Reeks MW. (2021) [The Development and Application of a Kinetic Theory for Modeling Dispersed Particle Flows](#). *Journal of Fluids Engineering*, 143(8), 080803

Copyright:

Copyright © 2021 by ASME. Distributed under the [Creative Commons Attribution License](#) (CC BY).

DOI link to article:

<https://doi.org/10.1115/1.4051289>

Date deposited:

08/10/2021

This work is licensed under a [Creative Commons Attribution 4.0 International License](#)

The Development and Application of a Kinetic Theory for Modeling Dispersed Particle Flows

Michael W. Reeks

School of Engineering,
Newcastle University,
Newcastle upon Tyne NE1 7RU, UK
e-mail: mike.reeks@ncl.ac.uk

This Freeman Scholar article reviews the formulation and application of a kinetic theory for modeling the transport and dispersion of small particles in turbulent gas-flows. The theory has been developed and refined by numerous authors and now forms a rational basis for modeling complex particle laden flows. The formalism and methodology of this approach are discussed and the choice of closure of the kinetic equations involved ensures realizability and well posedness with exact closure for Gaussian carrier flow fields. The historical development is presented and how single-particle kinetic equations resolve the problem of closure of the transport equations for particle mass, momentum, and kinetic energy/stress (the so-called continuum equations) and the treatment of the dispersed phase as a fluid. The mass fluxes associated with the turbulent aerodynamic driving forces and interfacial stresses are shown to be both dispersive and convective in inhomogeneous turbulence with implications for the build-up of particles concentration in near wall turbulent boundary layers and particle pair concentration at small separation. It is shown how this approach deals with the natural wall boundary conditions for a flowing particle suspension and examples are given of partially absorbing surfaces with particle scattering and gravitational settling; how this approach has revealed the existence of contra gradient diffusion in a developing shear flow and the influence of the turbulence on gravitational settling (the Maxey effect). Particular consideration is given to the general problem of particle transport and deposition in turbulent boundary layers including particle resuspension. Finally, the application of a particle pair formulation for both monodisperse and bidisperse particle flows is reviewed where the differences between the two are compared through the influence of collisions on the particle continuum equations and the particle collision kernel for the clustering of particles and the degree of random uncorrelated motion (RUM) at the small scales of the turbulence. The inclusion of bidisperse particle suspensions implies the application to polydisperse flows and the evolution of particle size distribution. [DOI: 10.1115/1.4051289]

1 Introduction

Flows of small particles¹ and droplets suspended in a turbulent gas abound in nature from clouds, mists, and fogs to the long-range transport of fine dust released in desert storms and volcanic eruptions as well as the spread both locally and globally of infectious diseases. They control the weather and influence the climate. They play key roles in many industrial processes, from spray drying, pneumatic and slurry transport, fluidized beds to mixing and combustion processes. Modeling their behavior is therefore important in our control of the environment, in the design and improvement of industrial processes, and their impact upon our health and well-being. We need to know, for instance, how individual particles are dispersed by a turbulent carrier flow, how they interact with one another, and with the underlying flow either through an exchange of mass (evaporation or condensation), momentum (drag and lift), or by energy (heat transfer). An important feature of all these processes is that they are statistical—they

occur both randomly in space and time. So successful modeling of these processes means not only understanding the basic physics but how to average and in what way.

This review is about the development and application of a particular approach to modeling the transport of small particles in a turbulent flow analogous to the kinetic theory of gases. More specifically it's about the derivation and application of kinetic equations that are equivalent to the Maxwell–Boltzmann equation of classical kinetic theory (CKT). The particles themselves are not passive scalars, they do not follow the motion of the carrier flow, neither the mean flow nor the large or small scales of the underlying turbulence. The particles are what are frequently referred to as *inertial* particles. So this review is about the way these inertial particles respond collectively to the mean flow and the large and small scales of the turbulence and through their inertial response, how the turbulence disperses and mixes them, how it deposits them to surfaces exposed to the flow, and how it influences their collision process by bringing the individual particles closer together.

This kinetic-probability density function (pdf) approach (as it is often referred to) underwrites what is called a two-fluid model of a particle laden flow in which both particle and carrier phases are described by continuum equations that represent the conservation of mass, momentum, and energy in both phases within some elemental volume of the mixture. Computationally it is more efficient to use this two-fluid (Eulerian) approach than a particle tracking (Lagrangian) approach where individual particles are tracked

¹Particle equivalent diameters $\ll$ the Kolmogorov dissipating length scales of the turbulence. See the Maxey and Riley definition [1].

Based originally on the Freeman Scholar Lecture 2010 on 'the PDF approach for modelling dispersed flows and subsequently extended to the present time.

Contributed by the Fluids Engineering Division of ASME for publication in the JOURNAL OF FLUIDS ENGINEERING. Manuscript received September 27, 2020; final manuscript received May 1, 2021; published online xx xx, xxxx. Editor: Francine Battaglia.

through a turbulent carrier flow field by solving their individual equations of motion. However, since its inception, much controversy has surrounded the forms of the continuum equations themselves and the constitutive relations that are necessary to solve them [2]. For example, it has been traditionally assumed without any formal justification, that the particle phase behaves as a simple Newtonian fluid, implying that the particle kinetic (Reynolds) stresses are proportional to the mean symmetric rate of strain of the particle flow [3]. The constant of proportionality naturally defines a particle eddy viscosity that traditionally is related to that of the carrier flow in some empirical, ad hoc way. In addition, natural boundary conditions involving particle-wall interactions (determining, for instance, whether an individual particle bounces or is deposited at a wall) are impossible to deal with without imposing some artificial restraint on the particle mean flow and kinetic stresses near or at the wall. What has been lacking is a *rational*² approach in which the continuum equations are derived in a strictly formal way, in exact agreement with those in simple generic turbulent flows whilst providing a basic procedure and platform for dealing with complex flows with particle-wall interactions of a general nature.

Furthermore, over the last 15 years, there has been considerable interest in the way small particles interact with vortices [4] and most recently with the small scale structures in a turbulent flow [5] and how this leads to clustering and demixing of the particles and enhanced collision rates [6]. Whilst studies have identified numerous interesting features associated with this demixing process, e.g., the existence of caustics and singularities [7] in the particle concentration field and the occurrence of random uncorrelated motion (RUM) [8], these features are not an intrinsic part of a traditional two-fluid model and call for an alternative rational and more general approach.

This Freeman Scholar review is about the development and application of such an approach³ in which we trace its historical development over the last 30 years showing how it has resolved some of the outstanding problems in particle transport in turbulent flows and has been used to tackle practical engineering problems as diverse as emissions of radioactive aerosols from nuclear reactors and transport flasks [9–11] to the collision and precipitation of water droplets in clouds [12]. Indeed the approach provides a basic framework for formulating a whole range of industrial and environmental particulate flows [13]. In the process, the successes are highlighted, where it has added insight and understanding and where the challenges lie in the future.

The kinetic-pdf approach provides a general theoretical framework in which the behavior of a reacting turbulent dispersed flow of particles can be formulated. The formulation refers not only to the particle transport by the carrier phase but also to the particle-wall interactions that constitute the natural boundary conditions of the flow. So as required, the method can handle the physics of particle surface interactions in a way that is part of the underlying formulation. The approach is similar to the classical kinetic theory of gases in that the continuum equations and the associated constitutive relations of the dispersed phase can be derived in a strictly formal way from a master equation for the pdf (the kinetic equation) analogous to the Maxwell-Boltzmann equation. Indeed many of the methods and approximations in CKT are explicitly used. Throughout this review, we shall refer to it as the kinetic-pdf approach or simply the kinetic approach.

Two forms of the kinetic approach are currently in use and both approaches will be reviewed here, comparing and contrasting the two and indicating the conditions under which they become

identical. The first approach referred to here as the kinetic method (KM)⁴ is based on the traditional form of pdf used in classical kinetic theory for the particle position $\mathbf{x}$ and velocity $\mathbf{v}$ at time t and the second approach is based on a pdf associated with an additional phase space variable, namely, the carrier flows velocity encountered by a particle at $(\mathbf{x}, \mathbf{v})$ at time t . The second approach has been referred to as the generalized Langevin model (GLM) because the equations for the carrier flow are based on a generalized Langevin equation similar to the Langevin equation used in the study of Brownian motion and in more recent times used extensively by Pope and others to model turbulence [14] and turbulence related phenomena such as combustion [15] and atmospheric dispersion [16]. The use of such a GLM means that the process is realizable for which the kinetic equation is an exact statistical representation of the model.

It is shown how these two forms of the kinetic equation can be used to derive the continuum equations and constitutive relations for the dispersed phase as well as providing at the same time, forms for the momentum coupling between phases due to the turbulence. In either case, the approximations used to close the continuum equations are based on methods used in classical kinetic theory. An important part of the review will be to show how these methods reproduce exact results for dispersion in statistically stationary and homogeneous turbulence and in simple shear flows⁵ indicating in the latter that the forms of the particle kinetic stresses do not behave as in a simple Newtonian fluid. In general, both kinetic-pdf approaches provide a set of continuum equations for the dispersed phase together with their constitutive relations which have been tested successfully on a variety of turbulent dispersed flows from separating flows, turbulent boundary layers and jets, and in many cases comparisons have been made with results from direct numerical simulation (DNS) and large eddy simulation (LES) where the flows can be well simulated.

An important consideration in this proposed review will be the application of this kinetic approach to modeling particle transport in turbulent boundary layers and in particular to the prediction of particle deposition and resuspension from surfaces exposed to a turbulent flow. The transport of particles illustrates important features which are uniquely handled by this approach, in particular the particle-surface interactions (particle bouncing and subsequent resuspension) together with its influence on near-wall behavior. In strongly inhomogeneous turbulence as in a turbulent boundary layer⁶ this leads to nonlocal transport and the concept of free flight to the wall used in simple but empirically based deposition models. It is shown how through the particle momentum equations, the divergence of the particle kinetic stress can give rise to a drift velocity toward the depositing wall, known as turbophoresis and which in many cases dominates the deposition process. The turbulent forces acting on the suspending particles reveal the particle mass flux to be both dispersive and convective with implications for the build-up of concentration in turbulent boundary layers. It is shown how considerable progress has been made in dealing with complex particle surface interactions and near-wall behavior using pdf methods, in particular in dealing with particles scattering off rough surfaces using novel computational methods to solve the kinetic equation in these circumstances. The work in this area forms part of an overall strategy for the application of two-fluid models in computational fluid dynamics (CFD) with the evaluation of wall functions based on the solution of pdf equations close to the wall that incorporate the natural boundary conditions of the dispersed particle phase.

