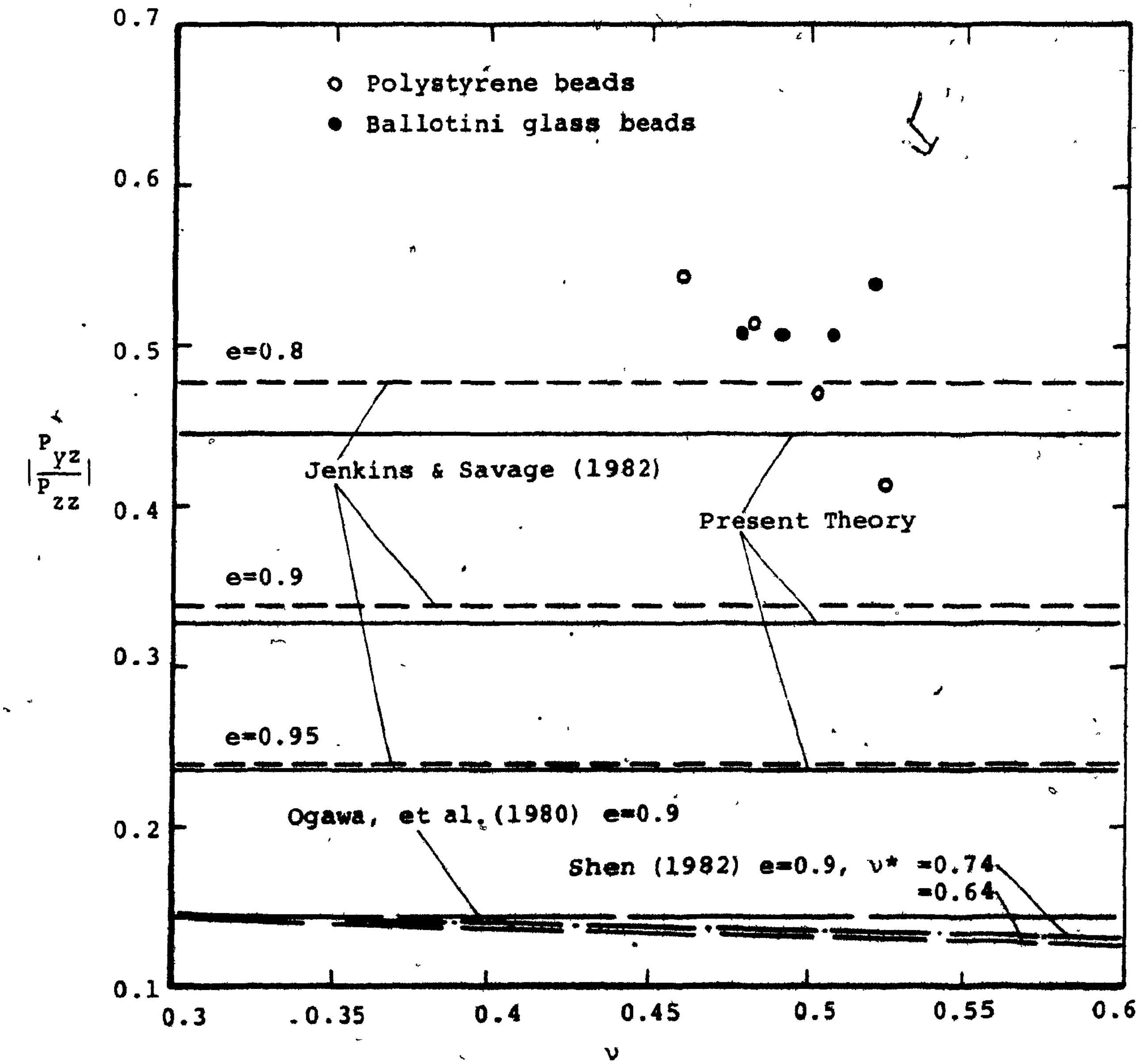


Fig. 20 Variation of the ratio of shear stress to normal stress with solids fraction ν for the case of simple shear. Comparison of various theories with experiments of Savage and Sayed (1980)

