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Kinetic Theory of Aggregation in Granular Flow

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Abstract

This paper presents a mathematical formulation of the aggregation kinetics in granular flow. The traditional kinetic theory and its generalised application to granular flow does not allow for particle size to change with time thus cannot be used to describe particle flow with aggregation taking place. In this paper, a collision success factor, quantifying the completely inelastic collision of particles, is introduced into the evaluation of collision rate. The kinetic transport equations are then transformed to include source terms that account for the effects of particle size and aggregation. The analytical solution of the collision success factor is obtained by integrating the relative velocity distribution function over its velocity domain from 0 to a critical value which corresponds a balance between the repulsion and attraction forces in a collision. The factor has been found to depend on the mixture granular energy and the critical relative collision energy.

Key words: Aggregation, Collision success factor, Granular flow, Kinetic theory, Population balance

Introduction

Attributed to the original work of Maxwell[1, 2] and Boltzmann[3], and further interpreted by Chapman[4, 5] and Enskog[6], kinetic theory was developed to describe the transport properties and constitutive relations of gases[7]. This theory was later generalised and applied to the flow of granular materials, which consist of particulates in granular scale flowing in a system under conditions such as fluidisation or shear, to study the behaviour and properties of granular particles[8]. Since the work of Bagnold[9] studying the collisions of identical spherical particles on the effects of mean shear rate on momentum and collision frequency, the application of kinetic theory of granular flow has been extensively investigated in engineering[10-14] and fundamental physics[15-22]. Blinowski[23] and Ogawa[10]

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formulated a theoretical work using velocity fluctuation. Jenkins and Savage[16] attempted to extend the theory to less elastic but identical and spherical particles. They obtained the balance equations by using a pair distribution function. Further attempts[24, 25] were also made to describe a dense binary and nearly elastic mixture of the granular flow of spherical particles and to compare the kinetic theory predictions with the discrete element simulation using the constitutive relations for dense granular flow[26]. A review on the application of kinetic theory to gas fluidised beds with mono dispersed particles can be found in the work of Gidaspow[27]. As pointed out by Sundaresan[28], formidable challenges still remain in developing continuum models to include particle size distribution to address the balances of the transport properties in order to predict the structure such as clusters and streamers of granular particles in various flow systems[28, 29].

Despite the broad studies of kinetic theory and its constitutive relations on granular flows[22, 26, 30-42], it is still true to say that the granular particles in such flows do not occur aggregation, i.e., completely inelastic collision; however, in granular flows with particle aggregation such as in fluidised bed granulation[43, 44], it is strongly necessary to take the completely inelastic collision into account in the configuration of kinetic transport equations so as to allow the kinetic theory able to predict the change of kinetic transport properties of particles such as the number density of particles in terms of their sizes in multiple dispersed granular flow systems.

The work presented in this paper is aimed to fundamentally reconstruct the transport equations in kinetic theory to allow particle aggregation to take place so that the theory can be applied to the particle size enlargement processes induced by aggregation. This gives rise to the evaluation of the collision rate that will have to take into account the completely inelastic collisions so that the kinetic transport equations can include the source terms that are to do with aggregation.

Assumptions

In order to carry out the evaluation of the collision rate and to form the kinetic transport equations, several assumptions are made as follows.

1. Inelastic and completely inelastic collisions.

It is allowed while some collisions between particles deviate slightly from full elasticity – characterised by a coefficient of restitution e – other collisions result in a completely inelastic process after which the colliding particles adhere to each other, and can be said to have aggregated and led to size enlargement, characterised by a collision success factor ψ .

2. Binary collision mechanism.

In order to evaluate the collision rate, the mechanism of the binary collision[1] is adopted since it is valid in relatively dilute systems[45]. This suggests when the concentration of granular particles becomes dense and the mode that the motion of particles is induced can be identified, for instance by shear or by fluidisation, it is necessary to replace the binary collision mechanism with the related ones such as the shear induced coagulation[46], the ortho-kinetic aggregation[47], Brownian motion[46] and some others as can be found in the work of Williams and Loyalka[48] in order for the constitutive relations and relevant transport equations of the theory to be valid in and applied to the specific particulate systems.

3. Maxwell's distribution of particles' velocity.

The distribution of particles' velocity used in this paper to derive the kinetic transport equations is regarded as Maxwellian. This distribution function captures the main features of the distribution of particles in velocity although it is the equilibrium form in Boltzmann's H-theorem[49]. It is thought that it is reasonable to start with this function in order to see the effects of the completely inelastic collisions on the velocity properties of the particles.

4. There is a critical relative collision velocity for the attraction and repulsion forces to reach a balance. Any collision with relative velocity smaller than that will lead to aggregation.

In particulate systems, where conditions exist to allow aggregation to occur that is for some of the collisions to be completely inelastic, it is understood that some mechanism must generate sufficient attraction force to overcome the repulsion force that would otherwise make the particles rebound. Because the exchange of the momentum takes place during a collision and the forces are essentially the rates of the exchanged momentum, it follows that the two forces must relate directly to and can be parameterised in terms of the initial relative velocity of two colliding particles. Here we assume that there is a critical relative collision velocity at which point the balance between the attraction and the repulsion forces is reached. This critical velocity indicates the maximum possibility from 0 to which two colliding particles could adhere to become an aggregate. This means that all the collisions between two kinds of particles having an initial relative velocity smaller than the critical one will lead to aggregation.

Velocity-size Distribution Function and Its Transport Properties

$f(v, \mathbf{c}_v, \mathbf{r}, t)$ is defined as the probability density function of particles with v (v is regarded as the volume of individual particles, hereafter throughout the paper 'particles v' means 'particles of volume v'), $\mathbf{c}_v$ (the velocity of particles v), $\mathbf{r}$ (spatial coordinates) and t (time) as the variables and is denoted as f_v. It is also called the velocity-size distribution function in this paper as velocity and size are its two main characteristics and all the derivations made in this paper are concerned with the properties of the two characteristics. Then, the number density of particles v, n_v, is

$$n_v = n(v, \mathbf{r}, t) = \int_{c_v} f_v d\mathbf{c}_v \; . \tag{1}$$

The total number of particles per unit spatial volume located in position $\mathbf{r}$ at time t, N, is

$$N(\mathbf{r}, t) = \int_v n_v dv \, , \tag{2a}$$

and the total volume fraction $\varepsilon_s(\mathbf{r}, t)$ and mass density $\varepsilon_s \rho_s$ (ρ_s is the average density of all particles) of the particles are

$$\varepsilon_s = \int_v v n_v dv \, , \tag{2b}$$

$$\varepsilon_s \rho_s = \int_v m_v n_v dv = \int_v \rho_v v n_v dv \, . \tag{2c}$$

where ρ_v is the density of particles v. Let $\phi_v = \phi(v, \mathbf{c}_v, \mathbf{r}, t)$ be a property of particles v in terms of their velocity, its ensemble average value, $\langle \phi_v \rangle = \langle \phi \rangle (v, \mathbf{r}, t)$, along the velocity coordinate, is

$$\langle \phi_v \rangle = \frac{\int_{c_v} \phi_v f_v d\mathbf{c}_v}{\int_{c_v} f_v d\mathbf{c}_v} = \frac{\int_{c_v} \phi_v f_v d\mathbf{c}_v}{n_v} \, . \tag{3}$$

The ensemble average velocity of the particles v, $\mathbf{u}_v = \mathbf{u}(v, \mathbf{r}, t)$, thus becomes

$$\mathbf{u}_v = \langle \mathbf{c}_v \rangle = \frac{\int_{c_v} \mathbf{c}_v f_v d\mathbf{c}_v}{n_v}. \quad (4)$$

$\mathbf{u}_s = \mathbf{u}(\mathbf{r}, t)$ is the bulk velocity of all particles in position $\mathbf{r}$ at time t calculated as

$$\mathbf{u}_s = \frac{\int_v \mathbf{u}_v v n_v dv}{\int_v v n_v dv} = \frac{\int_v \mathbf{u}_v v n_v dv}{\varepsilon_s}. \quad (5)$$

According to (5), the fluctuation velocity $\mathbf{C}_v$ is defined

$$\mathbf{C}_v = \mathbf{c}_v - \mathbf{u}_s. \quad (6)$$

The granular energy of particles v, $\theta_v = \theta(v, \mathbf{r}, t)$, and the mixture granular energy of all particles, $\theta_s = \theta(\mathbf{r}, t)$, are defined as

$$\theta_v = \frac{1}{3} m_v \langle C_v{}^2 \rangle, \quad (7)$$

$$\theta_s = \frac{\int_v \theta_v n_v dv}{\int_v n_v dv} = \frac{\int_v \theta_v n_v dv}{N}. \quad (8)$$

The diffusion velocity of particles v, $\mathbf{w}_v = \mathbf{w}(v, \mathbf{r}, t)$, can be expressed

$$\mathbf{w}_v = \langle \mathbf{C}_v \rangle = \mathbf{u}_v - \mathbf{u}_s, \quad (9a)$$

and the mixture diffusion velocity of all particles according to (5) is

$$\frac{\int_v \mathbf{w}_v v n_v dv}{\int_v v n_v dv} = \frac{\int_v (\mathbf{u}_v - \mathbf{u}_s) v n_v dv}{\varepsilon_s} = \mathbf{u}_s - \mathbf{u}_s = 0. \quad (9b)$$

A number density weighted diffusion velocity, $\mathbf{w}_s = \mathbf{w}(\mathbf{r}, t)$, is also defined as

$$\mathbf{w}_s = \frac{\int_v \mathbf{w}_v n_v dv}{\int_v n_v dv} = \frac{\int_v \mathbf{w}_v n_v dv}{N}. \quad (9c)$$

We now consider f_v for in a granular flow system, the Boltzmann's equation is written as

$$\frac{\partial f_v}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{c}_v f_v + \frac{\partial}{\partial \mathbf{c}_v} \cdot \frac{\mathbf{F}_v}{m_v} f_v + \frac{\partial}{\partial v \mathbf{k}} \cdot \mathbf{G}_v f_v = r_v. \quad (10)$$

where $\mathbf{F}_v$ is the external force imposed on particles v to maintain the flow of these particles and is a function of $\mathbf{c}_v$; $\mathbf{G}_v$ is called the growth rate and is a function of v. $\mathbf{G}_v = dv\mathbf{k}/dt$, here $\mathbf{k}$ denotes the unit vector, its direction is corresponding to that defined by the spatial coordinates, $\mathbf{r}$, for instance Cartesian, cylindrical or spherical system. It should be noted at this point, for the case that only aggregation is occurring, $\mathbf{G}_v = 0$ (means no molecular deposition on particles taking place). However, we still take $\mathbf{G}_v$ into further consideration without losing its general applicability.

For the property ϕ_v of particles v, the rate of the change of this property can be obtained by integrating (10) over the velocity domain. According to (3), the Maxwell's transport equation is given by

$$\frac{\partial\left(n_v\langle\phi_v\rangle\right)}{\partial t} + \frac{\partial}{\partial\mathbf{r}}\cdot n_v\langle\phi_v\mathbf{c}_v\rangle - n_v\left\langle\frac{\partial\phi_v}{\partial t}\right\rangle - n_v\left\langle\frac{\partial\phi}{\partial\mathbf{r}}\cdot\mathbf{c}_v\right\rangle - n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{c}_v}\cdot\frac{\mathbf{F}_v}{m_v}\right\rangle + \frac{\partial}{\partial v\mathbf{k}}\cdot n_v\langle\phi_v\mathbf{G}_v\rangle - \left\langle\frac{\partial\phi_v}{\partial v\mathbf{k}}\right\rangle\cdot n_v\mathbf{G}_v$$
$$= \int_{c_v}\phi_v r_v d\mathbf{c}_v\,. \tag{11a}$$

Re-arranging (11a), we have

$$\frac{\partial\left(n_v\langle\phi_v\rangle\right)}{\partial t} + \frac{\partial}{\partial\mathbf{r}}\cdot n_v\langle\phi_v\mathbf{c}_v\rangle + \frac{\partial}{\partial v\mathbf{k}}\cdot n_v\langle\phi_v\mathbf{G}_v\rangle$$
$$= \int_{c_v}\phi_v r_v d\mathbf{c}_v + n_v\left\langle\frac{\partial\phi_v}{\partial t}\right\rangle + n_v\left\langle\frac{\partial\phi}{\partial\mathbf{r}}\cdot\mathbf{c}_v\right\rangle + n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{c}_v}\cdot\frac{\mathbf{F}_v}{m_v}\right\rangle + \left\langle\frac{\partial\phi_v}{\partial v\mathbf{k}}\right\rangle\cdot n_v\mathbf{G}. \tag{11b}$$

On the left hand side of (11b), the first two terms describe the overall change of ϕ_v, which is associated with the number density n_v of particles v, in time and spatial coordinates; the third term explains the change of n_v associated with ϕ_v in particle size coordinate owing to the change of the particle size itself.