An important consideration in the application of the kinetic approach recognized early on in its development was the ability of this approach to deal with interparticle collisions following an obvious analogy with the Maxwell-Boltzmann equation and the

²i.e., it is a legitimate closure since the closure methods and approximations involved in its development are formally related to the underlying equations of motion of both fluid elements and particles, and preserve realizability. The “two-fluid” equations have thus a much sounder theoretical basis, the only constants involved being those of the particle equations of motion and statistics of the carrier flow itself.

³It is called a kinetic theory because it exploits the methods and approach of classical kinetic theory.

⁴This is not a model but a modeling approach.

⁵By this is meant the mean flow is a local linear shear and the turbulence is statistically homogeneous and stationary.

⁶And also particle pair dispersion in a homogeneous turbulent flow.

way it models molecular collisions. A crucial part of the success thus owes much to the application of the perturbation methods due to Grad, Chapman, and Enskog et al., to study the influence of molecular collisions on the constitutive relations for gas in kinetic theory. There is however an assumption made in CKT of *molecular chaos* which is no longer valid in general for particle collisions in turbulent flows where the turbulence plays a role in particle transport. In this regard, the work of Simonin and latterly Zaichik has been crucial in the way they have modified the molecular chaos assumption to include the correlation with the carrier flow before and after the collision. As a consequence, they have been able to model the particle kinetic stresses in the dispersed phase from dilute to granular flows. This review will consider these important advances and the impact they have on the influence of both turbulence and particle collisions, comparing the kinetic-pdf theory predictions with those of direct particle simulations (DPS) with particle collisions.

All of this mentioned so far refers to single-particle dispersion or transport, i.e., the transport of single particles in a fixed frame of reference independent of the motion of any neighboring particles. To deal with the problem of segregation and clustering of particles by small scale turbulent structures, it is necessary to consider two-particle dispersion or more succinctly the motion of particle pairs. As far as kinetic methods are concerned, this is simply the extension of the kinetic approach from one particle to two particles. The relevant turbulent velocities of the carrier flow are in this case the carrier flow velocity difference encountered by particle pairs as a function of their separation whose statistical properties are reflected in the values of the statistical moments of the carrier flow velocity differences measured by particle pairs (related to the turbulent structure functions at various orders). In this review paper, the progress is reviewed in applying the kinetic-pdf approach to particle pair dispersion, and collisions for both mono and bidisperse particles and in particular to the prediction of the radial distribution function (RDF), how it enhances collision rates, and how its dependence on the separation between particle pairs reflects a fractal nature to the segregation process. Here the comparison with DNS results has been most encouraging.

As a conclusion, the important features of this review are summarized and set out what is regarded as the important challenges for the future, identifying areas where the application of pdf methods can help to produce better and more reliable models, particularly in environmental and geophysical flows. The focus of most of the pdf modeling has been on gas-particle/droplet flows. Recently there has been a major effort to extend the approach to water droplets in oil flows where the ratio of densities of dispersed to continuous flow is such that there is a significant contribution from added mass forces [17].

2 Formulation of Kinetic-Probability Density Function Equations

There are currently two forms of kinetic-pdf equations in use. In the first form, the pdf, as in CKT, refers to the probability density that a particle has a certain velocity and position at a given time. This was referred to in the Introduction as the KM. It originated with the work of Buyevich [18–20] and has been developed since by a number of workers most notably Reeks [21–24], Swailes [25–28], Zaichik [29–32], Pozorski and Minier [33], and Zhou et al. [34,35]. In all these developments the kinetic-pdf approach was restricted to inert nonreactive particles. More recently Pandya and Mashayek [36] extended the approach to reactive condensing or evaporating particles in a turbulent gas. In contrast, the second form of the kinetic-pdf equation, first proposed by Simonin, Deutsch, and Minier (SDM) [37], is for a more general pdf which includes the velocity of the carrier flow local to the particle as a phase space variable as well as the particle position and velocity. As an example of how pdfs and kinetic-pdf equations are obtained, consider the motion of evaporating/

condensing particles (droplets) in a dilute suspension in which there are no interparticle collisions. Let $\mathbf{X}$ be the phase space vector at time t of a single particle as it moves through its phase space. So in this case

$$\mathbf{X} = [m, T, \mathbf{v}, \mathbf{x}] \quad (1)$$

where m is the mass of the particle, T its temperature and $\mathbf{v}$, $\mathbf{x}$ the velocity and position of its center of mass at time t . The number n of independent variables that defines the phase space dimension is thus $n = 8$. For a single realization of the underlying carrier flow velocity field $\mathbf{u}(\mathbf{x}, t)$ and temperature field $T(\mathbf{x}, t)$, the number of particles in an elemental volume $d^n \mathbf{X}$ of phase space located at $\mathbf{X}$ will be given by $W(\mathbf{X}, t)d^n \mathbf{X}$ where $W(\mathbf{X}, t)$ is the phase space density

$$\frac{\partial W}{\partial t} + \frac{\partial}{\partial \mathbf{X}} \cdot [W \dot{\mathbf{X}}] = 0 \quad (2)$$

So for the case of the evaporating droplet, we have explicitly

$$\dot{\mathbf{X}} = [\dot{m}, \dot{T}, \dot{\mathbf{v}}, \dot{\mathbf{x}}] \quad (3)$$

where the equations for components of $\dot{\mathbf{X}}$ represent the *particle equations of motion* in the most general sense and are derived from the mass-momentum-energy conservation equations for an individual particle/droplet, see, e.g., Crowe [2]. However because the underlying carrier flow field is turbulent, $\dot{\mathbf{X}}$ has a random component so we can only usefully refer to the pdf that a particle has a set of values $\mathbf{X}$ at any given time t . This is represented by the ensemble average of W over all realizations of the system, symbolically $\langle W \rangle$. The equation for $\langle W \rangle$ (the pdf equation) can be found by ensemble averaging the conservation equation for W (the Liouville equation). For convenience the instantaneous components of $\dot{\mathbf{X}}$ are decomposed into their mean components $\langle \dot{\mathbf{X}} \rangle$ and fluctuating (zero mean) components $\dot{\mathbf{X}}'$, noting that $\dot{\mathbf{x}} = \mathbf{v}$, so that explicitly the pdf equation for the evaporating/condensing particle is

$$\begin{aligned} \frac{\partial \langle W \rangle}{\partial t} + \left(\frac{\partial}{\partial m} \langle \dot{m} \rangle + \frac{\partial}{\partial T} \langle \dot{T} \rangle + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot \langle \dot{\mathbf{v}} \rangle \right) \langle W \rangle \\ = - \frac{\partial}{\partial m} \langle \dot{m}' W \rangle - \frac{\partial}{\partial T} \langle \dot{T}' W \rangle - \frac{\partial}{\partial \mathbf{v}} \cdot \langle \dot{\mathbf{v}}' W \rangle \end{aligned} \quad (4)$$

where on the left-hand side of Eq. (4) we have the convective part (the transport in the absence of the turbulence) and on the right-hand side, the dispersive part involving the gradients of the net fluxes due to the turbulence. To close the equation we need to relate the turbulent fluxes in some way, directly or indirectly, to $\langle W \rangle$ and its derivatives. That is, we have a closure problem to resolve which is the most important and crucial element of the kinetic-pdf approach.

To illustrate the way in which the values of $\dot{\mathbf{X}}$ depend upon the properties of the particle and the underlying carrier flow, let's consider the case of the evaporating droplet in more detail. From mass conservation of a spherical droplet of diameter d_p evaporating in a gas of material density ρ_g , we have the general relationship

$$\dot{m} = \pi \rho_g d_p D_v \text{Sh}(\text{Re}_p, \text{Sc}_c) \ln \left[\frac{1 - \alpha_v}{1 - \alpha_{vs}} \right] \quad (5)$$

where α_v is the mass fraction of vapor emitted by the particle in the locally undisturbed gas flow, α_{vs} is the saturated vapor mass fraction at the droplet/particle surface assumed to be in equilibrium with the particle so it depends directly on the absolute temperature T of the particle, D_v the molecular diffusion coefficient of the vapor, and Sh the droplet Sherwood number for mass transfer of vapor to or from the droplet which is a function of the vapor

Schmidt number S_c and the local particle Reynolds number Re_p given by

$$Re_p = \frac{d_p |\mathbf{v} - \mathbf{u}|}{\nu_f}; \quad Sc = \frac{D_v}{\nu_f} \quad (6)$$

where $\mathbf{u}(\mathbf{x}, t)$ is the gas velocity flow field local to the particle spatial position $\mathbf{x}$ at time t and ν_f is the kinematic viscosity of the carrier gas flow.

From momentum conservation [2] we have

$$m\dot{\mathbf{v}} = m\mathbf{g} - V \frac{\partial \cdot \boldsymbol{\sigma}}{\partial \mathbf{x}} + \mathbf{F}_A + (\mathbf{u} - \mathbf{v})\dot{m} \quad (7)$$

The first term on the right-hand side of this equation is the gravitational force. The second and third terms represent the force exerted by the surrounding gas flow from the external stresses $\boldsymbol{\sigma}$ and the aerodynamic force $\mathbf{F}_A$ which has both lift and drag components $\mathbf{F}_L$ and $\mathbf{F}_D$ arising from the locally disturbed gas flow field due to the presence of the particle which has a volume V . For a spherical particle, this is well represented by the drag force in most cases so that

$$\mathbf{F}_A \cong \mathbf{F}_D = -\frac{1}{2} \rho_g A C_D (Re_p) |\mathbf{v} - \mathbf{u}| (\mathbf{v} - \mathbf{u}) \quad (8)$$

where C_D is the drag coefficient and A the projected area of the particle normal to the flow. Note we have ignored any influence of flow curvature (Faxen force), flow boundaries, external pressure gradient, and forces generated through differences between the rotation of a particle and that of the local carrier flow (this precludes any coupling of rotation with the translational motion of the particles). However, even with these restrictions the chosen form for $\mathbf{F}_A$ encompasses several important practical forms of aerodynamic force used in gas-solid/liquid flow calculations.

From energy conservation, we would have an equation of the form

$$mC_p \dot{T} = S_r - \pi k_g d_p Nu(Re_p, Pr) + \Delta H \dot{m} \quad (9)$$

where C_p is the particle specific heat (assumed constant for small changes in temperature) and on the right-hand side of the equation, the first term S_r is the heat source due to the external field (radiation), the second term is the heat transfer rate from or to the particle to or from the surrounding gas where k_g is the thermal conductivity of the gas flow, Nu is the Nusselt number (depending upon the local particle Reynolds number Re_p and Pr , the Prandtl number of the gas/vapor mixture) and the third term ΔH the energy exchange rate during the evaporation/condensation which depends upon ΔH , the difference in enthalpy between the droplet and vapor mass flux.

The point to note here is that the equations of motion are all coupled and all depend upon the instantaneous particle Reynolds number Re_p based upon the relative velocity between particle and locally undisturbed gas.