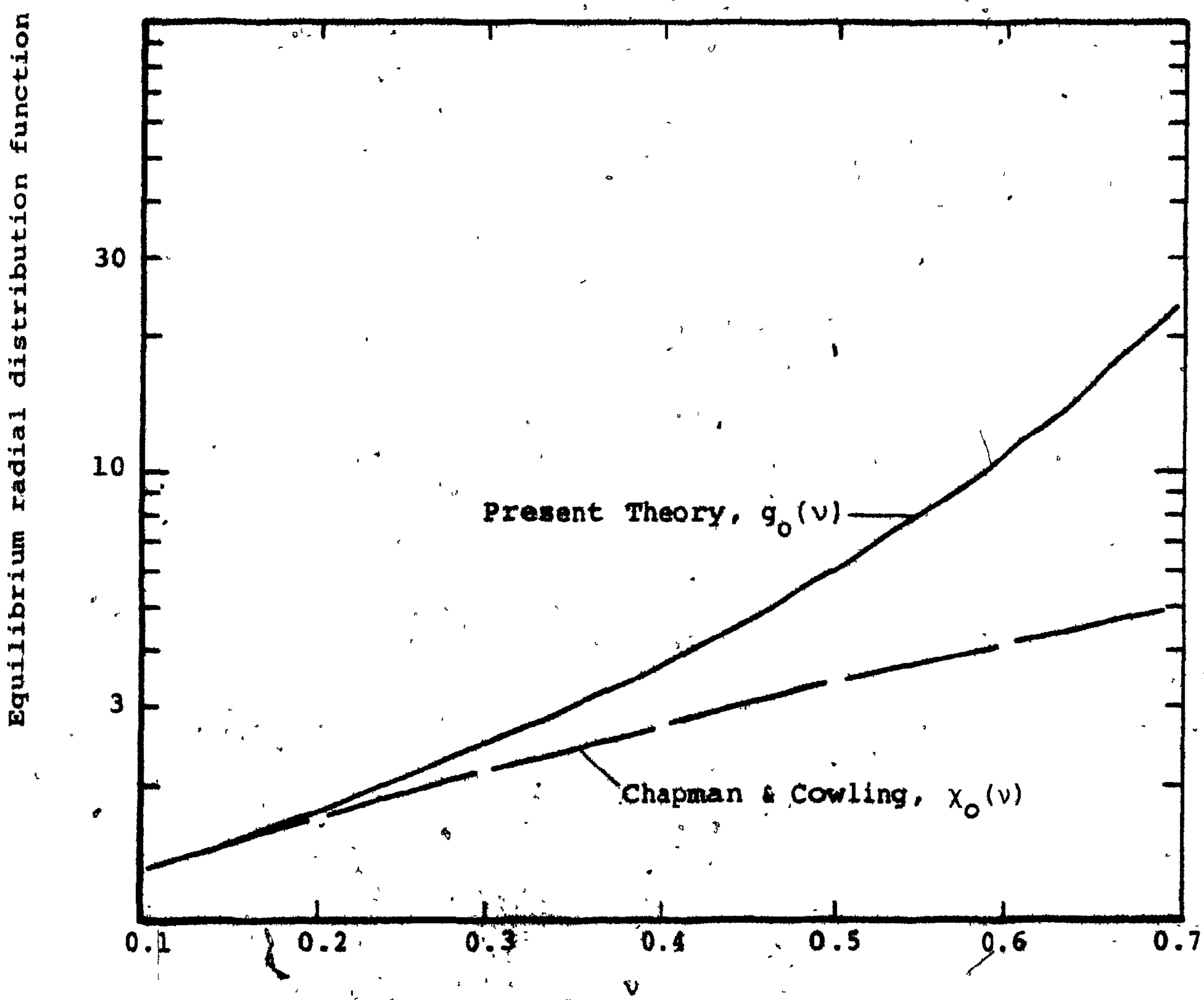


Fig. 21 Equilibrium radial distribution function $g_o(\nu)$ and $\chi_o(\nu)$

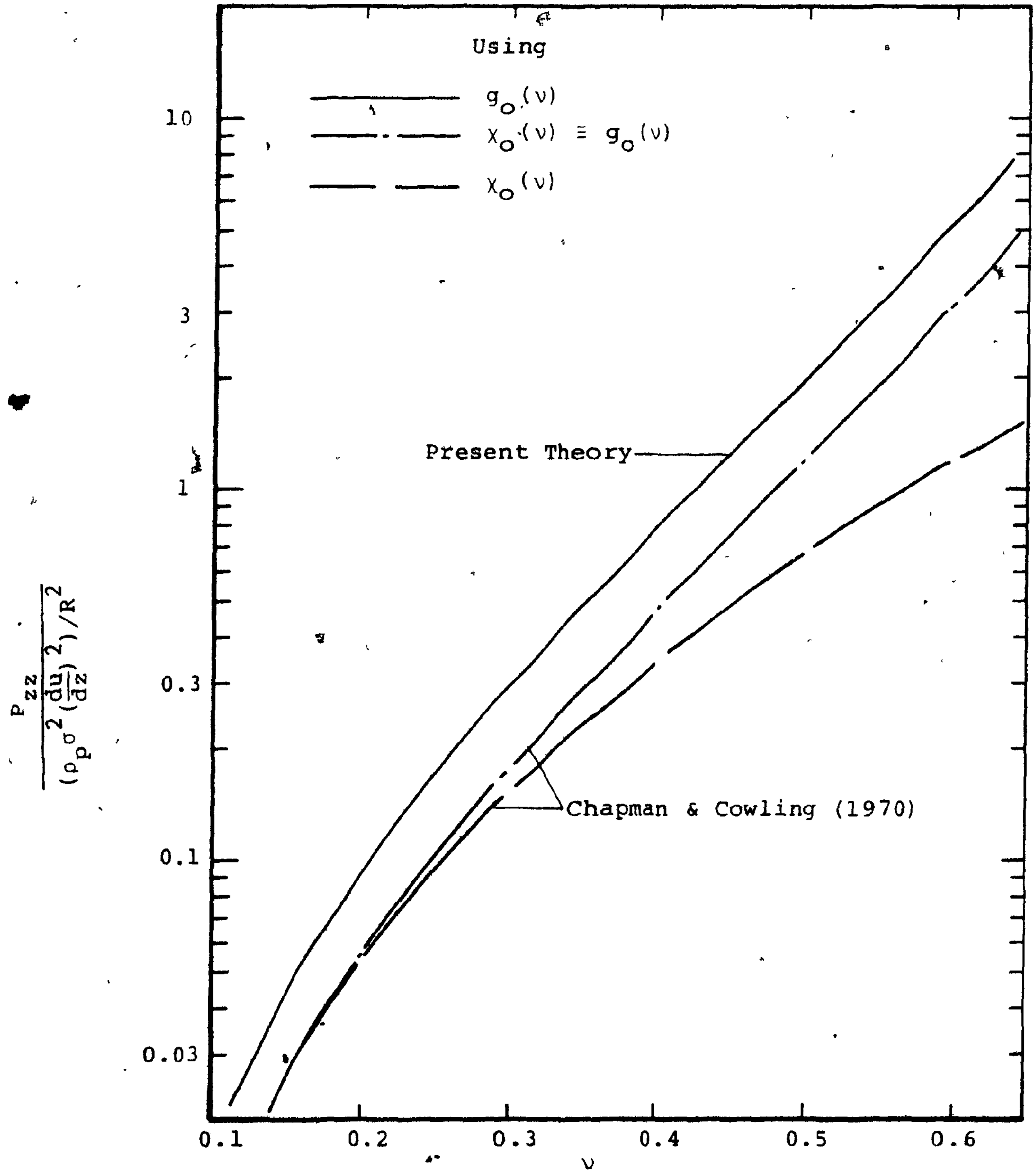


Fig. 22 Variation of non-dimensional normal stress with solids fraction ν for the case of simple shear. Comparison of present theory with the kinetic theory of dense gases of Enskog (Chapman and Cowling 1970)