The terms on the right hand side of (11b) account for the sources for the rate of the changes given on the left hand side of this equation. Thus, on the right hand side of (11b), the first term describes the change of ϕ_v attributed to the collisions that result in the change of number density of particles v with respect to their velocity and size characteristics; the second and third terms explain the change of ϕ_v itself in time and spatial coordinates; similarly the fourth and fifth terms describe the change of ϕ_v itself in velocity and size coordinates due to the external force $\mathbf{F}_v$ and the growth of particle size. It should be noted that on the left hand side of (11b), the overall rate of change of ϕ_v due to $\mathbf{F}_v$ in velocity coordinate, $\int_{\mathbf{c}_v} \frac{\partial}{\partial \mathbf{c}_v} \cdot \phi_v \frac{\mathbf{F}_v}{m_v} f_v d\mathbf{c}_v$, did not appear; this is due to the convergence of $\phi_v \frac{\mathbf{F}_v}{m_v} f$ as $\mathbf{c}_v$ approaches ∞ and $-\infty$.

It is worth mentioning that $r_v d\mathbf{c}_v$ describes the rate of change of particles v in the velocity ranging from $\mathbf{c}_v$ to $\mathbf{c}_v + d\mathbf{c}_v$, as a result, $\phi_v r_v d\mathbf{c}_v$ represents the rate of change of the property ϕ_v due to the change of the number of particles v resulting from collisions. Thus, $\int_{c_v} \phi_v r_v d\mathbf{c}_v$ measures the rate of change of ϕ_v carried by all the particles v through their velocity space. We then have

$$\int_{c_v} \phi_v r_v d\mathbf{c}_v = \Delta\langle n_v \phi_v \rangle = n_v \Delta\langle \phi_v \rangle + \langle \phi_v \rangle \Delta n_v . \tag{12}$$

It is seen from (11a) with (12), by replacing ϕ_v with 1, m_v, $m_v\mathbf{c}_v$ and $m_v c_v^2/2$, the number and mass continuity, the momentum and the kinetic energy equations can be generated, respectively. Notwithstanding this, for systems with the change of number density of particles n_v taking place due to such as aggregation, or the ensemble average property $\langle \phi_v \rangle$ not conserved, e.g., the kinetic energy in inelastic collisions, the right hand side of this equation must be evaluated thus requires f_v to be known.

Collision Rate and the Transport of a Property of particles

For the particles specified by size v and velocity $\mathbf{c}_v$, the rate of collisions is considered in such a way that contributes in quantity to these two characteristics. The detailed derivation of the collision rate and the transport of a property of particles is given in Appendix. Here we only describe those results. The collision rate is written as

$$
\begin{aligned}
r_v = & \iiint \left[e_{\varepsilon v}{}^2 (1-\psi_{\varepsilon v}') f_v' f_\varepsilon' \chi_{\varepsilon v}' g_{\varepsilon v}' - (1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \right] \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon \\
& + \int_0^v \iint \frac{1}{2M_{v-\varepsilon}{}^2} \psi_{\varepsilon, v-\varepsilon} f_{v-\varepsilon} f_\varepsilon \chi_{\varepsilon, v-\varepsilon} g_{\varepsilon, v-\varepsilon} \frac{\sigma_{\varepsilon, v-\varepsilon}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon \\
& - \iiint \psi_{\varepsilon v} f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon .
\end{aligned}
\qquad \text{(A10)}
$$

In (A10), f with subscripts v, ε and $v-\varepsilon$ refers to the probability density function for different kinds of particles specified by their sizes (and velocities abbreviated). Symbols with "′" refer to the properties of reverse collisions. $\mathbf{c}_{\varepsilon v} = \mathbf{c}_\varepsilon - \mathbf{c}_v$ is the relative collision velocity between particles v and ε and σ is the inter-distance of the two colliding particles referring to half of the addition of their diameters (of volume equivalent spheres). $g_{\varepsilon v}$ is the radial distribution function[7]. $e_{\varepsilon v}$ is given by $\mathbf{c}_{\varepsilon v}' = -e_{\varepsilon v}\mathbf{c}_{\varepsilon v}$. ψ with subscripts specifies its value (the probability) for a particular collision to succeed for an aggregation. χ is the Taylor's expansion when the sizes of two particles are taken into account in a collision to give the relative position of the two colliding particles. $M_{v-\varepsilon}$ is the mass ratio between the mass of particle $v-\varepsilon$, $m_{v-\varepsilon}$, and the addition of the masses $(m_{v-\varepsilon} + m_\varepsilon)$ of particles $v-\varepsilon$ and ε, which means $M_{v-\varepsilon} = m_{v-\varepsilon} / (m_{v-\varepsilon} + m_\varepsilon)$. $d\Omega$ is the differential angle multiplied by the square of a sphere radius to characterise the differential area of a spherical surface with $\int_\Omega d\Omega = \int_0^\pi \sin\omega d\omega \int_0^{2\pi} d\varphi = 4\pi$, here ω and φ represent the filling angles in spherical coordinates.

On the right hand side of (A10), the first term describes the net increase of particles v in terms of their velocity characteristic attributed to the forward and reverse collisions (without changing the number density n_v of the particles in their size v). The second term gives the birth rate of the particles with regard to their size v, which is due to the completely inelastic collisions between particles ε and $v-\varepsilon$; the third term shows the death rate of the particles v owing to the completely inelastic collisions between particles v and any sizes of particles. Together the second and third terms detail the net increase of particles v in terms of their size (number density n_v of the particles v has been changed).

The transport of the property ϕ_v is calculated as $\int \phi_v r_v d\mathbf{c}_v$ and given by (A11) as

$$\begin{aligned}
&\frac{\partial\left(n_v\langle\phi_v\rangle\right)}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot n_v\langle\phi_v\mathbf{c}_v\rangle - n_v\left\langle\frac{\partial\phi_v}{\partial t}\right\rangle - n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{r}}\cdot\mathbf{c}_v\right\rangle - n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{c}_v}\cdot\frac{\mathbf{F}_v}{m_v}\right\rangle+\frac{\partial}{\partial v\mathbf{k}}\cdot n_v\langle\phi_v\mathbf{G}_v\rangle - \left\langle\frac{\partial\phi_v}{\partial v\mathbf{k}}\right\rangle\cdot n_v\mathbf{G}_v \\
&= \int\iiint(\phi_v'-\phi_v)(1-\psi_{\varepsilon v})f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v \\
&+\iiint\phi_v\left[\int_0^v\frac{1}{2M_{v-\varepsilon}{}^2}\psi_{\varepsilon,v-\varepsilon}f_{v-\varepsilon}f_\varepsilon\chi_{\varepsilon,v-\varepsilon}g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon\right. \\
&\qquad\left.-\int_0^\infty\psi_{\varepsilon v}f_v f_\varepsilon\chi_{\varepsilon v}g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon\right]d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v.
\end{aligned} \tag{A11}$$

As can be seen from the right hand side of (A11), the first term is the rate of net change of ϕ_v contributed from the collisions with regard to the velocity characteristic of f_v (without changing n_v); the second and third terms together give the rate of ϕ_v attributed to the change of f_v in terms of its size characteristic (with n_v changed). Thus, according to (12), we have the following relations

$$n_v\Delta\langle\phi_v\rangle = \int\iiint(\phi_v'-\phi_v)(1-\psi_{\varepsilon v})f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v\,, \tag{13a}$$

$$\begin{aligned}
\langle\phi_v\rangle\Delta n_v = \iiint\phi_v&\left[\int_0^v\frac{1}{2M_{v-\varepsilon}{}^2}\psi_{\varepsilon,v-\varepsilon}f_{v-\varepsilon}f_\varepsilon\chi_{\varepsilon,v-\varepsilon}g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon\right. \\
&\left.-\int_0^\infty\psi_{\varepsilon v}f_v f_\varepsilon\chi_{\varepsilon v}g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\varepsilon\right]d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v.
\end{aligned} \tag{13b}$$

As a simplified case for (A11), let $\phi_v = 1$, then $\phi_v' = 1$, also $\psi_{\varepsilon v} = 0$ (without aggregation of particles) and $\mathbf{G}_v = 0$ (without molecular deposition for particles' growth), (A11) becomes $\frac{\partial n_v}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot n_v\mathbf{u}_v = 0$, multiplying both sides of it by v and integrating over v space, we then have $\frac{\partial\varepsilon_s}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot\varepsilon_s\mathbf{u}_s = 0$. These are the typical continuity equations in multiple phase flow[27] without the change of particle size and number density taking place.

However, with $\psi_{\varepsilon v} \neq 0$ and ϕ_v becoming more complicated such as $m_v\mathbf{c}_v$ and $m_v c_v^{\ 2}/2$, evaluation of (13a-b), i.e., the right hand side of (A11), becomes necessary and is presented in the next section for deriving the kinetic transport equations. It is worth noting at this stage that the transport equations for continuity, momentum and kinetic energy for all the particles, the conservation of mass and momentum needs to be proven and the dissipation of the kinetic energy needs to be given since $\psi_{\varepsilon v} \neq 0$ and the restitution of coefficient $e_{\varepsilon v}$ are involved in the evaluation, i.e., either (13a), (13b) or both not equal to 0 thus require detailed calculation.