2.1 The Kinetic-Probability Density Function Equation for Inertial Particles. As said earlier, there are currently two kinetic-pdf approaches in use which we refer to as the KM and the GLM, respectively. To illustrate the differences and similarities between these approaches, we consider here the simplest case of transport of inertial nonreacting solid particles in a turbulent gas flow which we will assume all to be identical to one another. To simplify the situation still further we will linearize the drag force $\mathbf{F}_A$ in Eq. (7) acting on a single particle with respect to the relative velocity between the particle and local carrier flow, i.e.,

$$\mathbf{F}_A \cong \eta(\mathbf{u} - \mathbf{v}) \quad (10)$$

where referring to Eq. (10) η is the net friction coefficient and given by

$$\eta = \frac{1}{2} \rho_g A C_D (\overline{Re_p}) |\bar{\mathbf{u}} - \bar{\mathbf{v}}| \quad (11)$$

where $\bar{\mathbf{v}}$ is the net particle velocity and $\overline{Re_p}$ is the value of the particle Reynolds number based on the net relative velocity between particle and local carrier flow. See Simonin [13]. The equations of motion for identical particles are thus

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \quad (12)$$

$$\frac{d\mathbf{v}}{dt} = \beta(\mathbf{u} - \mathbf{v}) \quad (13)$$

where β is the inverse particle response time and given by $m^{-1}\eta$ for a particle of mass m : in the case of $Re_p \ll 1$ corresponding to Stokes drag, β is a constant of the motion (for later use β^{-1} will be referred to as the particle response time τ_p). A more general way of linearizing the nonlinear drag to account for the dependence of the drag coefficient on the particle Reynolds number is given in Reeks [24]. To the particle equations of motion is added an equation of motion of the carrier flow velocity $\mathbf{u}$ along a particle trajectory, namely,

$$\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \quad (14)$$

In KM we consider continuum equations derived from an equation for the phase space density $W(\mathbf{v}, \mathbf{x}, t)$ in which $\mathbf{u}(\mathbf{x}, t)$ is a random function of $\mathbf{x}, t$ and $\mathbf{v}$ and $\mathbf{x}$ are independent random variables. In the GLM approach, the continuum equations are derived from a conservation equation for the phase space density $P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ where $\mathbf{v}, \mathbf{u}, \mathbf{x}$ form a set of independent variables. The transport/conservation equations for $W(\mathbf{v}, \mathbf{x}, t)$ and $P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ are, respectively,

$$\left\{ \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial}{\partial \mathbf{v}} \cdot \beta(\mathbf{u}(\mathbf{x}, t) - \mathbf{v}) \right\} W(\mathbf{v}, \mathbf{x}, t) = 0 \quad (15)$$

$$\left\{ \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial}{\partial \mathbf{v}} \cdot \beta(\mathbf{u} - \mathbf{v}) + \frac{\partial}{\partial \mathbf{u}} \cdot \mathbf{F}(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \right\} P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) = 0 \quad (16)$$

Note integrating the equation for P over all $\mathbf{u}$ gives the equation for W . We resolve $\mathbf{u}(\mathbf{x}, t)$ and $\mathbf{F}(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ into mean and fluctuating parts

$$\mathbf{u} = \langle \mathbf{u} \rangle + \mathbf{u}''; \quad \mathbf{F} = \langle \mathbf{F} \rangle + \mathbf{F}'' \quad (17)$$

where $\langle \dots \rangle$ represents an ensemble average. Then the transport equations for mean values of W and P , namely, $\langle W \rangle$ and $\langle P \rangle$ are

$$\left\{ \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial}{\partial \mathbf{v}} \cdot \beta(\langle \mathbf{u} \rangle - \mathbf{v}) \right\} \langle W \rangle = -\frac{\partial}{\partial \mathbf{v}} \cdot \beta \langle \mathbf{u}'' W \rangle \quad (18)$$

$$\left\{ \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} + \beta \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{u} - \mathbf{v}) + \frac{\partial}{\partial \mathbf{u}} \cdot \langle \mathbf{F} \rangle \right\} \langle P \rangle = -\frac{\partial}{\partial \mathbf{u}} \cdot \langle \mathbf{F}'' P \rangle \quad (19)$$

when suitably normalized $\langle W \rangle$ and $\langle P \rangle$ represent the probability density at time t , that a particle has the values $(\mathbf{v}, \mathbf{x})$ and $(\mathbf{v}, \mathbf{x}, \mathbf{u})$, respectively. To solve these equations requires closure relations for $\langle \mathbf{u}'' W \rangle$ and $\langle \mathbf{F}'' P \rangle$. For simplicity, we shall just deal with the case where β is a constant for given particle size.

2.2 Closure Approximations for Nonreactive Gas-Particle Flows

2.2.1 Kinetic Method. A range of strategies for closing the turbulent flux can be found in the literature. The methodologies underpinning these approaches can be divided into three distinct categories: (a) Furutsu–Novikov-based (FN) methods [25,38–45], (b) Lagrangian history direct interaction methods (LHDI) methods [24], and (c) Van Kampen (VK) operator representation methods [33,36]. These different approaches have been reviewed and analyzed recently by Bragg and Swailes [26]. Recent work has suggested that the corresponding kinetic equations are essentially equivalent [36]. However whilst the three closure expressions exhibit superficial similarities, Bragg et al. have shown that there are fundamental differences that have an important bearing on their validity in inhomogeneous turbulence. What all three methods do have in common is they represent the net force due to the turbulence $\beta(\mathbf{u}''W)$ by contributions from gradient diffusion of the net phase space density both in velocity and position and from a body force (per unit mass) dependent on the statistical inhomogeneity of the turbulence, i.e., it is zero in statistically stationary homogeneous turbulence). Thus in general

$$\langle f_i W \rangle = - \left(\frac{\partial}{\partial x_j} \langle W \rangle \lambda_{ji} + \frac{\partial}{\partial v_j} \langle W \rangle \mu_{ji} - \kappa_i \langle W \rangle \right) \quad (20)$$

where for convenience we have written f_i for $\beta u_i''$. Note that dispersion coefficients appear on the other side of the gradients in velocity and position than is normal. So in this context, they are more appropriately the components of stress tensors λ and μ (per unit particle mass) rather than diffusion coefficients. κ_i represent the components of a body force per particle mass. Reeks [23,24,46,47] has shown that this form is a general requirement of random Galilean transformation invariance [48,49]. Taking the forms for λ and μ and κ given by the FN method

$$\begin{aligned} \lambda_{ji} &= \int_0^t \langle \mathcal{G}_{jk}(t|s) R_{ki}(\mathbf{x}_p(t|s), s; \mathbf{x}, t) \rangle ds \\ \mu_{ji} &= \int_0^t \langle \dot{\mathcal{G}}_{jk}(t|s) R_{ki}(\mathbf{x}_p(t|s), s; \mathbf{x}, t) \rangle ds \\ \kappa_i &= \int_0^t \langle \mathcal{G}_{jk}(t|s) \frac{\partial}{\partial x_j} R_{ki}(\mathbf{x}_p(t|s), s; \mathbf{x}, t) \rangle ds \end{aligned} \quad (21)$$

in which R_{ki} denotes an Eulerian two-point, two-time carrier flow velocity correlation tensor of the turbulent force field $\mathbf{f}$, that is

$$R_{ki}(\mathbf{y}, s; \mathbf{x}, t) = \langle f_k(\mathbf{y}, s) f_i(\mathbf{x}, t) \rangle \quad (22)$$

where $\mathbf{x}_p(t|s)$ is the particle position evaluated at time s along all particle trajectories passing through $\mathbf{x}$ and $\mathbf{v}$ at time t , i.e., in Eq. (22) $\mathbf{y} = \mathbf{x}_p(t|s)$, with $\mathbf{x}_p(t|t) = \mathbf{x}$ and $\dot{\mathbf{x}}(t|t) = \mathbf{v}$. $\mathcal{G}_{jk}(t|s)$ are the components of a response tensor $\mathcal{G}$ given formally by the functional derivative

$$\mathcal{G}_{jk}(t|s) = \frac{\delta x_{p,j}(t|t)}{\delta f_k(\mathbf{x}_p(t|s), s)} \quad (23)$$

That is they describe the effect of a perturbation in the force field $\mathbf{f}(\mathbf{x}, s)$ applied at the particle position $\mathbf{x}_p(t|s)$ at time s upon the position of the particle at time t . This can be obtained by taking the functional derivative with respect to $\delta \mathbf{f}(\mathbf{x}, s)$ of the particle equation of motion Eq. (13), so that

$$\ddot{\mathcal{G}}_{jk} + \beta \dot{\mathcal{G}}_{jk} - \beta \left(\frac{\partial \langle u_j \rangle}{\partial x_k} + \frac{\partial u_j''}{\partial x_k} \right) \mathcal{G}_{jk} = 0 \quad (24)$$

with the “initial” conditions $\mathcal{G}_{jk}(s|s) = 0$, $\dot{\mathcal{G}}_{jk}(s|s) = \delta_{jk}$. In Eq. (24) the spatial derivatives of $\langle \mathbf{u} \rangle$ and $\mathbf{u}''$ are evaluated along

the particle trajectories $\mathbf{x}_p(t|s)$. The closure term given by Eq. (20) based on the forms for λ , μ and κ given by Eq. (21) is exact if the flow field $\mathbf{f}(\mathbf{x}, t)$ is Gaussian. We note that in the case of high inertial particles, i.e., $\beta \rightarrow \infty$, the velocity gradient term in Eq. (20) dominates and the kinetic equation reduces to the well-known Fokker–Planck equation. The forms for λ , μ , and κ based on the LHDI approach [24] are the same as those based on the Furutsu–Novikov method except that the Eulerian correlation $\mathbf{R}$ is replaced by $\langle f_k(\mathbf{x}_p(s), s) f_i(\mathbf{x}, t) \rangle$. Thus it is Lagrangian correlations that are involved rather than Eulerian correlations. In addition, the stochastic response functions $\mathcal{G}_{jk}$ are replaced by its deterministic components $\langle \mathcal{G}_{jk} \rangle$, so that the equation for $\langle \mathcal{G}_{jk} \rangle$ is given by

$$\langle \ddot{\mathcal{G}}_{jk} \rangle + \beta \langle \dot{\mathcal{G}}_{jk} \rangle - \beta \frac{\partial \langle u_j \rangle}{\partial x_k} \langle \mathcal{G}_{jk} \rangle = \delta(t-s) \delta_{jk} \quad (25)$$