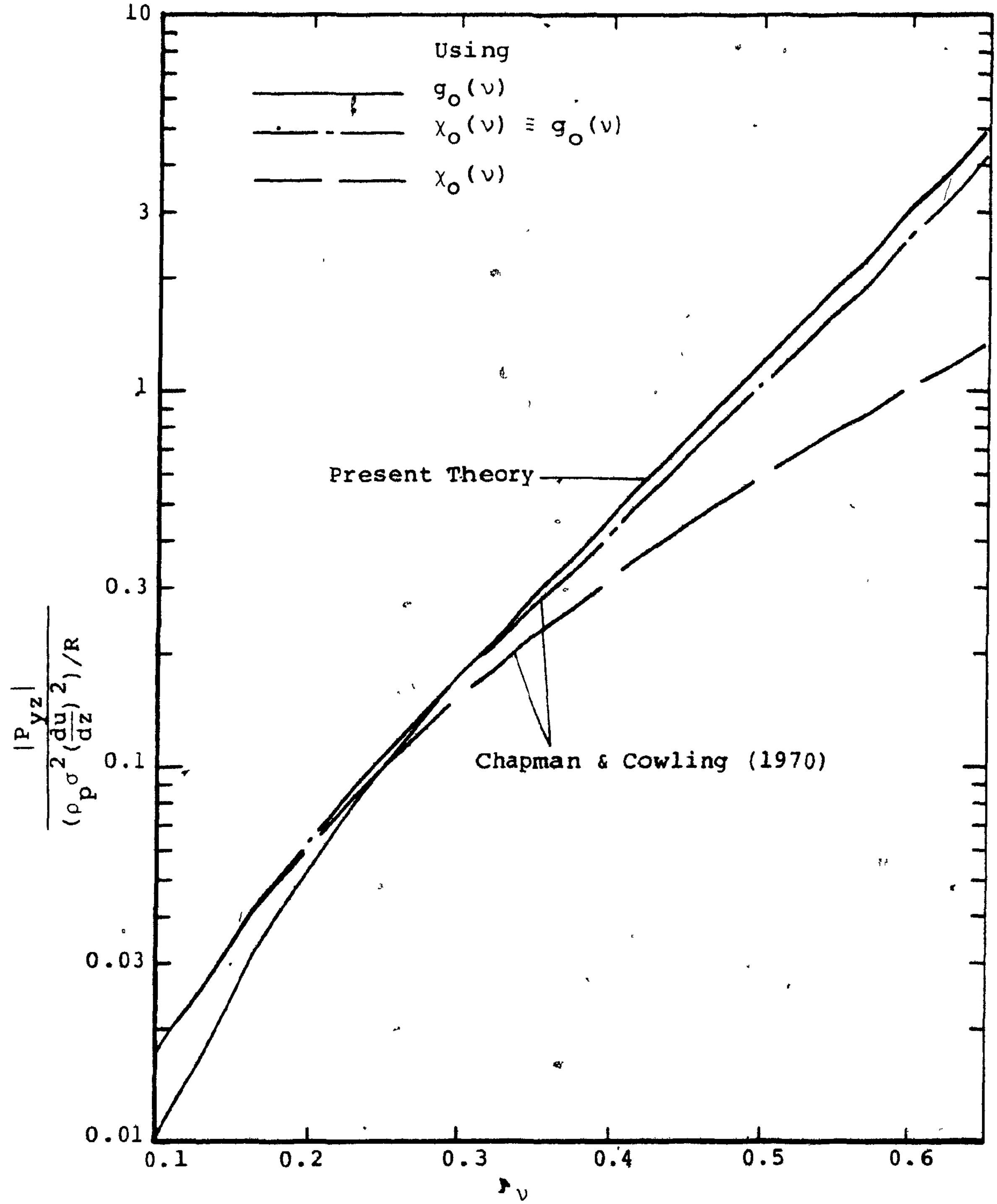


Fig. 23 Variation of non-dimensional shear stress with solids fraction ν for the case of simple shear. Comparison of present theory with the kinetic theory of dense gases of Enskog (Chapman and Cowling 1970)