Kinetic Transport Equations

To generate the kinetic transport equations, i.e., to evaluate (13a) and (13b), it is necessary to know the mathematical form of f_v. As indicated in (1), the following approximation is made

$$f_v = f(v, \mathbf{c}_v, \mathbf{r}, t) \cong n(v, \mathbf{r}, t)\lambda(\mathbf{c}_v, \mathbf{r}, t) = n_v\lambda_v\,, \tag{14}$$

where $\lambda(\mathbf{c}_v, \mathbf{r}, t) = \lambda_v$ and is corresponding to the normalised velocity distribution function of particles v. This approximation suggests a mutually independent behaviour between the particle size and velocity expressed in f_v. Thus, λ_v implies the probability of the particles with size v appearing to have velocity $\mathbf{c}_v$. According to Assumption 3, λ_v takes the form of Maxwell's distribution, we then have

$$f_v = n_v\left(\frac{m_v}{2\pi\theta_s}\right)^{\frac{3}{2}} \exp\left[-\frac{m_v(\mathbf{c}_v - \mathbf{u}_s)^2}{2\theta_s}\right], \tag{15a}$$

where θ_s is the mixture granular energy defined in (8). It is worth pointing out that this function can be extended to higher orders according to Chapman-Enskog's approximation[7] but it has captured the main features of the distribution of the particles in terms of their velocity. According to (6) for the fluctuation velocity of particles, (15a) becomes

$$f_v = n_v\left(\frac{m_v}{2\pi\theta_s}\right)^{\frac{3}{2}} \exp\left(-\frac{m_v C_v^{\ 2}}{2\theta_s}\right) \tag{15b}$$

Taking the 0th order of $\chi_{\varepsilon v}$ (means relatively dilute systems, the distance of particles to travel for a collision is much greater than the sizes of the particles), i.e., $\chi_{\varepsilon v}=1$, (A11) is changed to

$$\frac{\partial\left(n_v\langle\phi_v\rangle\right)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot n_v\langle\phi_v\mathbf{c}_v\rangle-n_v\left\langle\frac{\partial\phi_v}{\partial t}\right\rangle-n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{r}}\cdot\mathbf{c}_v\right\rangle-n_v\left\langle\frac{\partial\phi_v}{\partial\mathbf{c}_v}\cdot\frac{\mathbf{F}_v}{m_v}\right\rangle+\frac{\partial}{\partial v\mathbf{k}}\cdot n_v\langle\phi_v\mathbf{G}_v\rangle-\left\langle\frac{\partial\phi_v}{\partial v\mathbf{k}}\right\rangle\cdot n_v\mathbf{G}_v$$

$$\begin{aligned}&=n_v\int_0^\infty n_\varepsilon g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}\iiint(\phi_v'-\phi_v)(1-\psi_{\varepsilon v})\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon\\&+\int_0^v\frac{1}{2M_{v-\varepsilon}{}^2}\psi_{\varepsilon,v-\varepsilon}n_{v-\varepsilon}n_\varepsilon g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}{}^2}{4}\iiint\phi_v\lambda_{v-\varepsilon}\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon\\&-n_v\int_0^\infty\psi_{\varepsilon v}n_\varepsilon g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}\iiint\phi_v\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon.\end{aligned}\tag{16}$$

The above transformation is carried out with $f(\mathbf{c}_v,v,\mathbf{r},t)d\mathbf{c}_v=f(\mathbf{C}_v,v,\mathbf{r},t)d\mathbf{C}_v$ and

$$\lambda_v\lambda_\varepsilon(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{c}_v d\mathbf{c}_\varepsilon=\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_v d\mathbf{C}_\varepsilon,\tag{17}$$

where $\mathbf{C}_{\varepsilon v}=\mathbf{C}_\varepsilon-\mathbf{C}_v$ is the relative fluctuation velocity. Additionally, $d\mathbf{C}_v d\mathbf{C}_\varepsilon$ can be changed to the form of $d\mathbf{C}_c d\mathbf{C}_{\varepsilon v}$ ($\mathbf{C}_c$ is the mass centre velocity of particles v and ε as defined similarly to that in (A9)) with

$$d\mathbf{C}_v d\mathbf{C}_\varepsilon=\left|\frac{\partial(\mathbf{C}_v,\mathbf{C}_\varepsilon)}{\partial(\mathbf{C}_c,\mathbf{C}_{\varepsilon v})}\right|d\mathbf{C}_c d\mathbf{C}_{\varepsilon v}=d\mathbf{C}_c d\mathbf{C}_{\varepsilon v},\tag{18}$$

and the following expressions[7]

$$\begin{aligned}&d\mathbf{C}_{\varepsilon v}=(d\mathbf{C}_{\varepsilon v})_x(d\mathbf{C}_{\varepsilon v})_y(d\mathbf{C}_{\varepsilon v})_z=C_{\varepsilon v}{}^2d\mathbf{C}_{\varepsilon v}d\Omega,\\&d\mathbf{C}_c=C_c{}^2d\mathbf{C}_c d\Omega,\ d\mathbf{C}_{\varepsilon v}d\mathbf{C}_c=C_{\varepsilon v}{}^2d\mathbf{C}_{\varepsilon v}d\Omega C_c{}^2d\mathbf{C}_c d\Omega.\end{aligned}\tag{19}$$

The continuity equations

The continuity equation for the number density n_v of particles v can be obtained from (16) by letting $\phi_v=1$, then $\phi_v'=1$ as follows

$$\begin{aligned}&\frac{\partial n_v}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot n_v\mathbf{u}_v+\frac{\partial}{\partial v\mathbf{k}}\cdot n_v\mathbf{G}_v\\&=\int_0^v\frac{1}{2M_{v-\varepsilon}{}^2}\psi_{\varepsilon,v-\varepsilon}n_{v-\varepsilon}n_\varepsilon g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}{}^2}{4}d\varepsilon\iiint\lambda_{v-\varepsilon}\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v\\&-n_v\int_0^\infty\psi_{\varepsilon v}n_\varepsilon g_{\varepsilon v}\frac{\sigma_{\varepsilon v}{}^2}{4}d\varepsilon\iiint\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v.\end{aligned}\tag{20}$$

On the right hand side of (20), the triple integrations of the normalised Maxwell's velocity distribution functions $\lambda_{v-\varepsilon}$, λ_{ε} and λ_{v} over the domains of $\mathbf{\Omega}$, $\mathbf{C}_{\varepsilon}$ and $\mathbf{C}_{v}$ can be calculated according to (18) and (19) for the values of $\mathbf{C}_{c}$ and $\mathbf{C}_{\varepsilon v}$ ranging from 0 to ∞; (20) thus becomes

$$\frac{\partial n_v}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot n_v\mathbf{u}_v+\frac{\partial}{\partial v\mathbf{k}}\cdot n_v\mathbf{G}_v$$
$$=\frac{1}{2}\int_0^v\left[\frac{8\pi\theta_s\left(m_{v-\varepsilon}+m_\varepsilon\right)}{m_{v-\varepsilon}m_\varepsilon}\right]^{\frac{1}{2}}\psi_{\varepsilon,v-\varepsilon}g_{\varepsilon,v-\varepsilon}\sigma_{\varepsilon,v-\varepsilon}{}^2n_{v-\varepsilon}n_\varepsilon d\varepsilon-n_v\int_0^\infty\left[\frac{8\pi\theta_s\left(m_v+m_\varepsilon\right)}{m_vm_\varepsilon}\right]^{\frac{1}{2}}\psi_{\varepsilon v}g_{\varepsilon v}\sigma_{\varepsilon v}{}^2n_\varepsilon d\varepsilon. \quad (21)$$

This is the standard population balance equation[46, 50-53] in the form of aggregation and growth and has been widely used in the modelling and simulation of engineering particulate systems[54, 55] to predict the particle size distributions[51, 53] when size enlargement events occurred.

(21) has some interesting features presented as the following. Let $\xi(v)$ be a property of size v, multiply it to both sides of (21) then integrate the equation over v in the domain (0, ∞), also according to (9a) for $\mathbf{u}_v=\mathbf{u}_s+\mathbf{w}_v$, we have

$$\int_0^\infty\xi(v)\frac{\partial n_v}{\partial t}dv+\int_0^\infty\xi(v)\frac{\partial}{\partial \mathbf{r}}\cdot n_v(\mathbf{u}_s+\mathbf{w}_v)dv+\int_0^\infty\xi(v)\frac{\partial}{\partial v\mathbf{k}}\cdot n_v\mathbf{G}_vdv$$
$$=\frac{1}{2}\int_0^\infty\int_0^\infty\xi(v)\left[\frac{8\pi\theta_s\left(m_\zeta+m_\varepsilon\right)}{m_\zeta m_\varepsilon}\right]^{\frac{1}{2}}\psi_{\varepsilon\zeta}g_{\varepsilon\zeta}\sigma_{\varepsilon\zeta}{}^2n_\zeta n_\varepsilon d\zeta d\varepsilon \quad (22)$$
$$-\int_0^\infty\int_0^\infty\xi(v)\left[\frac{8\pi\theta_s\left(m_v+m_\varepsilon\right)}{m_vm_\varepsilon}\right]^{\frac{1}{2}}\psi_{\varepsilon v}g_{\varepsilon v}\sigma_{\varepsilon v}{}^2n_vn_\varepsilon d\varepsilon dv.$$

The first term on the right hand side of (22) is obtained by exchanging the order of the integrations for $v-\varepsilon$ and ε and then letting $\zeta=v-\varepsilon$ thus $\zeta\in(0,\infty)$.

Replacing $\xi(v)$ with 1 in (22), according to (2a) and (9c), the continuity equation for the total number of particles is

$$\frac{\partial N}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot N(\mathbf{u}_s+\mathbf{w}_s)=-\frac{1}{2}\int_0^\infty\int_0^\infty\left[\frac{8\pi\theta_s\left(m_v+m_\varepsilon\right)}{m_vm_\varepsilon}\right]^{\frac{1}{2}}\psi_{\varepsilon v}g_{\varepsilon v}\sigma_{\varepsilon v}{}^2n_vn_\varepsilon d\varepsilon dv. \quad (23a)$$

In (23a), the term $\int_0^\infty \frac{\partial}{\partial v\mathbf{k}} \cdot n_v \mathbf{G}_v dv = 0$ is due to the fact that $n_v \mathbf{G}_v \rightarrow 0$ as particle size $v \rightarrow 0$ and ∞. Note in this equation, the convective flux is with velocity $\mathbf{u}_s + \mathbf{w}_s$ as $\mathbf{u}_s$ is the particles volume fraction weighted bulk velocity instead of number weighted thus the number weighted diffusion velocity $\mathbf{w}_s$ is generated as an extra term. It is worth pointing out that (23a) explains the decrease of the total number of particles in a quantitative way for the systems where aggregation takes place.

Similarly, let $\xi(v) = v$ and m_v (note, $v = v - \varepsilon + \varepsilon = \zeta + \varepsilon$ and $m_v = m_{v-\varepsilon} + m_\varepsilon = m_\zeta + m_\varepsilon$ the right hand of (22) is equal to 0), the continuity equations for the volume fraction and mass density of all particles according to (2b), (2c), $\partial v / \partial t = 0$, $\partial v / \partial \mathbf{r} = 0$, $\partial m_v / \partial t = 0$ and $\partial m_v / \partial \mathbf{r} = 0$ are

$$\frac{\partial \varepsilon_s}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \varepsilon_s \mathbf{u}_s = 0, \tag{23b}$$

$$\frac{\partial (\varepsilon_s \rho_s)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\varepsilon_s \rho_s \mathbf{u}_s) = 0. \tag{23c}$$

(23b) and (23c) demonstrate the conservation of the total volume and mass of particles, respectively, for the aggregation of particles in granular flow systems.

The momentum equations

Similar to generating the continuity equations, the establishment of momentum and granular energy equations is as well for both the particles with a specific size v and all the particles in the system. The purpose to establish the equations for all the particles is to prove the conservativity (total momentum) and dissipativity (total kinetic energy) of the particles in the case of aggregation; and in particular to calculate the dissipation of the total kinetic energy due to the inelastic collisions and aggregation of particles.