In the LHDI case then

$$\begin{aligned} \lambda_{ji} &= \langle \Delta x_j(t) f_i(\mathbf{x}, t) \rangle \mu_{ij} = \langle \Delta v_j(t) f_i(\mathbf{x}, t) \rangle \\ \kappa_i &= \left\langle \Delta x_j(t) \frac{\partial f_i(\mathbf{x}, t)}{\partial x_j} \right\rangle \end{aligned} \quad (26)$$

where explicitly $\Delta x_j(t)$ and $\Delta v_j(t)$ are short-hands for $\Delta x_j(\mathbf{x}, t|0)$ and $\Delta v_j(\mathbf{x}, \mathbf{v}, t|0)$, denoting changes in the particle position and velocity for a particle starting somewhere in the particle phase space at some initial time $s=0$ and arriving at the point $\mathbf{x}, \mathbf{v}$ at time $s=t$. In terms of the deterministic response functions $\langle \mathcal{G}_{ik} \rangle$, these changes are given by

$$\begin{aligned} \Delta x_j(\mathbf{x}, \mathbf{v}, t|0) &= \int_0^t ds \langle \mathcal{G}_{jk} \rangle(t|s) f_k(\mathbf{x}_p(t|s), s) \\ \Delta v_j(\mathbf{x}, \mathbf{v}, t|0) &= \int_0^t ds \langle \dot{\mathcal{G}}_{jk} \rangle(t|s) f_k(\mathbf{x}_p(t|s), s) \end{aligned} \quad (27)$$

The result is exact for a process in which the displacements $\Delta x_i(\mathbf{x}, \mathbf{v}, t|0)$, $\Delta v_i(\mathbf{x}, \mathbf{v}, t|0)$ form a Gaussian process. Whilst both LHDI and FN closures would both claim to be exact for Gaussian processes, the Gaussian process to which they refer are not the same: in the case of LHDI, the Gaussian process refers to the Lagrangian statistics of $\mathbf{f}(\mathbf{x}(s), s)$ along a particle trajectory in phase space whilst in the FN case it refers to the field $\mathbf{f}(\mathbf{x}, t)$; given that one process is prescribed as Gaussian does not imply that the other is Gaussian. Bragg et al. [26] point out that in previous FN formulations, the deterministic response functions $\langle \mathcal{G}_{jk}(t|s) \rangle$ were used in place of $\mathcal{G}_{jk}$ so that the contribution of the fluctuations in the spatial gradients of $\mathbf{f}(\mathbf{x}, t)$ was omitted. Whilst using this nonrandom form for $\mathcal{G}$ formally closes the equation for $\langle \mathbf{f}W \rangle$, Bragg et al. [26] have shown that the inclusion of this random term ensures that the fully mixed criterion for a passive scalar (particle Stokes number $St \rightarrow 0$),⁷ i.e., the absence of spurious drift. We will need to refer to this feature in more detail later on (see Sec. 4.1). There is good reason however to use $\langle \mathcal{G}_{ji} \rangle$ instead of $\mathcal{G}_{ji}$ other than practicality. Calculations of the value of the dispersion coefficients by Bragg et al. [50] in a fully developed kinematically simulated (KS) of a turbulent boundary using both $\langle \mathcal{G}_{ji} \rangle$ and $\mathcal{G}_{ji}$ show little difference for $St = 0.3$, the negligible difference at $St = 0.8$, and an imperceptible difference at $St = 3$. Using the deterministic response $\langle \mathcal{G}_{ji} \rangle$ shows a resemblance between the FN and LHDI approaches that is reminiscent of Corrsin’s independence hypothesis [51] which gives an approximate relationship between Lagrangian and Eulerian timescales. So the Lagrangian correlation

⁷By Stokes number St is meant the ratio of β^{-1}/τ_f where τ_f is the typical timescale of the turbulence encountered by a particle.

$$\begin{aligned} \langle f_j(\mathbf{x}, \mathbf{v}, t) f_i(\mathbf{x}, t) \rangle &\simeq \int R_{ji}(\mathbf{x}, t'; \mathbf{x}, t) \langle \delta(\mathbf{x} - \mathbf{x}(t')) \rangle d^3\mathbf{x} \\ &= \int d^3\mathbf{x} R_{ki}(\mathbf{x}, t'; \mathbf{x}, t) G(\mathbf{x} - \mathbf{x}, t - t') \end{aligned} \quad (28)$$

where $G(\mathbf{x} - \mathbf{x}, t - t')$ is the Green's function solution for an instantaneous point source $\delta(\mathbf{x} - \mathbf{x})\delta(t' - t)$. This relationship arises naturally through the comparison between LHDI and FN approaches without the necessity of invoking Corrsin's hypothesis [51].

Finally, we mention briefly the operator representation of VK which was used by Pozorski and Minier [33] to obtain a kinetic equation. This third form of the kinetic equation is formally consistent with the fully mixed condition but fails to account for a nonzero scalar flux contribution associated with nonuniform scalar distributions in inhomogeneous, incompressible flows. Furthermore, this VK closure is based on an expansion in terms of a small parameter reflecting the magnitude of turbulence intensity relative to a rate scale for the decorrelation of turbulent flow velocities (weak turbulence approximation). Correlations are based on mean trajectories, i.e., due to the mean flow, ignoring the influence of the turbulence, and whilst this affords a significant simplification to the closure problem, removing conditional averages within the dispersion tensors makes the validity of such an approximation in strongly inhomogeneous flows highly questionable. In addition as Bragg and Swailes [50] point out, even for the simpler case of dispersion in isotropic turbulence there seems to be a serious issue with the VK formulation. The VK diffusion coefficients for fluid-point dispersion in isotropic turbulence suggest that the dispersion rate should be proportional to the Eulerian integral time scale, rather than the Lagrangian integral time scale. This is incorrect and arises precisely because the VK dispersion tensors contain correlations of the flow velocity field evaluated along mean trajectories. Therefore the question of the validity of the VK closure relates not only to inhomogeneous flows but also to homogeneous, isotropic flows. This is not as we shall see the case with FN and LHDI formulations.

2.2.2 Closure of Kinetic Equations for Non-Gaussian Processes. We have noted that the form of $\langle fW \rangle$ based on either Furutsu–Novikov or LHDI formulations preserves random Galilean transformation (RGT) invariance. The terminology and usage are due to Kraichnan [46] and means applying to each realization of the carrier flow a translational velocity, constant in space and time but varying randomly in value from one realization to the next; in Kraichnan's usage of RGT, the distribution of velocities is taken to be Gaussian for convenience. Clearly, the internal dynamics should be unaffected by this transformation and should be reflected in the equations that describe the average behavior of the resulting system. In the case of the classical Fokker Planck (FP) equation, the terms that describe the dispersion due to the aerodynamic driving force and that due to the translational velocity should be separate. Whilst this separation does occur in an FP formulation, the form of the dispersion term due to the random translational velocity is incorrect. More precisely this failure to preserve RGT invariance means failure to reproduce the correct equation of state for the dispersed phase (except in the case of very inert particles for $St \gg 1$)

Following the approach given in Reeks [23], we generalize the method used to obtain a closed expression for $\langle fW \rangle$ by considering $f(s)$ as continuous random process random referring to $(\mathbf{v}, \mathbf{x}, t|s)$, i.e., the aerodynamic force measured at time s along a particle trajectory which passes through the point $(\mathbf{v}, \mathbf{x})$ at time t . So

$$f(t) = f(\mathbf{v}, \mathbf{x}, t|t) = f(\mathbf{x}, t)$$

Using similar arguments to invoke RGT invariance, we can write

$$\begin{aligned} \langle W \rangle &= \langle W^{(0)} \left(\mathbf{v} - \int_0^t \mathbf{f}(s) \dot{g}(s-t) ds, \right. \\ &\quad \left. \mathbf{x} - \int_0^t \mathbf{f}(s) g(s-t) ds, t \right) \rangle \\ &\text{with } g(s) = 1 - e^{-\beta s} \end{aligned} \quad (29)$$

where $W^{(0)}(\mathbf{v}, \mathbf{x}, t)$ is the particle phase space density in the absence of turbulence, i.e., with $\mathbf{f}(s) = 0$. In the case of an instantaneous point source, $W^{(0)}(\mathbf{v}, \mathbf{x}, t) = \delta(\mathbf{v} - \mathbf{v}_0)\delta(\mathbf{x} - \mathbf{x}_0)\delta(t - t_0)$. Expanding the right-hand side in terms of a Taylor series gives formally

$$\langle W \rangle = \left\langle \exp \left(- \int_0^t ds \mathbf{f}(s) \cdot \left\{ \dot{g}(s-t) \frac{\partial}{\partial \mathbf{v}} + g(s-t) \frac{\partial}{\partial \mathbf{x}} \right\} \right) \right\rangle W^{(0)}(\mathbf{v}, \mathbf{x}, t)$$

which we can write as

$$\begin{aligned} \langle W \rangle &= M[\phi(s)] W^{(0)} \\ \text{with } \phi(s) &= \Psi(s-t) = i \left\{ \dot{g}(s-t) \frac{\partial}{\partial \mathbf{v}} + g(s-t) \frac{\partial}{\partial \mathbf{x}} \right\} \end{aligned}$$

where $M[\phi(s)]$ is the characteristic functional of $\mathbf{f}(s)$, namely,

$$\begin{aligned} M[\phi(s)] &= \left\langle \exp i \int_0^t \phi(s) \cdot \mathbf{f}(s) ds \right\rangle, \text{ for which} \\ \langle f(\mathbf{x}, t) W(\mathbf{v}, \mathbf{x}, t) \rangle &= -i \frac{\delta M[\phi(s)]}{\delta \phi(t)} \end{aligned} \quad (30)$$

where $\delta/\delta\phi(t)$ means a functional derivative of $\phi(s)$ for small changes of $\phi(s)$ about t .