CHAPTER 6 CONCLUSION

In this study, the conservation laws and constitutive integrals appropriate for the flow of identical, smooth, inelastic, spherical granular materials are formulated in the context of the transport theory of dense gases. The rapid simple shear flow of granular materials is studied in particular. With the use of the pair velocity distribution function proposed by Savage and Jeffrey (1981), the constitutive integrals for the collisional stresses and the rate of energy dissipation are approximated by asymptotic expansions and series transformations in terms of a parameter R which is defined as the ratio of mean shear characteristic velocity to the r.m.s. of the fluctuation velocity of the particles. The parameter R is found to depend upon the coefficient of restitution of the particles through the balance of energy. Thus, the stresses and the rate of energy dissipation are determined uniquely by the dissipative material property, the coefficient of restitution e of the particles.

The present study is compared with previous theoretical investigations and experiments. All the theories exhibit general agreement in the form of the constitutive relationships developed for the case of simple shear. Although the theories are based upon different statistical averaging methods and dynamic considerations the relationships between the parameter R and the coefficient of restitution e are quite similar. In the comparison of stresses between experiments and theoretical predictions, the theories of Ogawa, et al. (1980) and Shen (1982) yield stresses generally lower than the measurements. The stresses predicted by the theory of Jenkins and Savage (1982) and the present analysis show the correct order of magnitude. Furthermore, the small R solutions of the stresses of the present theory, which are exactly those derived by Jenkins and Savage (1982), indicate fair agreement with the stresses predicted by the kinetic theory of dense gases using the hard sphere model.

The present analysis has considered only the translational aspect of the particles in the granular flow system of simple shear. The effect of dry friction and the rotational motion of the particles are both plausible extensions that can be made in the theory. These two aspects are expected to become more important especially at high concentration. The collisional stresses are assumed to be the dominant stress contributions at high concentration, whereas the kinetic or diffusional part of the stresses can be expected to play a major role at low concentration. Numerous refinements can be made in the theory. The full potential of the approach of kinetic theory of dense gases for the investigation of the flow of granular materials has yet to be explored.

APPENDIX A

Collisional Change of Dynamical Quantity

In Chapter 2, we have formulated the collisional change ψ_{col} of the mean value of dynamical quanitity ϕ of the particle in a binary collision. In this appendix, we will discuss in some length the physical arguments involved in the decomposition of ψ_{col} into a flux term $\theta(\phi)$ and a sink term $\chi(\phi)$ as presented in equations (2.20) to (2.21). It will be shown that although the formulation and final expressions for ψ_{col} in the present analysis are slightly different from those of Jenkins and Savage (1982) and Condiff, Lu and Dahler (1965), the results from all these analysis are essentially equivalent.

Consider the collisional change of ϕ at position $\underline{r}$ in a volume element $d\underline{r}$ as shown in Fig. 2. The change of the dynamical quantity of particle 1 at $\underline{r}$ is $\phi_1' - \phi_1$, where primed quantity denotes value after the collision. Thus, equation (2.17) as previously presented in Chapter 2 is

$$\psi_{col} = d\underline{r}\; dt\; \sigma^2 \int_{\underline{k}\cdot\underline{q}>0} (\underline{k}\cdot\underline{q})\; f^{(2)}(\underline{r},\underline{c}_1,\underline{r}+\sigma\underline{k},\underline{c}_2,t)\,d\underline{k}\,d\underline{c}_1\,d\underline{c}_2\,(\phi_1'-\phi_1) \quad (A.1)$$

Since particle 1 and 2 are identical, we may interchange their roles or correspondingly their subscript 1 and 2 and note that $\underline{q}\to-\underline{q}$ and $\underline{k}\to-\underline{k}$. Expression (A.1) may be written as

$$\psi_{col} = d\underline{r}\,dt\,\sigma^2 \int_{\underline{k}\cdot\underline{q}>0} (\underline{k}\cdot\underline{q})\; f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\,d\underline{k}\,d\underline{c}_1\,d\underline{c}_2\,(\phi_2'-\phi_2) \quad (A.2)$$