For the momentum equation of particles v, by letting $\phi_v = m_v \mathbf{c}_v$, after the collisions with particles ε, the momentum of particles v is changed to $\phi_v' = m_v \mathbf{c}_v'$, thus we obtain

$$\phi_v' - \phi_v = m_v (\mathbf{c}_v' - \mathbf{c}_v) = m_v M_\varepsilon (1 + e_{\varepsilon v}) \mathbf{C}_{\varepsilon v}, \tag{24}$$

which is due to $\mathbf{c}_v = \mathbf{c}_c - M_\varepsilon \mathbf{c}_{\varepsilon v}$, $\mathbf{c}_v' = \mathbf{c}_c - M_\varepsilon \mathbf{c}_{\varepsilon v}'$, $\mathbf{c}_c = \mathbf{C}_c$, $\mathbf{c}_{\varepsilon v} = \mathbf{C}_{\varepsilon v}$, $\mathbf{c}_{\varepsilon v}' = \mathbf{C}_{\varepsilon v}'$ and $\mathbf{C}_{\varepsilon v} = -e_{\varepsilon v} \mathbf{C}_{\varepsilon v}'$. Then, the momentum equation for particles v according to (16), $\partial \mathbf{c}_v / \partial t = 0$, $\partial \mathbf{c}_v / \partial \mathbf{r} = 0$ and $\partial \mathbf{C}_v / \partial \mathbf{r} = 0$ ($\mathbf{c}_v$ and $\mathbf{C}_v$ are not the functions of $\mathbf{r}$ and t) is

$$\begin{aligned}
&\frac{\partial (n_v m_v \mathbf{u}_v)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot [n_v m_v \mathbf{u}_s (\mathbf{u}_v + \mathbf{w}_v)] + \frac{\partial}{\partial v \mathbf{k}} \cdot (n_v m_v \mathbf{u}_v \mathbf{G}_v) + \frac{\partial P_v}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{r}} \cdot \bar{\bar{\boldsymbol{\tau}}}_v - n_v \langle \mathbf{F}_v \rangle \\
&= n_v \int_0^\infty n_\varepsilon (1 - \psi_{\varepsilon v})(1 + e_{\varepsilon v}) g_{\varepsilon v} 3\pi \theta_s \sigma_{\varepsilon v}{}^2 \mathbf{k} d\varepsilon \\
&\quad + \int_0^v n_{v-\varepsilon} n_\varepsilon \psi_{\varepsilon, v-\varepsilon} g_{\varepsilon, v-\varepsilon} \sigma_{\varepsilon, v-\varepsilon}{}^2 \left\{ \frac{4\theta_s m_v \mathbf{k}}{(m_{v-\varepsilon} m_\varepsilon)^{\frac{1}{2}}} + m_v \mathbf{u}_s \left[\frac{2\pi\theta_s (m_{v-\varepsilon} + m_\varepsilon)}{m_{v-\varepsilon} m_\varepsilon} \right]^{\frac{1}{2}} \right\} d\varepsilon \\
&\quad - n_v \int_0^\infty n_\varepsilon \psi_{\varepsilon v} g_{\varepsilon v} \sigma_{\varepsilon v}{}^2 \left\{ \theta_s \left(8\sqrt{\frac{m_v}{m_\varepsilon}} - 3\pi \right) \mathbf{k} + \mathbf{u}_s \left[\frac{8\pi\theta_s (m_v + m_\varepsilon) m_v}{m_\varepsilon} \right]^{\frac{1}{2}} \right\} d\varepsilon,
\end{aligned} \tag{25}$$

where P_v and $\bar{\bar{\boldsymbol{\tau}}}_v$ are the normal solid pressure and stress tensor of particles v, respectively.

$$P_v = n_v m_v \langle (\mathbf{C}_v)_i (\mathbf{C}_v)_i \rangle, \tag{26a}$$

$$\bar{\bar{\boldsymbol{\tau}}}_v = n_v m_v \langle (\mathbf{C}_v)_i (\mathbf{C}_v)_j \rangle_{i \neq j}. \tag{26b}$$

(25) essentially explains all the forces that are imposed on particles v, causing the change of the momentum of these particles as a whole in time, spatial and size coordinates. The change of the momentum of particles v is thus attributed to the external force $\mathbf{F}_v$, collisions that particles v encountered (the first term of the right hand side of (25)) and the net change of the number of particles v owing to aggregation (the second and third terms of the right hand side of (25)).

The total momentum of particles can be obtained by integrating both sides of (25) over v domain (0, ∞), the left hand side of this equation thus becomes

$$\frac{\partial (\varepsilon_s \rho_s \mathbf{u}_s)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\varepsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) + \frac{\partial P_s}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{r}} \cdot \bar{\bar{\boldsymbol{\tau}}}_s - N \langle \mathbf{F}_v \rangle, \tag{27}$$

where the transformation is made according to (2c), (5), (9b), $\int_0^\infty P_v dv = P_s$ and $\int_0^\infty \bar{\bar{\boldsymbol{\tau}}}_v dv = \bar{\bar{\boldsymbol{\tau}}}_s$.

To obtain the integrated terms on the right hand side of (38), it is necessary to trace back (16). For the first term of the right hand side of (16), as $\phi_v' - \phi_v = m_v (\mathbf{c}_v' - \mathbf{c}_v)$ and the integration over the entire domain of size v is being made, it then represents the change of the total momentum of particles v and ε due to all the collisions between them. This term can thus be written as

$$\begin{aligned}&\int_0^\infty n_v \int_0^\infty n_\varepsilon g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^{\ 2}}{4} \iiint m_v (\mathbf{c}_v' - \mathbf{c}_v)(1-\psi_{\varepsilon v})\lambda_v \lambda_\varepsilon (\mathbf{C}_{\varepsilon v}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv \\ &= \frac{1}{2}\int_0^\infty n_v \int_0^\infty n_\varepsilon g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^{\ 2}}{4} \iiint (m_v \mathbf{c}_v' - m_v \mathbf{c}_v + m_\varepsilon \mathbf{c}_\varepsilon' - m_\varepsilon \mathbf{c}_\varepsilon)(1-\psi_{\varepsilon v})\lambda_v \lambda_\varepsilon (\mathbf{C}_{\varepsilon v}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv,\end{aligned} \tag{28}$$

which is equal to 0 as $m_v \mathbf{c}_v + m_\varepsilon \mathbf{c}_\varepsilon = m_v \mathbf{c}_v' + m_\varepsilon \mathbf{c}_\varepsilon'$.

With $\phi_v = m_v \mathbf{c}_v$ and $m_v = m_{v-\varepsilon} + m_\varepsilon$, the second term of the right hand side of (16) after integration over v domain becomes

$$\begin{aligned}&\int_0^\infty \int_0^v \frac{1}{2M_{v-\varepsilon}^{\ 2}} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\ 2}}{4} \iiint m_v \mathbf{c}_v \lambda_{v-\varepsilon} \lambda_\varepsilon (\mathbf{C}_{\varepsilon v}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv \\ &= \int_0^\infty \int_0^v \frac{1}{2} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\ 2}}{4} \iiint (m_{v-\varepsilon} \mathbf{c}_{v-\varepsilon} + m_\varepsilon \mathbf{c}_\varepsilon) \lambda_{v-\varepsilon} \lambda_\varepsilon (\mathbf{C}_{\varepsilon,v-\varepsilon}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_{v-\varepsilon} d\varepsilon dv,\end{aligned} \tag{29}$$

in which $m_v \mathbf{c}_v = m_\varepsilon \mathbf{c}_\varepsilon + m_{v-\varepsilon} \mathbf{c}_{v-\varepsilon}$ is due to the fact that $\mathbf{c}_v$ is the mass centre velocity of particles ε and $v-\varepsilon$ as expressed in (A9). Similar treatment to that in (22) by exchanging the order of the integrations for ε and v and letting $v-\varepsilon = \zeta$ transforms (29) into

$$\begin{aligned}&\int_0^\infty \int_\varepsilon^\infty \frac{1}{2} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\ 2}}{4} \iiint (m_{v-\varepsilon} \mathbf{c}_{v-\varepsilon} + m_\varepsilon \mathbf{c}_\varepsilon) \lambda_{v-\varepsilon} \lambda_\varepsilon (\mathbf{C}_{\varepsilon,v-\varepsilon}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_{v-\varepsilon} dv d\varepsilon \\ &= \int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\ 2}}{4} \iiint (m_{v-\varepsilon} \mathbf{c}_{v-\varepsilon} + m_\varepsilon \mathbf{c}_\varepsilon) \lambda_{v-\varepsilon} \lambda_\varepsilon (\mathbf{C}_{\varepsilon,v-\varepsilon}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_{v-\varepsilon} d(v-\varepsilon) d\varepsilon \\ &= \int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,\zeta} n_\zeta n_\varepsilon g_{\varepsilon,\zeta} \frac{\sigma_{\varepsilon,\zeta}^{\ 2}}{4} \iiint (m_\zeta \mathbf{c}_\zeta + m_\varepsilon \mathbf{c}_\varepsilon) \lambda_\zeta \lambda_\varepsilon (\mathbf{C}_{\varepsilon,\zeta}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_\zeta d\zeta d\varepsilon.\end{aligned} \tag{30}$$

As particles ζ and ε in (30) are in-distinguished and the integrations over their entire domains are being carried out, (30) can be written as

$$\int_0^\infty \int_0^\infty \psi_{\varepsilon,v} n_v n_\varepsilon g_{\varepsilon,v} \frac{\sigma_{\varepsilon,v}^{\ 2}}{4} \iiint m_v \mathbf{c}_v \lambda_v \lambda_\varepsilon (\mathbf{C}_{\varepsilon,v}\cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v dv d\varepsilon \,, \tag{31}$$

which is essentially the same as the integration of the third term of the right hand side of (16) over v domain with $\phi_v = m_v \mathbf{c}_v$. Thus, the second and the third terms of the right hand side of (16) after the integration over v with $\phi_v = m_v\mathbf{c}_v$ are cancelled. The momentum equation for all the particles taking (27) forward hence becomes

$$\frac{\partial(\varepsilon_s\rho_s\mathbf{u}_s)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot(\varepsilon_s\rho_s\mathbf{u}_s\mathbf{u}_s)+\frac{\partial P_s}{\partial\mathbf{r}}+\frac{\partial}{\partial\mathbf{r}}\cdot\bar{\bar{\boldsymbol{\tau}}}_s-N\langle\mathbf{F}_v\rangle=0\,. \tag{32}$$

This has given a detailed mathematical proof for the conservation of the total momentum of all the particles in a system when aggregation occurs.

The granular energy equations

The granular energy equation of particles v can be obtained by replacing ϕ_v with $m_v {c_v}^2/2$ into (16). Since the granular energy is defined with fluctuation velocity as expressed in (7) and by carrying out the integration for the right hand side of (16) for $\phi_v = m_v {c_v}^2/2$, for particles v, their granular energy equation becomes

$$\begin{aligned}
&\frac{3}{2}\left[\frac{\partial(n_v\theta_v)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot(n_v\theta_v\mathbf{u}_s)\right]+\frac{1}{2}\left\{\frac{\partial\left(n_v m_v {u_s}^2\right)}{\partial t}+\frac{\partial}{\partial\mathbf{r}}\cdot\left[n_v m_v {u_s}^2(\mathbf{u}_v+\mathbf{w}_v)\right]\right\}+\left\{\frac{\partial[n_v m_v(\mathbf{u}_s\cdot\mathbf{w}_v)]}{\partial t}\right.\\
&\left.+\frac{\partial}{\partial\mathbf{r}}\cdot[n_v m_v(\mathbf{u}_s\cdot\mathbf{w}_v)\cdot\mathbf{u}_s]\right\}+\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{q}_v+P_v\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{u}_s+\bar{\bar{\boldsymbol{\tau}}}_v:\frac{\partial}{\partial\mathbf{r}}\mathbf{u}_s+\frac{3}{2}\frac{\partial}{\partial v\mathbf{k}}\cdot(n_v\theta_v\mathbf{G}_v)-n_v m_v\langle(\mathbf{C}_v+\mathbf{u}_s)\cdot\mathbf{F}_v\rangle\\
&=n_v\int_0^\infty n_\varepsilon(1-\psi_{\varepsilon v})g_{\varepsilon v}{\sigma_{\varepsilon v}}^2\left\{\frac{2\sqrt{2\pi}{\theta_s}^{\frac{3}{2}}(1+e_{\varepsilon v})m_\varepsilon^{\frac{1}{2}}}{(m_v+m_\varepsilon)^{\frac{1}{2}}}\left[\frac{2(e_{\varepsilon v}-1)}{m_v^{\frac{1}{2}}}+\frac{3}{m_\varepsilon^{\frac{1}{2}}}\right]+3\pi\theta_s(1+e_{\varepsilon v})(\mathbf{u}_s\cdot\mathbf{k})\right\}d\varepsilon\\
&+\int_0^v n_{v-\varepsilon}n_\varepsilon\psi_{\varepsilon,v-\varepsilon}g_{\varepsilon,v-\varepsilon}{\sigma_{\varepsilon,v-\varepsilon}}^2 m_v\left\{\frac{3\sqrt{2\pi}{\theta_s}^{\frac{3}{2}}}{2(m_\varepsilon+m_{v-\varepsilon})^{\frac{1}{2}}(m_\varepsilon m_{v-\varepsilon})^{\frac{1}{2}}}+\left[\frac{\pi\theta_s(m_\varepsilon+m_{v-\varepsilon})}{2m_\varepsilon m_{v-\varepsilon}}\right]^{\frac{1}{2}}{u_s}^2+\frac{4\pi\theta_s(\mathbf{u}_s\cdot\mathbf{k})}{(m_\varepsilon m_{v-\varepsilon})^{\frac{1}{2}}}\right\}d\varepsilon\\
&-n_v\int_0^\infty n_\varepsilon\psi_{\varepsilon v}g_{\varepsilon v}{\sigma_{\varepsilon v}}^2\left\{\frac{\sqrt{2\pi}{\theta_s}^{\frac{3}{2}}}{(m_\varepsilon+m_v)^{\frac{1}{2}}}\left[3\left(\frac{m_v}{m_\varepsilon}\right)^{\frac{1}{2}}+8\left(\frac{m_\varepsilon}{m_v}\right)^{\frac{1}{2}}-6\right]+8\theta_s(\mathbf{u}_s\cdot\mathbf{k})\left(\frac{m_v}{m_\varepsilon}\right)^{\frac{1}{2}}\right.\\
&\qquad\qquad\left.-3\pi\theta_s(\mathbf{u}_s\cdot\mathbf{k})+m_v{u_s}^2\left[\frac{2\pi\theta_s(m_\varepsilon+m_{v-\varepsilon})}{m_\varepsilon m_v}\right]^{\frac{1}{2}}\right\}d\varepsilon\,,
\end{aligned}\tag{33}$$