$M[\phi(s)]$ is now represented as a cumulant expansion

$$\begin{aligned} M[\phi(s)] &= \sum_{n=1}^{\infty} \frac{i^{2n}}{\{2n\}!} \int_0^t ds_1 \dots \int_0^t ds_n \\ &\quad \times \mathbf{K}^n \{ f_{i_1}(s_1) \phi_{i_1}(s_1), \dots, f_{i_n}(s_n) \phi_{i_n}(s_n), \mathbf{f}(t) \} \end{aligned}$$

where $\mathbf{K}^n\{\}$ is the cumulant involving the averages associated with $\{f_{i_1}(s_1) \phi_{i_1}(s_1), \dots, f_{i_n}(s_n) \phi_{i_n}(s_n), \mathbf{f}(t)\}$. Substituting this in Eq. (30) we obtain

$$\begin{aligned} \langle f(\mathbf{x}, t) W(\mathbf{v}, \mathbf{x}, t) \rangle &= \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_0^t ds_1 \dots \int_0^t ds_n \\ &\quad \times \mathbf{K}^n \{ f_{i_1}(t-s_1) \psi_{i_1}(t-s_1), \dots, f_{i_n}(s_n) \psi_{i_n}(t-s_n), \mathbf{f}(t) \} \\ &\quad \langle W(\mathbf{v}, \mathbf{x}, t) \rangle \end{aligned} \quad (31)$$

It is noteworthy as shown in Reeks [23] that RGT invariance is satisfied at each order of the cumulant expansion. Furthermore, if $f(t)$ is a Gaussian random process, every term in the expansion apart from the first is zero and we have after some manipulation and differentiation by parts

$$\langle f(\mathbf{x}, t) W(\mathbf{v}, \mathbf{x}, t) \rangle = - \left(\frac{\partial}{\partial \mathbf{x}} \cdot \boldsymbol{\lambda} + \frac{\partial}{\partial \mathbf{v}} \cdot \boldsymbol{\mu} + \boldsymbol{\kappa} \right) \langle W \rangle$$

identical to the LHDI form in Eq. (26). (See also Swailes and Darbyshire [52] for the FN cumulant expansion) The value of the cumulant expansion in Eq. (31) would be the hope that truncating the expansion at higher and higher-order (cumulant neglect hypothesis) would achieve successively better approximations for $\langle W \rangle$ for a non-Gaussian $\mathbf{f}(\mathbf{v}, \mathbf{x}, t|s)$. Unfortunately, the expansion is not uniformly convergent; furthermore, it is well "known" [46] that realizable solutions for $\langle W \rangle$ can only be achieved by truncating the expansion after the first term or including all the terms in the expansion. Ultimately this nonrealizability can be traced to the

use of a truncated cumulant expansion for the characteristic functional for $f(s)$ which does not satisfy realizability for the corresponding probability functional for $f(t)$ [53]. However, this does not rule out the use of such expansions. Whilst solutions for $\langle W \rangle$ may be negative for some regions of phase space, such regions may be regions where $\langle W \rangle$ is in reality very small in value; over regions where $\langle W(\mathbf{v}, \mathbf{x}, t) \rangle$ is appreciable, better approximations can be obtained by taking more than one term in the expansion. However, since the expansion is not uniformly convergent one has no a priori rule for assessing how many terms are required. Ultimately we are limited by our knowledge of $f(\cdot|s)$ as a random process. No exact theory exists for determining this process from the underlying random velocity field of the carrier flow from which it is derived. What does exist are approximate methods for determining the second moments of $f(\mathbf{x}, t)$. Experimental determinations are similarly limited to measurements of this quantity. In view of these limitations it would be pointless from a practical point of view to consider currently more than the first term in the expansion which at least corresponds to a realizable process and one for which as we have shown becomes the dominant term in the expansion when $f(t)$ behaves as white noise.

2.2.3 Generalized Langevin Model. Simonin, Deutsch, and Minier (SDM) [37] derived an equation of motion for the flow velocity along a particle trajectory by starting with the Langevin equation which Pope [14] has used as the analog of the Navier–Stokes equation for fluid point motion. Thus along a fluid point trajectory

$$\frac{du_i}{dt} = -\alpha_{ij}(\mathbf{x})u_j'' + f_i(\mathbf{x}) + f_i''(t) \quad (32)$$

where $f_i(\mathbf{x})$ is the net viscous and pressure force per unit mass of fluid and $f_i''(t)$ is a white noise function of time. Both SDM and Pope consider the equation of motion in differential form because the white noise is assumed nondifferentiable. For convenience, we have assumed that the white noise, like all turbulence-related functions is differentiable: it has white noise properties simply because it has a timescale much shorter than the timescale over which $\mathbf{u}(t)$ varies along a fluid point trajectory $O(\alpha^{-1})$. For future reference, we note that

$$f_i(\mathbf{x}) = \frac{D_f \langle u_i \rangle}{Dt} - \frac{\partial \langle u_j'' u_i'' \rangle}{\partial x_j} \quad (33)$$

where

$$\frac{D_f}{Dt} = \frac{\partial}{\partial t} + \langle u_j \rangle \frac{\partial}{\partial x_j} \quad (34)$$

Simonin, Deutsch, and Minier use this equation to generate an equation of motion for the fluid velocity along a particle trajectory. That is if $\frac{d\mathbf{x}}{dt}$ is the time derivative of the fluid velocity along a particle trajectory and similarly $\frac{d\mathbf{v}}{dt}$ along a fluid point trajectory, then we have

$$\begin{aligned} \frac{d_p u_i}{dt} &= \left(\frac{\partial}{\partial t} + \mathbf{v}_j \frac{\partial}{\partial x_j} \right) u_i(\mathbf{x}, t) \\ &= (\mathbf{v}_j - u_j) \frac{\partial u_i(\mathbf{x}, t)}{\partial x_j} + \frac{d_f u_i}{dt} \\ &= (\mathbf{v}_j - u_j) \frac{\partial u_i(\mathbf{x}, t)}{\partial x_j} \\ &\quad - \alpha_{ij} u_j'' + f_i(\mathbf{x}) + f_i''(\mathbf{x}) + f_i''(t) \end{aligned} \quad (35)$$

Simonin, Deutsch, and Minier consider only the contribution from the gradient of the mean fluid velocity in this equation of

motion for the fluid velocity along a particle trajectory. That is they consider the equation

$$\frac{d_p u_i}{dt} = (\mathbf{v}_j - u_j) \frac{\partial \langle u_i(\mathbf{x}, t) \rangle}{\partial x_j} - \alpha_{ij} u_j'' + f_i(\mathbf{x}) + f_i''(t) \quad (36)$$

In effect this is equivalent to assuming that the contribution of the fluctuating fluid velocity gradient is absorbed into the white noise function $f_i''(t)$. In the case of the white noise function, the equation for $\langle P \rangle$ can be closed exactly, namely,⁸

$$\begin{aligned} \langle F_i''(\mathbf{x}, t) P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \rangle &= \langle f_i''(t) P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \rangle \\ &= - \int_0^\infty \langle f_i''(0) f_j''(s) \rangle ds \frac{\partial \langle P \rangle}{\partial u_j} \end{aligned} \quad (37)$$

Then from Eq. (19), the equation for $\langle P \rangle$ used by SDM is

$$\begin{aligned} \frac{\partial \langle P \rangle}{\partial t} + \frac{\partial}{\partial x_i} \mathbf{v}_i \langle P \rangle + \frac{\partial}{\partial \mathbf{v}_i} \beta(u_j - \mathbf{v}_j) \langle P \rangle \\ + \frac{\partial}{\partial u_i} \left[-\alpha_{ij} u_j'' + f_i(\mathbf{x}) + (\mathbf{v}_j - u_j) \frac{\partial \langle u_i \rangle}{\partial x_j} \right] \langle P \rangle \\ = \int_0^\infty \langle f_i''(0) f_j''(s) \rangle ds \frac{\partial^2 \langle P \rangle}{\partial u_i \partial u_j} \end{aligned} \quad (38)$$

and are spatially independent but varying in time.

3 Analytic Solutions for Dispersion in Generic Flows and Very Inert Particles

In cases where the turbulence is homogeneous and stationary and the mean carrier flow is a linear flow field, the pdf equations for both KM and GLM have analytic solutions that are exact solutions for a Gaussian process for the flow velocity sampled along a particle trajectory. Moreover, in this case, both kinetic-pdf methods, given the same form for the carrier flow correlation along a particle trajectory, will give identical results [54].⁹ Furthermore, these solutions can be used as a basis for dealing with more complex flow fields (e.g., in constructing appropriate constitutive relations), give some insights into the basic diffusion process, and can be used as test cases to check out numerical methods that are appropriate in more general cases. In this section we will present some results for the dispersion of point sources in mean flows which are (a) uniform, (b) simple shear, and (c) rotational. The results are taken from Hyland et al. [55], Swailes and Darbyshire [25], and Reeks [54]. As a preliminary, we note as in Swailes and Darbyshire [25] that if for convenience we introduce the phase space variable $\underline{\varrho}$, then the solution of the pdf equation for an instantaneous point source is a Gaussian $G(\underline{\varrho}, t)$ given by

$$G(\underline{\varrho}, t) = (2\pi)^{-n} \det\{\underline{\Theta}\}^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} (\underline{\varrho} - \mathbf{m}) \cdot \underline{\Theta}^{-1} (\underline{\varrho} - \mathbf{m}) \right\} \quad (39)$$

where $\underline{\Theta}$ is the matrix of ensemble covariances of $\underline{\varrho}$ as a function of time t and $\mathbf{m} = (\hat{\mathbf{x}}, \hat{\mathbf{v}})$ where $\hat{\mathbf{x}}$ and $\hat{\mathbf{v}}$ are the solutions of $\mathbf{x}(t)$ and $\mathbf{v}(t)$, respectively, in the absence of turbulence starting from some initial values $\mathbf{x}$ and $\mathbf{v}^0$ at time zero (the point of release) and $\det \underline{\Theta}(0) = 0$. The solution for the particle spatial concentration at $\mathbf{x}$ in a frame of reference moving with velocity $\hat{\mathbf{v}}(t)$ whose origin coincides with the point of release $\mathbf{x}$ at time zero satisfies the simple diffusion equation

⁸Note the closure is also exact if $f''(t)$ is Gaussian nonwhite but will include gradients of $\langle P \rangle$ in $\mathbf{x}$ and $\mathbf{v}$ as well.

⁹However, it is important to point out that the fluid velocity correlations as a function of time used in the GLM are also predicted by the model itself. In KM there is complete freedom to choose any form based on simulation or experiment.

$$\frac{\partial \langle \rho \rangle}{\partial t} = \frac{\partial}{\partial x_i^*} D_{ij}(t) \frac{\partial}{\partial x_j^*} \langle \rho \rangle + \delta(\mathbf{x}) \delta(t) \quad (40)$$

where the diffusion $D_{ij}(t)$ is the particle ensemble covariances. The solution is a Gaussian in $\mathbf{x}$ of the general form

$$G(\mathbf{x}^*, t) = (2\pi)^{-3/2} \det(\langle \mathbf{x}^* \mathbf{x}^* \rangle)^{-1/2} \times \exp\left(-\frac{1}{2} \mathbf{x}^* \langle \mathbf{x}^* \mathbf{x}^* \rangle^{-1} \mathbf{x}^*\right) \quad (41)$$

That is in the fixed frame of reference the contours of constant concentration will be concentric ellipses (in 2D) centered at $\hat{\mathbf{x}}(t)$. For the mean density weighted particle velocity we have

$$\bar{\mathbf{v}} = \hat{\mathbf{v}} + \langle \mathbf{v}^* \mathbf{x}^* \rangle \langle \mathbf{x}^* \mathbf{x}^* \rangle^{-1} \mathbf{x}^* \quad (42)$$

that is the mean particle flow field is linear in $\mathbf{x}$ and for the density weighted particle velocity covariances we have

$$\overline{\mathbf{v}^* \mathbf{v}^*} = \langle \mathbf{v}^* \mathbf{v}^* \rangle - \langle \mathbf{v}^* \mathbf{x}^* \rangle \langle \mathbf{x}^* \mathbf{x}^* \rangle^{-1} \langle \mathbf{x}^* \mathbf{x}^* \rangle \quad (43)$$

and are spatially independent but varying in time.