The pair velocity distribution function $f^{(2)}(\underline{X})$ in equation (A.1) is evaluated at the point $\underline{X} = (\underline{r},\underline{c}_1,\underline{r}+\sigma\underline{k},\underline{c}_2,t)$

in a phase space of 12 dimensions. Similarly, the pair velocity distribution function in equation (A.2) $f^{(2)}(\underline{Y})$ is evaluated at the point $\underline{Y} = (\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)$ in the phase space. We assume that $f^{(2)}$ and its partial derivatives up to the order n are continuous in the neighbourhood R of $\underline{Y}$. Since $\underline{X}$ differs only spatially from $\underline{Y}$ by an amount $\sigma\underline{k}$, $\underline{X}$ is assumed to be well within the region R. Thus we may relate $f^{(2)}(\underline{X})$ in (A.1) and $f^{(2)}(\underline{Y})$ in (A.2) in the following way. Firstly, we re-write $f^{(2)}(\underline{X})$ to be $f^{(2)}(\underline{r}_i,\underline{c}_i,t)$ where i = 1,2. Similarly, $f^{(2)}(\underline{Y})$ may be written as $f^{(2)}(\underline{r}_i-\sigma\underline{k},\underline{c}_i,t)$. Using a Taylor expansion (Fulks 1961) we may express $f^{(2)}(\underline{r}_i,\underline{c}_i,t)$ in terms of $f^{(2)}(\underline{r}_i-\sigma\underline{k},\underline{c}_i,t)$ spatially as

$$f^{(2)}(\underline{r}_i,\underline{c}_i,t)=[1+\sigma\underline{k}\cdot\nabla+\tfrac{1}{2}(\sigma\underline{k}\cdot\nabla)^2+\ldots+\frac{1}{n!}(\sigma\underline{k}\cdot\nabla)^n+\ldots]f^{(2)}(\underline{r}_i-\sigma\underline{k},\underline{c}_i,t) \tag{A.3}$$

By so doing, we may evaluate the change of the dynamical quantity due to collision of particles 1 and 2 at the same phase point. In the present case, $f^{(2)}$ is evaluated at point $\underline{Y}$ in the phase space so that all the macroscopic variables due to collisions may be weighted by the same kernel or weighting function. Taking half the sum of (A.1) and (A.2) and using (A.3) the collisional change may be expressed in the form of

$$\psi_{col} = [-\nabla\cdot\theta(\phi) + \chi(\phi)]\, d\underline{r}dt \tag{A.4}$$

where

$$\theta(\phi) = -\frac{\sigma^3}{2}\int_{\underline{k}\cdot\underline{g}>0}(\phi_1'-\phi_1)(\underline{k}\cdot\underline{g})\underline{k}[1+\frac{1}{2!}\sigma\underline{k}\cdot\nabla+\frac{1}{3!}(\sigma\underline{k}\cdot\nabla)^2+\ldots]$$
$$f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\,d\underline{k}d\underline{c}_1d\underline{c}_2 \tag{A.5}$$

and $$\chi(\phi) = \frac{\sigma^2}{2} \int_{\underline{k}\cdot\underline{g}>0} (\phi_1'+\phi_2'-\phi_1-\phi_2)(\underline{k}\cdot\underline{g}) f^{(2)}(\underline{r}-\sigma\underline{k},\underline{c}_1,\underline{r},\underline{c}_2,t)\, d\underline{k}d\underline{c}_1 d\underline{c}_2 \tag{A.6}$$

The collisional transfer contribution $\theta(\phi)$ may be interpreted as the flux of change of dynamical quantity of the particle at $\underline{r}$ in the $\underline{k}$ direction due to the collision. The contribution $\chi(\phi)$ may be considered as a term for the sink of dynamical quantity at $\underline{r}$ since it represents the total change of ϕ of the particles in the binary collision. For example, if the dynamical quantity is the translational energy of the particle, i.e. $\phi = \frac{1}{2} mc^2$, then $\theta(\frac{1}{2}mc^2)$ will represent the flux of kinetic energy and $\chi(\frac{1}{2}mc^2)$ will represent the loss of kinetic energy due to the inelastic collision of particles.