where $\mathbf{q}_v$ is the heat flux defined as $\mathbf{q}_v = n_v m_v\left\langle {C_v}^2\mathbf{C}_v\right\rangle/2$.

As the property being transported is the actual kinetic energy ($m_v {c_v}^2/2$) but θ_v is related to the dot product of $\mathbf{C}_v$ ($\langle\mathbf{C}_v\cdot\mathbf{C}_v\rangle$) with also $\mathbf{c}_v=\mathbf{C}_v+\mathbf{u}_s$, it is thus seen that on the left hand side of

(33), two extra total differential terms are generated with respect to the bulk velocity $\mathbf{u}_s$. They are explained as follows.

The second group (two terms with u_s^2 in {}) describes the transfer of the kinetic energy of particles v moving as a whole with all other particles; the third group (two terms with ($\mathbf{u}_s \cdot \mathbf{w}_v$) in {}) is understood as the transfer of the kinetic energy of particles v due to their diffusion with a velocity $\mathbf{w}_v$ relative to the bulk particles with the ensemble average velocity $\mathbf{u}_s$.

The physical meanings of other terms on the left hand side of (33) are similar to that explained in the works of Davidson and Harrison[56], Kunii and Levenspiel[57] and Gidaspow[27].

The mixture granular energy of all particles can then be generated by integrating both sides of (33) over particle size domain (0, ∞); thus the left hand side of (33) becomes

$$\frac{3}{2}\left[\frac{\partial(N\theta_s)}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot(N\theta_s\mathbf{u}_s)\right]+\frac{1}{2}\left[\frac{\partial\left(\varepsilon_s\rho_s u_s^2\right)}{\partial t}+\frac{\partial}{\partial \mathbf{r}}\cdot\left(\varepsilon_s\rho_s u_s^2\mathbf{u}_s\right)\right]$$
$$+\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{q}_s+P_s\frac{\partial}{\partial \mathbf{r}}\cdot\mathbf{u}_s+\bar{\bar{\boldsymbol{\tau}}}_s:\frac{\partial}{\partial \mathbf{r}}\mathbf{u}_s-\varepsilon_s\rho_s\left\langle(\mathbf{C}_v+\mathbf{u}_s)\cdot\mathbf{F}_v\right\rangle, \quad (34)$$

where $\mathbf{q}_s=\int_0^\infty \mathbf{q}_v dv$, $n_v\theta_v\mathbf{G}_v$ converges with $v\to 0$ and ∞; and the terms with the dot product of diffusion velocity $\mathbf{w}_v$ after integration are equal to 0 according to (9b).

For the integration of the right hand side of (33) over v, considering the terms of the right hand side of (16), a similar treatment can be made as to that for the total momentum equation of all particles. Therefore, the kinetic energy dissipation due to the inelastic collisions, ΔE_c, the first term of the right hand side of (16) for $\phi_v = m_v c_v^2/2$, with the integrations over v and ε from 0 to ∞ being carried out, which indicates particles v and ε are in-distinguished, becomes

$$\Delta E_c=\int_0^\infty n_v\int_0^\infty n_\varepsilon g_{\varepsilon v}\frac{\sigma_{\varepsilon v}^2}{4}\iiint\frac{1}{2}m_v\left(c_v'^2-c_v^2\right)(1-\psi_{\varepsilon v})\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv$$
$$=\frac{1}{4}\int_0^\infty n_v\int_0^\infty n_\varepsilon g_{\varepsilon v}\frac{\sigma_{\varepsilon v}^2}{4}\iiint\left(m_v c_v'^2-m_v c_v^2+m_\varepsilon c_\varepsilon'^2-m_\varepsilon c_\varepsilon^2\right)(1-\psi_{\varepsilon v})\lambda_v\lambda_\varepsilon(\mathbf{C}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv \quad (35)$$
$$=\int_0^\infty n_v\int_0^\infty n_\varepsilon(1-\psi_{\varepsilon v})g_{\varepsilon v}\sigma_{\varepsilon v}^2\left(e_{\varepsilon v}^2-1\right)\left[\frac{8\pi\theta_s^3(m_\varepsilon+m_v)}{m_\varepsilon m_v}\right]^{\frac{1}{2}}d\varepsilon dv.$$

As can be seen in (35), because $e_{\varepsilon v} \le 1$ and $\psi_{\varepsilon v} \le 1$, then $\Delta E_c \le 0$.

The second term of the right hand side of (16) for $\phi_v = m_v c_v^{\,2}/2$ with also the integration over v becomes

$$\begin{aligned}
&\int_0^\infty \int_0^v \frac{1}{2M_{v-\varepsilon}^{\,2}} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\,2}}{4} \iiint \frac{1}{2} m_v c_v^{\,2} \lambda_{v-\varepsilon} \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon v} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv \\
&= \int_0^\infty \int_0^v \frac{1}{2} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\,2}}{4} \iiint \frac{1}{2} (m_{v-\varepsilon} + m_\varepsilon) c_v^{\,2} \lambda_{v-\varepsilon} \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,v-\varepsilon} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_{v-\varepsilon} d\varepsilon dv \\
&= \int_0^\infty \int_0^v \frac{1}{2} \psi_{\varepsilon,v-\varepsilon} n_{v-\varepsilon} n_\varepsilon g_{\varepsilon,v-\varepsilon} \frac{\sigma_{\varepsilon,v-\varepsilon}^{\,2}}{4} \times \\
&\quad \iiint \frac{1}{2} \Big(M_{v-\varepsilon} c_{v-\varepsilon}^{\,2} + M_\varepsilon c_\varepsilon^{\,2} + \frac{2 m_{v-\varepsilon} m_\varepsilon c_{v-\varepsilon} c_\varepsilon}{m_{v-\varepsilon} + m_\varepsilon}\Big) \lambda_{v-\varepsilon} \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,v-\varepsilon} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_{v-\varepsilon} d\varepsilon dv \\
&= \int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,\zeta} n_\zeta n_\varepsilon g_{\varepsilon,\zeta} \frac{\sigma_{\varepsilon,\zeta}^{\,2}}{4} \iiint \frac{1}{2} (M_\zeta c_\zeta^{\,2} + M_\varepsilon c_\varepsilon^{\,2}) \lambda_\zeta \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,\zeta} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_\zeta d\varepsilon d\zeta \\
&+ \int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,\zeta} n_\zeta n_\varepsilon g_{\varepsilon,\zeta} \frac{\sigma_{\varepsilon,\zeta}^{\,2}}{4} \iiint \frac{1}{2} \frac{2 m_\zeta m_\varepsilon c_\zeta c_\varepsilon}{m_\zeta + m_\varepsilon} \lambda_\zeta \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,\zeta} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_\zeta d\varepsilon d\zeta ,
\end{aligned} \tag{36}$$

where $v - \varepsilon = \zeta$. As $M_\zeta + M_\varepsilon = 1$, in (36), this term $\int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,\zeta} n_\zeta n_\varepsilon g_{\varepsilon,\zeta} \frac{\sigma_{\varepsilon,\zeta}^{\,2}}{4} \times$ $\iiint \frac{1}{2} (M_\zeta c_\zeta^{\,2} + M_\varepsilon c_\varepsilon^{\,2}) \lambda_\zeta \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,\zeta} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_\zeta d\varepsilon d\zeta$ is cancelled with half of the integrated third term of the right hand side of (16) over v with $\phi_v = m_v c_v^{\,2}/2$, the kinetic energy dissipation due to aggregation, ΔE_a, is then written as

$$\begin{aligned}
\Delta E_a = &\int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,\zeta} n_\zeta n_\varepsilon g_{\varepsilon,\zeta} \frac{\sigma_{\varepsilon,\zeta}^{\,2}}{4} \iiint \frac{1}{2} \frac{2 m_\zeta m_\varepsilon c_\zeta c_\varepsilon}{m_\zeta + m_\varepsilon} \lambda_\zeta \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,\zeta} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_\zeta d\varepsilon d\zeta \\
&- \int_0^\infty \int_0^\infty \frac{1}{2} \psi_{\varepsilon,v} n_v n_\varepsilon g_{\varepsilon,v} \frac{\sigma_{\varepsilon,v}^{\,2}}{4} \iiint \frac{1}{2} m_v c_v^{\,2} \lambda_v \lambda_\varepsilon \left(\mathbf{C}_{\varepsilon,v} \cdot \mathbf{k}\right) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v d\varepsilon dv.
\end{aligned} \tag{37}$$

It is worth pointing out in (37), as the integrations over all the size and velocity domains are being made, v, ε and ζ then become in-distinguishable particles, thus, $m_v c_v^{\,2}$ can be understood as $\frac{m_\zeta c_\zeta^{\,2}}{m_\zeta + m_\varepsilon} + \frac{m_\varepsilon c_\varepsilon^{\,2}}{m_\zeta + m_\varepsilon}$, then $\Delta E_a \le 0$. With $\mathbf{c}_\zeta = \mathbf{C}_\zeta + \mathbf{u}_s$, $\mathbf{c}_\varepsilon = \mathbf{C}_\varepsilon + \mathbf{u}_s$, $\mathbf{C}_\zeta = \mathbf{C}_c - M_\varepsilon \mathbf{c}_{\varepsilon\zeta}$ and $\mathbf{C}_\varepsilon = \mathbf{C}_c + M_\zeta \mathbf{c}_{\varepsilon\zeta}$, after the integrations over Ω and $\mathbf{C}$ carried out, (37) is

$$\Delta E_a = \int_0^\infty \int_0^\infty \psi_{\varepsilon,v} n_v n_\varepsilon g_{\varepsilon,v} \sigma_{\varepsilon,v}{}^2 \beta d\varepsilon dv, \tag{38}$$

where

$$\beta = \frac{1}{2(m_\varepsilon + m_v)}\sqrt{\frac{2\pi}{m_\varepsilon m_v}}\left\{\left[\frac{3\theta_s^{\frac{3}{2}}}{\sqrt{m_\varepsilon + m_v}} + \theta_s^{\frac{1}{2}}\sqrt{m_\varepsilon + m_v}\,u_s{}^2 + \frac{4\sqrt{2}\theta_s(\mathbf{u}_s \cdot \mathbf{k})}{\sqrt{\pi}}\right](m_\varepsilon - m_v)m_v \right.$$
$$\left. + \frac{12\theta_s^{\frac{3}{2}} m_v^{\frac{3}{2}} m_\varepsilon}{\sqrt{m_\varepsilon + m_v}} + \frac{8\theta_s^{\frac{3}{2}} m_\varepsilon (m_v - m_\varepsilon)}{\sqrt{(m_\varepsilon + m_v)}} + \frac{3\sqrt{2\pi}}{2}\theta_s m_v^{\frac{3}{2}} m_\varepsilon (\mathbf{u}_s \cdot \mathbf{k})\right\}. \tag{39}$$