3.1 Uniform Flows. The features of dispersion in this flow have been extensively simulated and measured, particularly the particle diffusion coefficient and particle velocity covariances (see Stock [56]). Forms for the long time particle diffusion coefficient $D_p(\infty)$ have been much quoted in isotropic turbulence both with and without gravitational settling, e.g., Reeks [57]. The kinetic-pdf equation reproduces the right result, namely, for Stokes drag

$$D_p(\infty) = \frac{1}{3} \int_0^\infty \langle \mathbf{u}(0) \mathbf{u}(s) \rangle ds \quad (44)$$

where we have used $\mathbf{u}(s)$ as shorthand for $\mathbf{u}(\mathbf{x}|s)$ the carrier flow velocity along a particle trajectory measured at time s with position $\mathbf{x}$ at $s=0$. The absence of $\mathbf{x}$ in Eq. (44) is meant to imply independence on the initial position at $s=0$. It is a result we shall deduce later from the momentum equation and shows that the particle response time (inertia) dependence is reflected only in the way this quantity determines the timescale of $\mathbf{u}(s)$ along a particle trajectory: whether the carrier flow timescales along a particle trajectory are greater or smaller than those along a fluid element trajectory. In fact, particles with more inertia appear to have a long time diffusion coefficient that is greater than that for a fluid element or passive tracer. This is shown in Fig. 1 based on the results

obtained by Squires and Eaton [58] for particle diffusion in DNS statistically stationary isotropic homogeneous turbulence. The vertical axis is the ratio of the particle diffusion coefficient compared to that of the fluid or passive scalar. The calculations were done for a range of particle Stokes numbers St from 0.06 to 0.35 where Stokes number is the ratio of the particle response time τ_p to integral timescale of the flow T_f . You can see that for all the Stokes numbers, the longtime values of the diffusion coefficient are greater than that of the carrier flow, the greatest value being for $St=0.35$ but with little difference between this value and the value for $St=1.09$. The formula in Eq. (44) is also appropriate for particles settling under gravity or in an electric field as with the measurements of Wells and Stock [59]. The timescales of fluid motion along a particle trajectory depend upon the time it takes for a particle to move from one eddy to another in the flow field. The faster the particle moves the shorter the timescale of the fluid motion it encounters, assuming that the eddy lifetime is much longer than the transit time of the particle. If v_g is the settling velocity and l_e the spatial length scale then $l_e/v_g \ll \tau_e$ where τ_e is the eddy decay time. Since $\tau_e \sim l_e/u'$ (where u' is the fluid rms velocity), this implies $u'/v_g \ll 1$ in which case

$$D_p(\infty) = \int_0^\infty R_E(0, \mathbf{v}_g t) dt \quad (45)$$

where $R_E(0, y)$ is the carrier flow spatial velocity correlation in a frame moving with the settling velocity with a separation measured in the direction of gravity. D_p in this case refers to the diffusion coefficient for diffusion in the direction of gravity. The phenomenon is often referred to as crossing trajectories, see Csáraday [60]. In this case, the particle diffusion coefficient in the direction of the settling velocity reduces to the form given by Csáraday [60]. Reeks [23] shows how the phase space density changes with time as it moves toward its long term form in which case the velocity distribution is a Maxwell-Boltzmann distribution with a mean square velocity given by

$$\langle v^2(\infty) \rangle = \beta \int_0^\infty e^{-\beta s} \langle \mathbf{u}(0) \cdot \mathbf{u}(s) \rangle ds \quad (46)$$

where $v = |\mathbf{v}|$.

3.2 Simple Shear and Rotational Flows for Kinetic Method and Generalized Langevin Model. Whilst the KM and GLM approaches are compatible with one another for a Gaussian process in the case of homogeneous and statistically stationary turbulence, there is an important difference between the two

Fig. 1 Ratio of long term particle diffusion coefficient $D_p(\infty)$ to long term fluid element diffusion coefficient $D_f(\infty)$ in homogeneous isotropic turbulence, u' = rms fluid velocity, DNS and experimental measurements: (a) shows the influence of particle inertia (Stokes number) $St = \tau_p/T_f$, $v_g = 0$; (b) the influence of settling velocity ratio v_g/u' , symbols represent a range of Reynolds number Re_λ based on Eq. (45) (taken from Squires and Eaton [58])

approaches, namely, the GLM approach provides a model for particle transport and at the same time a model for the turbulence encountered by the particle, which encompasses in the limit of very small particles, the turbulence of the carrier flow itself. In the KM approach, this information must be prescribed independently, either based on experiment, DNS or from a separate model like the GLM.

3.2.1 Analytical Solutions Based on the Kinetic Method. Using the general result in Eqs. (39) and (41) Swailes et al. [27] have evaluated the particle spatial concentration and mean velocity fields in simple shear and rotational mean carrier flow fields and compared them with results obtained from a random flight simulation in which the turbulence is Gaussian with an exponential decaying autocorrelation. Results were obtained for both Stokes drag and a combination of drag and lift appropriate for low particle Reynolds numbers. In all these cases the equation of motion of the particle is given by

$$\ddot{\mathbf{x}} = \dot{\mathbf{v}} = \beta(\mathbf{S} \cdot \mathbf{x} - \mathbf{v} + \mathbf{u}''(t))$$

where $\mathbf{S}$ is the strain rate tensor. Some of their results are reproduced in Fig. 2 for the case of Stokes drag with the particle response times and shear rates normalized on the fluid integral timescale along a particle trajectory. For the simple shear and rotating flow, we have, respectively,

$$\mathbf{S} = \begin{bmatrix} 0 & S \\ 0 & 0 \end{bmatrix} \quad \mathbf{S} = \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix}$$

For the sake of brevity, we show in Fig. 2 only analytic solutions for the form of the underlying mean particle flow for both these types of dispersion at some time after releasing the particles from the origin. Normalizing timescales on the integral timescale of the turbulence, the cases are shown in Fig. 2, correspond to $t = 1, \beta = 1, S = 1, \omega = 1$. We will consider the results for the particle concentration in the simple shear when we consider solutions based on the GLM in the next section for which KM using the same carrier flow autocorrelation along particle trajectories would give identical results. We note that for the simple shear flow the concentration contours are ellipses concentric about the origin of the shear whose principal axes rotate in time as the concentration decays until they align with the carrier mean shear. In

contrast in the rotating flow the concentration contours, like those in uniform flow, are all circles centered about the origin. The rate of diffusion outward is greater than that in the uniform flow because the mean spatial variation of the flow enhances the diffusion (the spreading of the particles).

3.2.2 GLM for a Simple Shear. In this regard, a more detailed analysis has been performed for particle dispersion in a simple shear based on Pope's GLM approach which demonstrates the compatibility of the two approaches whilst at the same time highlighting the extra information that the GLM approach provides relating to the underlying carrier flow encountered by the suspended particles. In this simple case, Pope's analog equation is

$$\begin{aligned} \frac{du_i}{dt} &= \alpha(S_{ij}x_j - u_i) + f_i''(t) \\ S_{ij} &= S\delta_{i1}\delta_{j2} \end{aligned} \quad (47)$$

where α in this case is assumed constant and isotropic.

Using a simple model for the Reynolds shear stresses based on Pope's GLM model [14], exact solutions have been obtained for the particle kinetic stresses (velocity covariances) and the particle diffusion coefficients associated with an instantaneous point source located at the center of the shear [54]. The results for the particle kinetic stresses are shown in Fig. 3(a) as a function of the particle response time suitably normalized on the timescale of the turbulence which is homogeneous and stationary (effectively the particle Stokes number St). x_1 is the streamwise direction and x_2 the cross-streamwise direction. What is plotted is the difference between the streamwise and cross-streamwise components for the normal stresses normalized on $S^2\langle u^2 \rangle$ where S is the strain rate normalized on the time scale of the turbulence. What is noticeable is that the difference is positive and increases with Stokes number. As particles cross the shear, they extract turbulent energy from the mean flow—it's the work done by shear stresses in the streamwise direction which appears as an increase of turbulent kinetic energy in the streamwise direction. The second graph in Fig. 3(b) is even more revealing. A calculation is made of the diffusion coefficients ε_{ij}^S which relate the diffusion current j_i to the gradients of the concentration gradient, i.e.,

$$j_i = \langle u_i \rangle \langle \rho \rangle - \varepsilon_{ij}^S \frac{\partial}{\partial x_j} \langle \rho \rangle \quad (48)$$

Fig. 2 Analytic solutions for the mean particle velocity field for an instantaneous point source at the center of a simple shear flow and a rotating flow: $\beta = 1$; $S = 1$, $\omega = 1$, $t = 1$ [27]

Fig. 3 Dispersion of particles in a simple shear based on Pope's GLM versus Stokes number β^{-1} . S is the strain rate normalized on turbulence integral time scale versus Stokes number β^{-1} . In the graphs $e_{ij}^S = \langle v_i' x_j' \rangle$ [54]

Here we see the particle current composed of a convective term proportional to the local mean carrier flow and a long term diffusive current. What is most interesting is the particle diffusion coefficient in the streamwise direction compared to that in the cross-streamwise direction. We note that for all Stokes numbers it is $-ve$, which includes that for a passive scalar! This does not imply however that contrary to the Second Law of Thermodynamics an elemental volume of particles will always contract rather than expand. These diffusion coefficients make a small contribution to the way an elemental particle volume will diffuse. Particles will diffuse in the streamwise direction because as they move upward or downward they will experience larger positive or negative velocities according to how far away they are from the origin. And that displacement from the origin is randomly positive or negative because it is determined by dispersion in the cross-streamwise direction. So it is this process that makes the elemental volume stretch in the streamwise direction. The $-ve$ diffusion coefficients reduce this process but never reverses it.

Figure 4 shows a picture of the concentration contours and the mean particle velocities at a time $\sim$ integral timescale after they were released from the center of the shear where the mean velocities are almost radial and later where they have rotated to align with the velocities of the shear during which time the contours have expanded. As noted previously the mean concentration contours at any given time are expanding ellipses possessing the same principal axes centered at the origin, which rotate first anticlockwise and then clockwise until the major principal axis aligns with the streamwise direction. The rotational component of the particle mean velocity follows a similar behavior though the changeover from anticlockwise to clockwise is much more gradual. Although one of the principal strain rates of the mean particle velocity field becomes compressible during the approach to equilibrium, the divergence of the mean particle velocity field is always positive ensuring the mean particle concentration decreases everywhere and for all time consistent with the second law of thermodynamics. See Fig. 4 for the corresponding concentration and mean velocity vectors during the dispersion.