A.1 Jenkins and Savage (1982)

Jenkins and Savage (1982) have formulated the collisional change of the mean value of dynamical quantity by using a slightly different approach of physical argument. A particle velocity $\underline{c}_1$ at $\underline{r}$ is considered to collide with a particle having velocity $\underline{c}_2$ at $\underline{r}+\sigma\underline{k}$ inside a volume element $d\underline{r}$ as shown in Fig. 2. By using the same kind of collisional consideration as in the present theory, the collisional change of the mean value of dynamical quantity at $\underline{r}$ is found to be given by equation (A.1). An identical collision is considered to occur between a particle with velocity $\underline{c}_1$ at $\underline{r}-\sigma\underline{k}$ and a particle with velocity $\underline{c}_2$ at $\underline{r}$. In this case ψ_{col} is given by (A.2)

Using the kind of Taylor expansion of $f^{(2)}$ as presented earlier, the collisional change of the mean value of dynamical quantity ψ_{col}, the flux term $\theta(\phi)$ and the sink term $\chi(\phi)$ are given by equations (A.4), (A.5) and (A.6) respectively. The formulation of Jenkins and Savage is equivalent to the present analysis, except that they consider two spatially different identical binary collisions while the present one considers the interchange of identical particles in the same collision.

A.2 Condiff, Lu and Dahler (1965)

Condiff, Lu and Dahler (1965) have dealt with the same subject from a somewhat different point of view. They consider a dilute gas of perfectly rough, elastic spheres. In their formulation, translational and rotational dynamical quantities of the molecules are exchanged due to particle interactions. Using an argument similar to that of the present theory, the collisional change of the mean value of dynamical quantity ψ_{col} is found to be given by equation (A.1) and (A.2). The obvious difference between the two theories is that a pair translational and rotational velocity distribution function $f^{(2)}(\underline{r},\underline{\tau}_1,\underline{r}+\sigma\underline{k},\underline{\tau}_2,t)$, where $\tau_1 = (\underline{c}_i,\underline{\omega}_i)$ and $\underline{\omega}_i$ is the rotational velocity, is required for their case. The decomposition of ψ_{col} into $\theta(\phi)$ and $\chi(\phi)$ as in equation (A.4) is used. However, their collisional transfer contribution terms $\theta(\phi)$ and $\chi(\phi)$ are presented in a different way from the present ones. In their theory, the integral of $\theta(\phi)$ is weighted by

$f^{(2)}(\underline{r},\underline{I}_1,\underline{r}+\sigma\underline{k},\underline{I}_2,t)$ while the integral of $\chi(\phi)$ is weighted by $f^{(2)}(\underline{r}-\sigma\underline{k},\underline{I}_1,\underline{r},\underline{I}_2,t)$. The reason for having $\theta(\phi)$ and $\chi(\phi)$ evaluated at different phase points is not clear and Condiff, et al. provide no explanation. The term $\theta(\phi)$ in their case represents the flux of the change of translational and rotational dynamical quantities of the particle. The term $\chi(\phi)$ represents the total exchange of translational and rotational dynamical quantities in a binary collision.

Analogous to the present analysis, we may ignore the rotational aspect of their formulation and take $\theta(\phi)$ to be the flux of only translational dynamical quantity of the particle and $\chi(\phi)$ to be the total change of translational dynamical quantity in a binary collision of smooth, inelastic particles. If we follow similar procedures of manipulation of the present theory - to rearrange the Taylor expansion of $f^{(2)}$ in their analysis, the same integral forms as given in equations (A.5) and (A.6) will be achieved readily.

APPENDIX B

Some standard integrations involving exponentials (Chapman & Cowling 1970) are presented below.

(a) If n is an even positive integer, then

$$\int_0^\infty e^{-\alpha t^2} t^n \, dt = \frac{\sqrt{\pi}}{2} \cdot \frac{1}{2} \cdot \frac{3}{2} \cdots \frac{n-1}{2} \alpha^{-(n+1)/2} \qquad \text{(B.1)}$$

(b) If n is an odd positive integer, then

$$\int_0^\infty e^{-\alpha t^2} t^n \, dt = \frac{1}{2} \alpha^{-(n+1)/2} \left(\frac{n-1}{2}\right)! \qquad \text{(B.2)}$$

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