The total kinetic energy dissipation due to inelastic collisions and aggregations thus becomes

$$\Delta E_d = \Delta E_c + \Delta E_a = \int_0^\infty \int_0^\infty n_v n_\varepsilon g_{\varepsilon,v} \sigma_{\varepsilon,v}{}^2 \left[(1 - \psi_{\varepsilon,v})(e_{\varepsilon v}{}^2 - 1)\alpha + \psi_{\varepsilon,v}\beta\right] d\varepsilon dv, \tag{40}$$

where $\alpha = \left[\frac{8\pi\theta_s{}^3(m_\varepsilon + m_v)}{m_\varepsilon m_v}\right]^{\frac{1}{2}}$. The mixture granular energy equation can then be expressed

$$\frac{3}{2}\left[\frac{\partial(N\theta_s)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (N\theta_s \mathbf{u}_s)\right] + \frac{1}{2}\left[\frac{\partial(\varepsilon_s \rho_s u_s{}^2)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\varepsilon_s \rho_s u_s{}^2 \mathbf{u}_s)\right]$$
$$+ \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{q}_s + P_s \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{u}_s + \bar{\bar{\boldsymbol{\tau}}}_s : \frac{\partial}{\partial \mathbf{r}} \mathbf{u}_s - \varepsilon_s \rho_s \langle (\mathbf{C}_v + \mathbf{u}_s) \cdot \mathbf{F}_v \rangle = \Delta E_d. \tag{41}$$

In this section, because the actual velocity $\mathbf{c}_v$ is used and the completely inelastic collisions are taken into account in the derivation of the kinetic transport equations, the effects of the bulk velocity $\mathbf{u}_s$ and the collision success factor on those transport properties particularly on those of the individual particle phases specified by their sizes are detailed. It can be seen in (21), (23a), (25), (33) and (41), by letting $\psi_{\varepsilon v} = 0$, those equation are then relaxed to the traditional ones in the classical kinetic theory of granular flow[24, 25, 27].

The Collision Frequency, Relative Velocity Distribution Function and Collision Success Factor

It should be mentioned that the constitutive relations[7, 24, 27], which are the properties of particles to do with the products of their velocities, for instance, the mathematical expressions for the normal pressure, stress tensor and heat flux, and the coefficients calculated in those products such as the shear and bulk viscosities and the granular heat conductivity, are not affected by the aggregation of particles thus remain the same in their forms and can be found in those references listed above. However, it must be pointed out that in granular flow systems where the aggregation of particles takes place, the values of those particle size related coefficients such as viscosities and conductivity are expected to change over time since the particle size is enlarged over time.

The collision frequency measures the number of collisions occurring to a particle in a unit time and a unit spatial volume. The number of collisions between particles v and ε , $N_{\varepsilon v}$, used to count the number of the collisions between the two kinds of particles occurring in a unit time and spatial volume, is expressed as

$$N_{\varepsilon v} = n_v v n_\varepsilon \varepsilon g_{\varepsilon v} \frac{{\sigma_{\varepsilon v}}^2}{4} \iiint \lambda_v \lambda_\varepsilon (\mathbf{C}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{C}_\varepsilon d\mathbf{C}_v , \quad (42a)$$

after the integrations carried out, it then becomes

$$N_{\varepsilon v} = N_v N_\varepsilon g_{\varepsilon v} {\sigma_{\varepsilon v}}^2 \left[\frac{8\pi\theta_s (m_v + m_\varepsilon)}{m_v m_\varepsilon} \right]^{\frac{1}{2}}, \quad (42b)$$

where $N_v = \mathrm{n}_v v$ and $N_\varepsilon = \mathrm{n}_\varepsilon \varepsilon$ are the numbers of particles with size v and ε per unit spatial volume, respectively. It should be noted that in (42a), for mono-dispersed systems, the right hand side of the expression should be multiplied by ½ in order to eliminate double counting. The collision frequencies of a particle v to all particles ε and to all other particles can thus be given by (43a) and (43b), respectively.

$$F_{\varepsilon v} = \frac{N_{\varepsilon v}}{N_v} = N_\varepsilon g_{\varepsilon v} {\sigma_{\varepsilon v}}^2 \left[\frac{8\pi\theta_s (m_v + m_\varepsilon)}{m_v m_\varepsilon} \right]^{\frac{1}{2}}, \quad (43a)$$

$$F_v = \int_0^\infty n_\varepsilon g_{\varepsilon v} {\sigma_{\varepsilon v}}^2 \left[\frac{8\pi\theta_s (m_v + m_\varepsilon)}{m_v m_\varepsilon} \right]^{\frac{1}{2}} d\varepsilon . \quad (43b)$$

The collision success factor, $\psi_{\varepsilon v}$, was introduced to quantify the fraction of the completely inelastic collisions between particles v and ε such as that seen in (A3). It is used to calculate the number of the collisions between the two kinds of particles that leads to aggregation. From a more fundamental point of view, for a single collision between a particle v and a particle ε , $\psi_{\varepsilon v}$ gives the probability of this collision to succeed for an aggregation event.

In order to obtain the analytical expression of $\psi_{\varepsilon v}$, we now consider the collisions between particles v and ε, $N_{\varepsilon v}$, as expressed in (42a); owing to $d\mathbf{C}_v d\mathbf{C}_\varepsilon = d\mathbf{C}_c d\mathbf{C}_{\varepsilon v}$, after the integration over the mass centre velocity $\mathbf{C}_c$ carried out, (42a) is then transformed into

$$N_{\varepsilon v} = N_v N_\varepsilon g_{\varepsilon v} \sigma_{\varepsilon v}{}^2 (2\pi)^2 \left[\frac{m_\varepsilon m_v}{2\pi (m_\varepsilon + m_v)\theta_s}\right]^{\frac{3}{2}} \int_0^\infty C_{\varepsilon v}{}^3 \exp\left[-\frac{m_\varepsilon m_v C_{\varepsilon v}{}^2}{2(m_\varepsilon + m_v)\theta_s}\right] dC_{\varepsilon v} . \quad (44)$$

So $dN_{\varepsilon v} / dC_{\varepsilon v}$ is the relative velocity distribution function, which is a density function that interprets the collisions between particles v and ε per unit spatial volume and time by the relative fluctuation velocity $\mathbf{C}_{\varepsilon v}$ between the two kinds of particles

$$\frac{dN_{\varepsilon v}}{dC_{\varepsilon v}} = N_v N_\varepsilon g_{\varepsilon v} \sigma_{\varepsilon v}{}^2 (2\pi)^2 \left[\frac{m_\varepsilon m_v}{2\pi (m_\varepsilon + m_v)\theta_s}\right]^{\frac{3}{2}} C_{\varepsilon v}{}^3 \exp\left[-\frac{m_\varepsilon m_v C_{\varepsilon v}{}^2}{2(m_\varepsilon + m_v)\theta_s}\right]. \quad (45)$$

The normalised relative velocity distribution function $f_{\varepsilon v} = dN_{\varepsilon v} /(N_{\varepsilon v} dC_{\varepsilon v})$ combined with (42b) is

$$\begin{aligned} f_{\varepsilon v} &= \frac{N_v N_\varepsilon g_{\varepsilon v} \sigma_{\varepsilon v}{}^2 (2\pi)^2 \left[\frac{m_\varepsilon m_v}{2\pi (m_\varepsilon + m_v)\theta_s}\right]^{\frac{3}{2}} C_{\varepsilon v}{}^3 \exp\left[-\frac{m_\varepsilon m_v C_{\varepsilon v}{}^2}{2(m_\varepsilon + m_v)\theta_s}\right]}{N_{\varepsilon v}} \\ &= \frac{1}{2}\left[\frac{m_\varepsilon m_v}{(m_\varepsilon + m_v)\theta_s}\right]^2 \exp\left[-\frac{m_\varepsilon m_v C_{\varepsilon v}{}^2}{2(m_\varepsilon + m_v)\theta_s}\right] C_{\varepsilon v}{}^3 . \end{aligned} \quad (46)$$

According to Assumption 4, the collision success factor $\psi_{\varepsilon v}$ can thus be obtained by integrating the normalised relative velocity distribution function $f_{\varepsilon v}$ over the domain of $C_{\varepsilon v}$, $[0, C_{\varepsilon v}{}^*)$; here $C_{\varepsilon v}{}^*$ is the magnitude of the critical relative collision velocity $\mathbf{C}_{\varepsilon v}{}^*$, then

$$\psi_{\varepsilon v} = \int_0^{C_{\varepsilon v}{}^*} f_{\varepsilon v} dC_{\varepsilon v} = 1 - \left[1 + \frac{m_\varepsilon m_v C_{\varepsilon v}{}^{*2}}{2(m_\varepsilon + m_v)\theta_s}\right] \exp\left[-\frac{m_\varepsilon m_v C_{\varepsilon v}{}^{*2}}{2(m_\varepsilon + m_v)\theta_s}\right]. \quad (47)$$

(47) has clearly shown the dependence of the success factor on particle sizes (as the masses of particles v and ε, m_ε and m_v, respectively, can be converted into their sizes) not only upon the

critical relative collision velocity and the mixture granular energy θ_s of all particles in the system. (47) also implies if $\psi_{\varepsilon v}$ and θ_s are known, it can be used to calculate the critical relative collision velocity – an import attribute in characterising the collisions of aggregating particles.

Defining a critical relative collision granular energy function, $\theta_{\varepsilon v}{}^{*} = \frac{m_\varepsilon m_v C_{\varepsilon v}{}^{*2}}{2(m_\varepsilon + m_v)}$, (47) becomes

$$\psi_{\varepsilon v} = 1 - \left(1 + \frac{\theta_{\varepsilon v}{}^{*}}{\theta_s}\right)\exp\left(-\frac{\theta_{\varepsilon v}{}^{*}}{\theta_s}\right). \tag{48}$$

Since $\theta_{\varepsilon v}{}^{*}$ is the kinetic energy property of an individual collision and θ_s is the mixture granular energy of all the particles in a granular flow system, (48) interprets that both the individual collision and the system's ensemble average kinetic energy characteristics determine the success of an aggregation. Figure 1 illustrates the change of $\psi_{\varepsilon v}$ in $\theta_{\varepsilon v}{}^{*}/\theta_s$.

(Figure 1)

From Figure 1, it can be seen when the value of $\theta_{\varepsilon v}{}^{*}/\theta_s$ reaches around 3.0, the dramatic increase (to nearly 0.8) of $\psi_{\varepsilon v}$ starts changing to a rather slow pace, which indicates that efforts on increasing the value of $\theta_{\varepsilon v}{}^{*}/\theta_s$ to increase $\psi_{\varepsilon v}$ will then becomes almost no efficiency and not worth experimenting. This figure can provide such useful information to identify the range of $\psi_{\varepsilon v}$ in which its large value can be achieved with little effort on increasing the ratio of $\theta_{\varepsilon v}{}^{*}/\theta_s$.