Fig. 4 Concentration contours and particle mean velocity; $St = 1$, normalized strain rate $S = 1$, at (a) $t = 1$, (b) $t = 6$ where t is in units of the integral timescale. Concentration contours represent a constant fraction f of the concentration at the center of the shear, $f = 1 - 0.02n$, $n = 1, 2, \dots, k$ [54].

848 The possibility of this occurring has been noted before for pas-
849 sive scalar diffusion [61].

850 **3.3 Analytic Solutions for the Dispersion of Very Inert**
851 **Particles With Nonlinear Drag.** Here we present analytic solu-
852 tions of the kinetic equation given by Reeks [21] for very inert
853 particles, i.e., $St \gg 1$ and in particular the formulae that arise for
854 the long term particle diffusion coefficient $D_p(\infty)$ and mean
855 square velocity $\langle v_i^2 \rangle$ in homogeneous isotropic turbulence. We
856 recall that for particle motion based on Stokes drag, i.e., constant
857 β in Sec. 3.1 for the case of dispersion in uniform flows, the long
858 term particle diffusion coefficient was given by the formula in
859 Eq. (45) which shows that there is no explicit dependence on the
860 particle response time (inertia); its influence is reflected only in
861 the way this quantity determines the timescale of $\mathbf{u}(s)$ along a par-
862 ticle trajectory: whether the carrier flow timescales along a par-
863 ticle trajectory are greater or smaller than those along a fluid
864 element trajectory. We noted that particles with more inertia have
865 a long time diffusion coefficient that is greater than that for a fluid
866 element or passive tracer (see Fig. 1). In the case of very inert par-
867 ticles where the particle drag coefficient is significantly nonlinear
868 in the particle Reynolds numbers, this lack of dependence on par-
869 ticle response time in the formula for the particle diffusion coeffi-
870 cient is still retained, but as it turns out only a very small
871 dependence of the long term diffusion coefficient on the particle
872 Reynolds number. Following [21] and with reference to Eq. (13)
873 we can write the particle equation of motion as:

$$\frac{d\mathbf{v}}{dt} = \beta \Psi[\mathbf{v}, \mathbf{u}(\mathbf{x}, t)] \quad (49)$$

874 where Ψ is a prescribed function of $\mathbf{v}$ and $\mathbf{u}$ whose statistical
875 behavior is derived from the statistics of the turbulent velocity
876 field $\mathbf{u}(\mathbf{x}, t)$. We define it such that when the particle Reynolds
877 number $\ll 1$ $\Psi = \mathbf{u} - \mathbf{v}$. In this way β^{-1} is identical to the particle
878 relaxation time τ_p for Stokes drag. For convenience, we suppose
879 that $\mathbf{v}, \mathbf{x}, \mathbf{u}, t$ are dimensionless variables by suitable scaling of the
880 measured variables on the turbulent intensity u_0 and T_E Eulerian
881 integral time scale of the carrier flow turbulence (which is the
882 timescale of the fluid motion appropriate for high inertia particles.
883 In this instance β^{-1} becomes the particle Stokes number $St =$
884 $\tau_p T_E$ where τ_p is the particle Stokes relaxation time in normal
885 units. By so doing, β is then a direct measure of the strength of the
886 interaction and Ψ a measure of the departure from Stokes drag.
887 High inertial particles for which $St \gg 1$ means that the particles
888 are sufficiently inert to possess velocities small in relation to the
889 turbulent intensity. Note that in the calculation

$$T_E/T_L = \int_0^\infty e^{-1/2z^2} dz = \sqrt{\pi/2} = 1.2533$$

890 T_L is the Lagrangian integral timescale of the fluid motion so
892 that for Stokes drag for very inert particles, the ratio of the long
893 term particle diffusion coefficient to that of the fluid element is
894 given by

$$D_p(\infty)/D_f(\infty) \rightarrow 1.2533 \quad \text{for } St \gg 1 \quad (50)$$

896 We write Ψ more explicitly as

$$\Psi = \Phi(Re_p |\mathbf{u} - \mathbf{v}|)(\mathbf{u} - \mathbf{v}) \quad (51)$$

898 where Re_p is the “turbulent” particle Reynolds number $u_0 d_p/\nu_f$,
899 with u_0 , the turbulent intensity, d_p the particle diameter, and ν_f the
900 kinematic viscosity. Φ is such that $\Phi(0) = 1$, and supposed to be
901 in a form amenable to a power series expansion in Re_p . For small
902 $\mathbf{v}$, the kinetic equation reduces to a Fokker-Planck equation, in
903 which case we have for an instantaneous point source of particles
at $\mathbf{v}, \mathbf{x}$ at time t'

$$\left\{ \frac{\partial}{\partial \tau} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} - \beta' \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} \right\} G(\mathbf{v}, \mathbf{x}, \tau; \mathbf{v}', \mathbf{x}', \tau') \quad (52)$$

$$= \mu \nabla_{\mathbf{v}}^2 G(\mathbf{v}, \mathbf{x}, \tau; \mathbf{v}', \mathbf{x}', \tau')$$

where the time τ is the normalized time t/T_L as with the other
variable and $G(\mathbf{v}, \mathbf{x}, \tau; \mathbf{v}', \mathbf{x}', \tau')$ is the point source of Green's
function phase space density. $\tilde{\Psi}$ is the fluctuating (zero mean)
component of Ψ and

$$\langle \tilde{\Psi}(0) \tilde{\Psi}(\tau) \rangle = \langle \tilde{\Psi}(\mathbf{v}, \mathbf{x}, 0) \tilde{\Psi}(\omega, \mathbf{y}, \tau) \rangle \approx \langle \tilde{\Psi}(0, 0) \tilde{\Psi}(0, 0, \tau) \rangle$$

$\langle \Psi \rangle$ for small $St \gg 1$ is given by $\beta' \mathbf{v}$ where $\beta' \propto St^{-1}$ for which
the constant of proportionality depends only upon Re_p . Precise
evaluation of β' and $\langle \tilde{\Psi}(0, 0) \tilde{\Psi}(0, 0, \tau) \rangle$ is based on an empirical
form for $\Phi(Re_p)$ reliable up to particle Reynolds numbers ~ 500 ,
and based on measurements of drag coefficients for spheres in
steady flow [62], namely,

$$\Phi(Re_p) = 1 + 0.158 Re_p^{2/3} \quad (53)$$

Thus

$$\beta' \simeq St^{-1} (1 + 0.2582 Re_p^{2/3}) \quad (54)$$

with $Re_p = u_0 d_p/\nu_f$ and using the following form for $f(\tau)$ the
Eulerian point time correlation:

$$\int_0^\infty \langle \tilde{\Psi}(0, 0) \tilde{\Psi}(0, 0, \tau) \rangle d\tau$$

$$= (T_E/T_L) (1 + 0.5165 Re_p^{2/3} + 0.0685 Re_p^{4/3})$$

Using these relations the long term particle diffusion coefficient
 $D_p(\infty)$ and the particle means square velocity along any direction
 $\langle v^2 \rangle$ are given by

$$\left(\frac{D_p(\infty)}{u_0^2 T_E} \right) = \left\{ \frac{1 + 0.5165 Re_p^{2/3} + 0.0685 Re_p^{4/3}}{(1 + 0.2582 Re_p^{2/3})^2} \right\} \quad (55)$$

Fig. 5 Particle rms velocity as a function of particle turbulent Reynolds number Re_p for $St \gg 1$ based on the formula in Eq. (46). Note the particle Stokes number $St = \tau_p/T_E$, where T_E is the Eulerian integral time scale of the carrier flow turbulence.

$$\langle v_i^2 \rangle / u_0^2 = \left(\frac{T_E}{\tau_p} \right) \frac{(1 + 0.5165 \text{Re}_p^{2/3} + 0.0685 \text{Re}_p^{4/3})}{(1 + 0.2582 \text{Re}_p^{2/3})}, \text{St} \gg 1 \quad (56)$$

Significantly as stated formula for the long term particle diffusion coefficient is independent of the particle Stokes number St and as it turns out, is very insensitive to the values of Re_p , e.g., the asymptotic value of the formula in Eq. (55) is close to 2% of its value of unity at $\text{Re}_p = 0$, i.e., the value of the particle diffusion coefficient for Stokes' drag (see Eq. (45)). Figure 5 shows the values of normalized particle rms velocity compared to the flow turbulence u_0 for a range of values of Re_p showing a significant enhancement of the particle rms with increasing values of Re_p .

4 Continuum equations and Constitutive Relations for the Dispersed Phase (Without Collisions)

The continuum equations refer to the equations for the transport of mass, momentum, and kinetic stress (which includes kinetic energy) of the particle phase and can be generated from the kinetic-pdf equations for $\langle P \rangle$ or $\langle W \rangle$ by multiplying them by an appropriate power of $m \mathbf{v}_j^p \mathbf{v}_j^q \mathbf{v}_k^r \dots$ and then integrating over all $\mathbf{u}$ and $\mathbf{v}$ (for $\langle P \rangle$) and overall $\mathbf{v}$ (for $\langle W \rangle$) where m is the mass of a particle (assuming that all the particles for the sake of simplicity have the same mass m) and $\mathbf{v}'$ is the fluctuating value of $\mathbf{v}$ relative to its mean density weighted value $\bar{\mathbf{v}}$

$$\text{mass} \langle \rho \rangle = m \int \langle P \rangle (\mathbf{v}, \mathbf{u}, \mathbf{x}) d\mathbf{v} d\mathbf{u} \quad (57)$$

$$\text{momentum} \langle \rho \rangle \bar{\mathbf{v}}_i = m \int \langle P \rangle (\mathbf{v}, \mathbf{u}, \mathbf{x}) v_i d\mathbf{v} d\mathbf{u} \quad (58)$$

$$\text{kinetic stress} \langle \rho \rangle \overline{\mathbf{v}'_i \mathbf{v}'_j} = m \int \langle P \rangle (\mathbf{v}, \mathbf{u}, \mathbf{x}) v'_i v'_j d\mathbf{v} d\mathbf{u} \quad (59)$$