When $\theta_{\varepsilon v}{}^{*}$ and θ_s are regarded as the mutually independent variables, a 3D plot of $\psi_{\varepsilon v}$ versus $\theta_{\varepsilon v}{}^{*}$ and θ_s is given in Figure 2.

(Figure 2)

The significance of Figure 2 is that it is able to point out the direction quantitatively to which the best match of $\theta_{\varepsilon v}{}^{*}$ and θ_s can give the most achievable $\psi_{\varepsilon v}$ value; for instance, in general as seen in this figure a large $\theta_{\varepsilon v}{}^{*}$ and a small θ_s would give a large $\psi_{\varepsilon v}$; however, if large value of $\theta_{\varepsilon v}{}^{*}$ cannot be achieved, it is still possible to obtain a large value of $\psi_{\varepsilon v}$ with a small value of θ_s

even the chance is slim but can still occur (indicated in the down-left corner but on the upper surface of Figure 2).

If for a system, aggregation is to be avoided, Figure 1 and 2 can give useful information for how the least value of $\psi_{\varepsilon v}$ can be obtained by changing the values of $\theta_{\varepsilon v}{}^{*}$ and θ_s.

It can also be suggested from Figure 1 and 2, since the collision success factor depends on the ratio of the critical relative collision granular energy to the mixture granular energy, under the condition that the flow of the granular particles can be maintained, the way to increase the efficiency of the successful aggregations is to increase the ratio by either reducing the turbulence of the granular flow system or increasing the critical velocity which for instance for a gas fluidised bed granulation system would be achieved by increasing the surface tension and viscosity of binders[44]. However, it may be worth pointing out that reducing system turbulence in order to increase the collision success factor should be taken cautiously as this may cause a system's momentum collapse (particles are not well suspended) thus particles may aggregate in a rather non-uniform way and their size distribution will not change in a gradually progressive fashion. The solution of the success factor suggests that, increasing the critical relative velocity, or, using the particles and binding materials resulting in higher critical velocity, and keeping a degree of system turbulence to maintain the momentum of the particles can help increase the successful collisions efficiently.

It is also worth mentioning that (48) has established a link between the fundamental understanding of successful particle collisions leading to aggregation and the engineering processes of particle size enlargement owing to aggregation. (48) provides a method to quantitatively control the growth of particle size in granular flow systems.

Since the normalised relative velocity distribution function $f_{\varepsilon v}$ is given by (46), it may be worth calculating the ensemble average relative velocity $\left\langle \mathbf{C}_{\varepsilon v} \right\rangle$ that measures the intensity of a collision in an overall perspective.

$$\left\langle \mathbf{C}_{\varepsilon v} \right\rangle = \int_0^\infty \mathbf{C}_{\varepsilon v} f_{\varepsilon v} dC_{\varepsilon v} = \left[\frac{72\pi \left(m_\varepsilon + m_v \right) \theta_s}{m_\varepsilon m_v} \right]^{\frac{1}{2}} \mathbf{k} . \tag{49}$$

It is seen in (49), the average collision intensity is related directly to the mixture granular energy of the granular flow system and the masses of the colliding particles.

Concluding Remarks

The work presented in this paper has given a mathematical description for the aggregation of particles in granular flow. It is seen from those derived kinetic transport equations that, for a flow system where aggregation of the particles takes place, those conservative equations were shown to be able to describe the balances of the population, momentum and kinetic energy of the particles characterised by their size and velocity. In particular the number continuity equation is transformed into the typical population balance equation in the form of aggregation and growth; while the momentum and kinetic energy equations for the particles of the individual phases have shown the significance of the aggregation depending on the value of the collision success factor. It is expected that solving the three types of conservative equations together would give a complete prediction to the distributions of particle velocity, kinetic energy particularly to the size of particles for the systems where the motion of particles in spatial coordinates, i.e., convection (segregation), and in their own sizes due to aggregation, are taking place simultaneously.

The dissipation of kinetic energy due to aggregations is expected to be highly related to the collision success factor, the mixture velocity and granular energy of all particles. Moreover, for a single particle phase, it also depends on the sizes of the colliding particles.

The solution of collision success factor gives the probability of a collision to succeed for an aggregation from the kinetic energy point of view although the critical relative collision velocity needs further research to detail its dependency on processing materials and conditions. It is still true to say that the success factor can provide a quantitative way to practically control the coefficient of particle collisions that result in aggregation. It can thus be used to assess the efficiency of the process of particle aggregation in granular flow systems.

It needs to be mentioned that particle aggregation does not affect the mathematical forms of the constitutive relations; however, when the probability density function is extended to the higher orders of the Chapman-Enskog approximation, the corresponding terms associated with the integration of the velocity distribution function in the kinetic transport equations should also be re-evaluated particularly for the kinetic energy dissipation and the collision success factor.

Finally, it also needs to be pointed out that a validation of this theory is needed, which is presented in a subsequent paper on the application of the kinetic theory of aggregation to a gas fluidised bed granulation system.

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Notations

Roman symbols

c	magnitude of actual velocity **c**	m s^{-1}
C	magnitude of fluctuation velocity **C**	m s^{-1}
e	restitution coefficient in the collision between particles	(-)
f	velocity-size distribution function	s^{3} m^{-9}
F	collision frequency	s^{-1}
g	radial distribution function	(-)
m	mass of a particle	kg
M	mass ratio of a particle to the total mass of the pair of collding particles	(-)
n	number density of particles	m^{-6}
N	total number of particles per unit volume	m^{-3}
$N_{\varepsilon v}$	total number of collisions between particles ε and v per unit time and volume	m^{-3} s^{-1}
P	normal pressure of particles	Pa m^{-3}
r	collision rate of particles	s^{4} m^{-10}
t	time	s

v	the size of individual particles in volume	m^3
Vectors		
c	actual velocity of particles	$m\ s^{-1}$
C	fluctuation velocity of particles	$m\ s^{-1}$
F	the external force	N
G	growth rate of particles in volume size	$m^3\ s^{-1}$
k	unit vector	(-)
q	heat flux	$W\ m^{-5}$
r	spatial position vector	m
u	ensemble average velocity	$m\ s^{-1}$
w	number density weighted diffusion velocity of particles	$m\ s^{-1}$
Tensors		
$\bar{\bar{\mathbf{I}}}$	unit tensor	(-)
$\bar{\bar{\boldsymbol{\tau}}}$	stress tensor	$Pa\ m^{-3}$
Greek symbols		
Δ	change of properties	
ε	the size of individual particles in volume	m^3
ϕ	property of particles in terms of their velocity	
φ	the filling angle in spherical coordinates	rad
λ	normalized velocity-size distribution function of particles	$s\ m^{-4}$
Ω	solid angle	rad
ψ	collision success factor	(-)
ρ	density of particles	$kg\ m^{-3}$
σ	inter-distance of two colliding particles	m
θ	granular energy of particles	J
ω	the filling angles in spherical coordinates	rad

χ	Taylor's expansion	
ξ	property of particles by volume size	
ζ	dummy variable for $v - \varepsilon$	m^3

Superscripts

'	reverse collision
*	critical property

Subscripts

s	ensemble particles
v	the size of individual particles in volume
ε	the size of individual particles in volume
εv	collisions between particles ε and v

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Appendix

The detailed derivation of the collision rate is presented in the work of Liu[44], in the following only a concise version of such a derivation is given.

Consider two kinds of particles with sizes v and ε respectively having collisions based on the mechanism of binary collision[1] (Assumption 2) in differential elements $d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt$, the rate of the forward collisions, which results in the decrease of the number of particles characterised by $\mathbf{c}_v$, is expressed in (A1). This expression also takes into the sizes of the colliding particles, i.e., if a particle v is situated at position $\mathbf{r}$ then the colliding particle ε must be at $\mathbf{r}+\sigma_{\varepsilon v}\mathbf{k}$.

$$f_v f_\varepsilon(\mathbf{r}+\sigma_{\varepsilon v}\mathbf{k}) g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k}) d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt, \tag{A1}$$

Using Taylor's expansion for $f_\varepsilon(\mathbf{r}+\sigma_{\varepsilon v}\mathbf{k})$, (A1) becomes

$$f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k}) d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt, \tag{A2}$$

where $\chi_{\varepsilon v} = \left[1+\sum_m \frac{1}{m!}\left(\sigma_{\varepsilon v}\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{r}}\right)^m f_\varepsilon\right]$.

According to Assumption 1 that some fraction $\psi_{\varepsilon v}$ of the collisions occurred in a completely inelastic way that leads to aggregation, (A2) can then be transformed into

$$\begin{aligned}&(1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k}) d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt\\ &+\psi_{\varepsilon v} f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k}) d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt.\end{aligned} \tag{A3}$$

Similarly, the collisions between particles v and ε with reverse velocities $\mathbf{c}_v'$ and $\mathbf{c}_\varepsilon'$ respectively resulting in the increase of the number of particles v characterised by $\mathbf{c}_v$, taking into account the completely inelastic collisions, can be expressed

$$(1-\psi_{\varepsilon v}') f_v' f_\varepsilon' \chi_{\varepsilon v}' g_{\varepsilon v}' \frac{\sigma_{\varepsilon v}'^2}{4}(\mathbf{c}_{\varepsilon v}'\cdot\mathbf{k}') d\Omega' d\mathbf{c}_v' dv d\mathbf{c}_\varepsilon' d\varepsilon d\mathbf{r} dt, \tag{A4}$$

where the symbols with "′" refer to the properties of the reverse collisions.

We also have the following relations

$$d\Omega' = d\Omega, \sigma_{\varepsilon v}' = \sigma_{\varepsilon v}, \mathbf{c}_{\varepsilon v}' = -e_{\varepsilon v}\mathbf{c}_{\varepsilon v}, \mathbf{k}' = \text{-}\mathbf{k},$$
$$\mathbf{c}_v' = \mathbf{c}_v + M_\varepsilon(1+e_{\varepsilon v})\mathbf{c}_{\varepsilon v}, \mathbf{c}_\varepsilon' = \mathbf{c}_\varepsilon - M_v(1+e_{\varepsilon v})\mathbf{c}_{\varepsilon v}, \tag{A5}$$
$$d\mathbf{c}_v' d\mathbf{c}_\varepsilon' = \left|\frac{\partial(\mathbf{c}_v', \mathbf{c}_\varepsilon')}{\partial(\mathbf{c}_v, \mathbf{c}_\varepsilon)}\right| d\mathbf{c}_v d\mathbf{c}_\varepsilon = e_{\varepsilon v}.$$

Subtracting (A3) from (A4) yields the net increase of the number of particles v characterised by $\mathbf{c}_v$. Also according to the relations in (A5), we have

$$\begin{aligned}&\left[e_{\varepsilon v}^2(1-\psi_{\varepsilon v}')f_v' f_\varepsilon' \chi_{\varepsilon v}' g_{\varepsilon v}' - (1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v}\right]\frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt \\ &-\psi_{\varepsilon v} f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v}\frac{\sigma_{\varepsilon v}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt.\end{aligned} \tag{A6}$$

It is clear that the completely inelastic collisions between particles $v-\varepsilon$ and ε can also result in the net increase of the number of particles v. This is given by

$$\frac{1}{2}\psi_{\varepsilon,v-\varepsilon} f_{v-\varepsilon} f_\varepsilon \chi_{\varepsilon,v-\varepsilon} g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}^2}{4}(\mathbf{c}_{\varepsilon,v-\varepsilon}\cdot\mathbf{k})d\Omega d\mathbf{c}_{v-\varepsilon} dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt, \tag{A7}$$

where ½ eliminates the double counting of the collisions, and, ε ranges from 0 to v. It is worth pointing out that there is no reverse collisions between particles $v-\varepsilon$ and ε contributing to the increase of the number of particles v as (A7) is only concerned with the size characteristic of $f_{v-\varepsilon}$ and f_ε. (A7) can also be transformed into

$$\frac{1}{2M_{v-\varepsilon}^2}\psi_{\varepsilon,v-\varepsilon} f_{v-\varepsilon} f_\varepsilon \chi_{\varepsilon,v-\varepsilon} g_{\varepsilon,v-\varepsilon}\frac{\sigma_{\varepsilon,v-\varepsilon}^2}{4}(\mathbf{c}_{\varepsilon v}\cdot\mathbf{k})d\Omega d\mathbf{c}_v dv d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{r} dt. \tag{A8}$$

This is because

$$\mathbf{c}_v = M_\varepsilon\mathbf{c}_\varepsilon + M_{v-\varepsilon}\mathbf{c}_{v-\varepsilon}, \mathbf{c}_{v-\varepsilon} = \mathbf{c}_v - M_\varepsilon\mathbf{c}_{\varepsilon,v-\varepsilon}, \mathbf{c}_\varepsilon = \mathbf{c}_v + M_{v-\varepsilon}\mathbf{c}_{\varepsilon,v-\varepsilon},$$
$$\mathbf{c}_{\varepsilon,v-\varepsilon} = \frac{\mathbf{c}_{\varepsilon v}}{M_{v-\varepsilon}}, d(v-\varepsilon) = dv, d\mathbf{c}_{v-\varepsilon} d\mathbf{c}_\varepsilon = \left|\frac{\partial(\mathbf{c}_{v-\varepsilon}, \mathbf{c}_\varepsilon)}{\partial(\mathbf{c}_v, \mathbf{c}_\varepsilon)}\right| d\mathbf{c}_v d\mathbf{c}_\varepsilon = \frac{1}{M_{v-\varepsilon}} d\mathbf{c}_v d\mathbf{c}_\varepsilon, \tag{A9}$$

where $\mathbf{c}_v$ is the mass centre velocity of particles $v-\varepsilon$ and ε, i.e., the velocity of particles v.

Adding (A8) into (A6) yields the differential form of the number of collisions occurring to particles v to give the net increase of the number of particles v in terms of their size v and velocity $\mathbf{c}_v$ characteristics. With the integrations over the domains of Ω, $\mathbf{c}_\varepsilon$ and ε, the total number of collisions occurring to particles v per unit time and spatial volume is obtained

$$
\begin{aligned}
r_v = & \iiint \left[e_{\varepsilon v}{}^2 (1-\psi_{\varepsilon v}{}') f_v{}' f_\varepsilon{}' \chi_{\varepsilon v}{}' g_{\varepsilon v}{}' - (1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \right] \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon \\
& + \int_0^v \iint \frac{1}{2M_{v-\varepsilon}{}^2} \psi_{\varepsilon, v-\varepsilon} f_{v-\varepsilon} f_\varepsilon \chi_{\varepsilon, v-\varepsilon} g_{\varepsilon, v-\varepsilon} \frac{\sigma_{\varepsilon, v-\varepsilon}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon \qquad \text{(A10)} \\
& - \iiint \psi_{\varepsilon v} f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon .
\end{aligned}
$$

As can be seen from (A10), the first term of the right hand side is the net birth rate contributing to the velocity characteristic of f_v; the second and third terms together give the net birth rate of particles contributing to the size characteristic of f_v.

For a property ϕ_v of particles v in terms of their velocity $\mathbf{c}_v$, the change of the property due to the collisions occurring to particles v is expressed as $\int \phi_v r_v d\mathbf{c}_v$; therefore, according to (A10), the transport equation (11a) is obtained

$$
\begin{aligned}
& \frac{\partial (n_v \langle \phi_v \rangle)}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot n_v \langle \phi_v \mathbf{c}_v \rangle - n_v \left\langle \frac{\partial \phi_v}{\partial t} \right\rangle - n_v \left\langle \frac{\partial \phi_v}{\partial \mathbf{r}} \cdot \mathbf{c}_v \right\rangle - n_v \left\langle \frac{\partial \phi_v}{\partial \mathbf{c}_v} \cdot \frac{\mathbf{F}_v}{m_v} \right\rangle + \frac{\partial}{\partial v \mathbf{k}} \cdot n_v \langle \phi_v \mathbf{G}_v \rangle - \left\langle \frac{\partial \phi_v}{\partial v \mathbf{k}} \right\rangle \cdot n_v \mathbf{G}_v \\
& = \int \iiint (\phi_v{}' - \phi_v)(1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\varepsilon d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v \\
& \quad + \iiint \phi_v \Bigg[\int_0^v \frac{1}{2M_{v-\varepsilon}{}^2} \psi_{\varepsilon, v-\varepsilon} f_{v-\varepsilon} f_\varepsilon \chi_{\varepsilon, v-\varepsilon} g_{\varepsilon, v-\varepsilon} \frac{\sigma_{\varepsilon, v-\varepsilon}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\varepsilon \qquad \text{(A11)} \\
& \qquad - \int_0^\infty \psi_{\varepsilon v} f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\varepsilon \Bigg] d\Omega d\mathbf{c}_\varepsilon d\mathbf{c}_v ,
\end{aligned}
$$

where the first term on the right hand side of (A11) is gained due to

$$
\begin{aligned}
& \int \iiint \phi_v e_{\varepsilon v}{}^2 (1-\psi_{\varepsilon v}{}') f_v{}' f_\varepsilon{}' \chi_{\varepsilon v}{}' g_{\varepsilon v}{}' \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{c}_v \\
& = \int \iiint \phi_v (1-\psi_{\varepsilon v}{}') f_v{}' f_\varepsilon{}' \chi_{\varepsilon v}{}' g_{\varepsilon v}{}' \frac{\sigma_{\varepsilon v}{}'^2}{4} (\mathbf{c}_{\varepsilon v}{}' \cdot \mathbf{k}') d\Omega' d\mathbf{c}_\varepsilon{}' d\varepsilon d\mathbf{c}_v{}' \qquad \text{(A12)} \\
& = \int \iiint \phi_v{}' (1-\psi_{\varepsilon v}) f_v f_\varepsilon \chi_{\varepsilon v} g_{\varepsilon v} \frac{\sigma_{\varepsilon v}{}^2}{4} (\mathbf{c}_{\varepsilon v} \cdot \mathbf{k}) d\Omega d\mathbf{c}_\varepsilon d\varepsilon d\mathbf{c}_v ,
\end{aligned}
$$

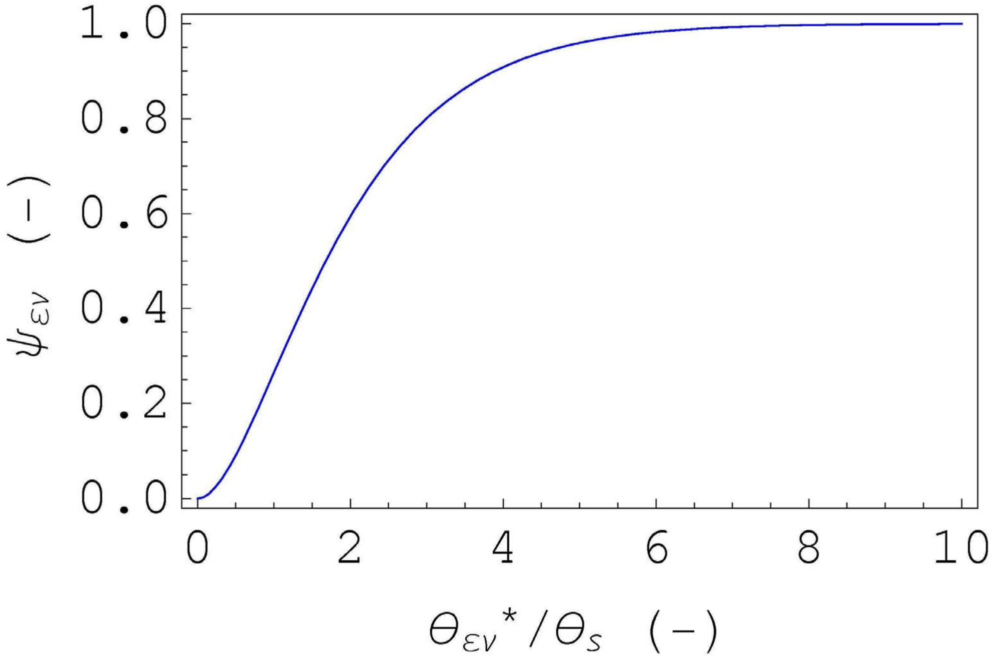
where $\phi_v{}'$ is the property of particles v after collisions and is the function of variables $(\Omega', \mathbf{c}_\varepsilon{}', \mathbf{c}_v{}')$.

(A12) can be understood that ϕ_v is being transported by the reverse collisions occurring to particles v. Since every reverse collision must corresponds to a forward collision, the properties with variable groups $(\Omega', \mathbf{c}_\varepsilon{}', \mathbf{c}_v{}')$ and $(\Omega, \mathbf{c}_\varepsilon, \mathbf{c}_v)$ can be exchanged[7] also $g_{\varepsilon v} = g_{\varepsilon v}{}'$ as the radial distribution function is considered to relate to the volume fraction of all particles only[7, 9, 10, 58].

Figure Captions

Figure 1. Dependence of $\psi_{\varepsilon\nu}$ on $\theta_{\varepsilon\nu}{}^{*}/\theta_{s}$.

Figure 2. Dependence of $\psi_{\varepsilon\nu}$ on $\theta_{\varepsilon\nu}{}^{*}$ and θ_{s}.



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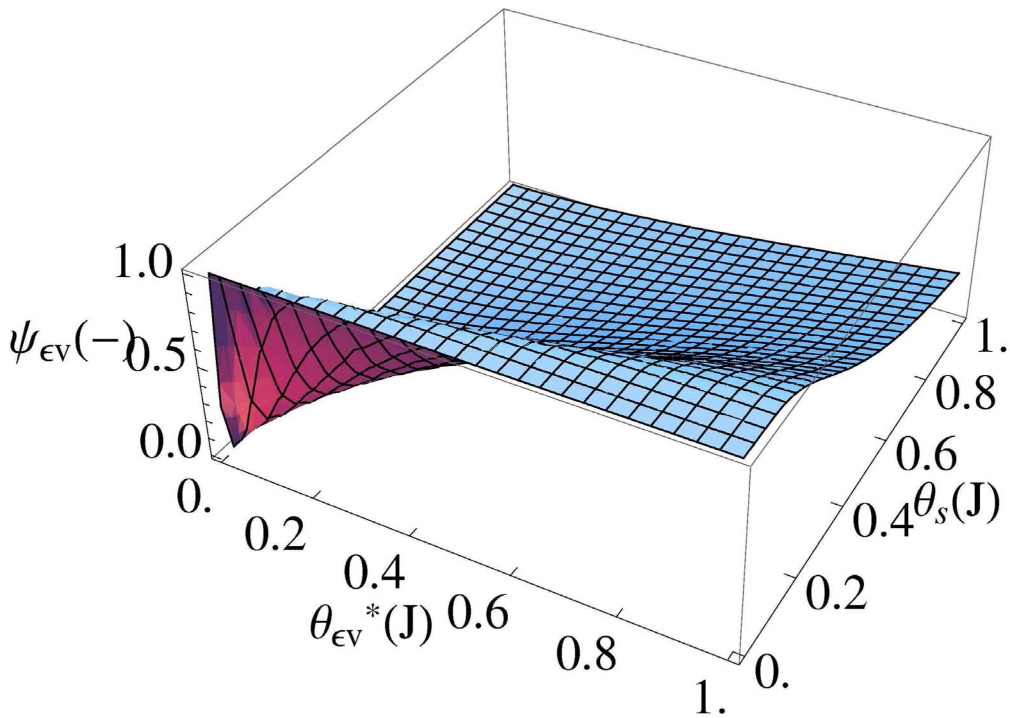

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