So ρ refers to the instantaneous mass density of the particle phase (i.e., for one realization of the flow field and $\langle \rho \rangle$ the ensemble average of ρ , with $\langle \cdot \rangle$ referring to an ensemble average. So the quantities $\bar{\mathbf{v}}_j$ and $\overline{\mathbf{v}'_j \mathbf{v}'_j}$ are the particle mass mean and mean covariance¹⁰ of the particle velocities at $(\mathbf{x}, t)$. The continuum equations are from Eq. (15)

$$\frac{\partial \langle \rho \rangle}{\partial t} + \frac{\partial}{\partial x_i} \langle \rho \rangle \bar{\mathbf{v}}_i = 0 \quad (60)$$

$$\langle \rho \rangle \frac{D_p}{Dt} \bar{\mathbf{v}}_i = - \frac{\partial}{\partial x_j} \langle \rho \rangle \overline{\mathbf{v}'_j \mathbf{v}'_i} + \langle \rho \rangle \beta \langle u_i \rangle - \bar{\mathbf{v}}_i + \beta \langle \rho \rangle \bar{u}_i' \quad (61)$$

$$\begin{aligned} \langle \rho \rangle \frac{D_p}{Dt} \overline{\mathbf{v}'_j \mathbf{v}'_j} = & - \frac{\partial}{\partial x_k} \langle \rho \rangle \overline{\mathbf{v}'_k \mathbf{v}'_j \mathbf{v}'_i} + \langle \rho \rangle \overline{\mathbf{v}'_j \mathbf{v}'_k} \frac{\partial \bar{\mathbf{v}}_i}{\partial x_k} + \langle \rho \rangle \overline{\mathbf{v}'_j \mathbf{v}'_k} \frac{\partial \bar{\mathbf{v}}_j}{\partial x_k} \\ & - \langle \rho \rangle \beta \left(2 \overline{\mathbf{v}'_i \mathbf{v}'_j} - \left\{ \overline{\mathbf{v}'_i u'_j} + \overline{\mathbf{v}'_j u'_i} \right\} \right) \end{aligned} \quad (62)$$

where $\frac{D_p}{Dt}$ is the particle substantial derivative, i.e.,

$$\frac{D_p}{Dt} = \frac{\partial}{\partial t} + \bar{\mathbf{v}}_j \frac{\partial}{\partial x_j}$$

So we require closed expressions for

(1) $\bar{\mathbf{u}}''$ the average carrier flow velocity relative to $\langle \mathbf{u} \rangle$ encountered by a particle.

- (2) The symmetric component of the covariance of the particle and carrier flow velocities $\mathbf{u}' \mathbf{v}'$.
- (3) $\langle \rho \mathbf{v}'_k \mathbf{v}'_j \mathbf{v}'_i \rangle$ the turbulent kinetic energy flux.

Note the distinction here between variables u''_i and u'_i . Here and throughout we shall use $''$ and $'$ to refer to random variables relative to $\langle \mathbf{u} \rangle$ and particle density weighted averages, respectively, e.g., $\mathbf{v}'' = \mathbf{v} - \langle \mathbf{u} \rangle$; $\mathbf{v}' = \mathbf{v} - \bar{\mathbf{v}}$.

Using the same integration of the closed form of the kinetic equation as was used to obtain the particle momentum equation Eq. (61), identifies the closed form $\bar{\mathbf{u}}''$ in KM as

$$\bar{\mathbf{u}}'' = \beta^{-1} \bar{\boldsymbol{\kappa}} - \langle \rho \rangle^{-1} \nabla \cdot \bar{\boldsymbol{\lambda}} \langle \rho \rangle \quad (63)$$

where $\bar{\boldsymbol{\lambda}}$ refers to an average of $\boldsymbol{\lambda}$ overall particle velocities at $\mathbf{x}$. We recognize $\bar{\boldsymbol{\lambda}} \langle \rho \rangle$ as a stress/pressure tensor which combines with the particle Reynolds stresses to give a pressure tensor $\mathbf{p}$ whose components are expressible in terms of an equation of state (for a fully mixed suspension in bounded homogeneous stationary turbulence), namely,

$$\mathbf{p} / \langle \rho \rangle = \bar{\boldsymbol{\lambda}} + \overline{\mathbf{v}' \mathbf{v}'} \quad (64)$$

where $\mathbf{v}'$ is the particle velocity fluctuation. Equation (64) in turn encapsulates a fundamental relationship between the components of $\mathbf{p}$ and a set of diffusion coefficients ε_{ij} , namely,

$$p_{ij} / \langle \rho \rangle = \beta \varepsilon_{ij}^\dagger \quad (65)$$

$$\varepsilon_{ij} = \beta^{-1} (\overline{\mathbf{v}'_i \mathbf{v}'_j} + \lambda_{ij}^\dagger) \quad (66)$$

where † refers to the transpose. Expressing the right-hand side in the way we have done, is meant to imply a close relationship to the particle diffusion coefficients ε_{ij} associated with particle dispersion in generic flows like those considered in Sec. 3. We note that it's these coefficients that are the analogs of temperature, not the particle kinetic energy. These results have also been derived independently using the Clausius virial theorem of classical kinetic theory [23].

4.1 The Particle Momentum Equation Interpreted as an Advection-Diffusion Equation. To demonstrate in more detail the close relationship between the particle momentum equation and an advection gradient diffusion equation, we rewrite the KM closed form for the particle momentum equation Eq. (61) as an equation for the particle flux $\langle \rho \rangle \bar{\mathbf{v}}$, namely,

$$\begin{aligned} \langle \rho \rangle \bar{\mathbf{v}} = \langle \rho \rangle \left(\underbrace{\langle \mathbf{u} \rangle + \mathbf{v}_g + \beta^{-1} \left\{ \underbrace{[\bar{\boldsymbol{\kappa}} - \nabla \cdot \bar{\boldsymbol{\lambda}}]}_{(1)} - \underbrace{\nabla \cdot \overline{\mathbf{v}' \mathbf{v}'}}_{(2)} - \underbrace{\frac{D_p}{Dt} \bar{\mathbf{v}}}_{(3)} \right\}}_{\text{convective flux}} \right) \\ \underbrace{- \beta^{-1} (\overline{\mathbf{v}' \mathbf{v}'} + \boldsymbol{\lambda}^\dagger) \cdot \nabla \langle \rho \rangle}_{\text{diffusive flux}} \end{aligned} \quad (67)$$

which we have separated into a convective flux and a diffusive flux. For completeness, we have included the gravitational settling velocity in quiescent fluid $\mathbf{v}_g = \beta^{-1} \mathbf{g}$. Term (1) refers to the convective velocity derived from the net turbulent driving force $\bar{\mathbf{f}}$ as the sum of $\bar{\boldsymbol{\kappa}}$ (the body force per unit particle mass) and a kinematic turbulent stress/surface force $-\nabla \cdot \bar{\boldsymbol{\lambda}}$. Term (2) is the turbophoretic force (per unit particle mass) [22] derived from the kinetic stress $-\nabla \cdot \overline{\mathbf{v}' \mathbf{v}'}$. The combination of turbulent and kinetic stresses defines the total pressure tensor $\mathbf{p}$ referred to in the equation of state Eq. (64). Term (3) is the inertial acceleration of the suspended particles which at equilibrium/steady-state conditions is zero or in general very small for weakly interacting

¹⁰Alternatively the particle kinematic kinetic stresses.

inertial particles. In general, it is an important consideration in particle transport in nonuniform inhomogeneous turbulent flows. It is important to point out that in some modeling approaches the turbulent body force given in (1) is either not recognized or unjustifiably set to zero [63]. In the GLM it is not a feature although it could be added to the particle equation of motion but without on its own any formal justification. We see later that the nonzero value of $\bar{\kappa}$ when particle are settling under gravity in a homogeneous flow is responsible for the enhancement of the gravitational settling due to the turbulence, see Sec. 7.7. The diffusive flux defines a diffusion tensor ε with components ε_{ij} as in Eq. (66). According to this approach, gradient diffusion is always the case for particles that follow the flow: indeed the set of diffusion coefficients ε_{ij} in the LHD version reduce to the local average

$$\varepsilon_{ij} = \langle u_i''(\mathbf{x}, t) \Delta x_j(\mathbf{x}, t|0) \rangle \quad (68)$$

In the case of statistical stationary homogeneous turbulence, advection diffusion applies to the case of inertial particles in the long term for dispersion in an unbounded flow when $\beta t \gg 1$, or when the particles are confined and the system approaches equilibrium in which case $\partial \rho / \partial \mathbf{x} \rightarrow 0$. In this case, substituting the formula $\langle v_i' v_j' \rangle = \beta \int_0^\infty e^{-\beta s} u_i''(0) u_j''(s) ds$ and $\Delta x_j(\mathbf{x}, t|0) = \int_0^\infty (1 - e^{-\beta s}) u_j''(s) ds$ into the formula for ε_{ij} in Eq. (66) we obtain the result in Eq. (44) for statistically stationary isotropic homogeneous turbulence.

4.1.1 In the Footsteps of Albert Einstein. It is instructive to point out that similar arguments were used by Einstein [64] to evaluate the diffusion coefficient of Brownian particles that lead to the well-known Stokes–Einstein relation. Here we have an almost identical particle equation of motion except for the driving force (due to the carrier flow turbulence) in our case is not limited to white noise as it is in the case of Brownian motion generated from the molecular bombardment of the suspended particles. What Einstein recognized was that the momentum equation (in his case the balance of the pressure gradient with the weight of the particles) implies a diffusion equation for the suspended particles as they approached their long term equilibrium state and in

particular as the average particle concentration gradient $\nabla \langle \rho \rangle \rightarrow 0$. So instead of an isothermal system, we have a statistical stationary homogeneous isotropic turbulent flow and consider an equilibrium state in which there is a balance between the pressure gradient and a body force acting on the particles, the obvious one being the weight of the particles; so in effect, we are considering the weight of an elemental volume of particles balanced by the pressure gradient acting on it as Einstein did for Brownian motion.

We note however that the coefficients ε_{ij} defined in general in Eq. (66) are not the same as the diffusion coefficients ε_{ij}^S for particle dispersion in a simple linear shear flow referred to in Eq. (48) except in the case of inertialess (passive scalar) particles that follow the flow $\beta^{-1} = 0$. In general

$$\varepsilon_{ij}^S = \langle v_i'' x_j \rangle \quad (69)$$

The reason for the discrepancy between ε_{ij} and ε_{ij}^S for particles with inertia is that while the process is still diffusive (for particles released from the center of the shear) the inertial acceleration term $D \bar{v}_i / Dt$ in the particle momentum Eq. (61) also makes a finite contribution to ε_{ij}^S along with the normal gradient diffusion term in the momentum equation from which ε_{ij} is derived.

4.2 $\overline{u_k' v_j'}$ the Carrier Flow-Particle Velocity Covariances. Referring to the transport Eq. (62) for the particle kinetic stresses (which includes the particles' turbulent kinetic energy), the particle-carrier flow velocity covariances are given in KM by

$$\{\overline{v_m' u_n'} + \overline{v_n' u_m'}\} = 2\mu_{mn}^S \quad (70)$$

Substituting these expressions into the transport Eq. (62) for the particle kinetic stresses gives

$$\begin{aligned} \langle \rho \rangle \frac{D}{Dt} \overline{v_m' v_n'} = & - \frac{\partial}{\partial x_i} \langle \rho v_i' v_m' v_n' \rangle - \left[\frac{\partial v_n'}{\partial x_l} p_{lm} + \frac{\partial v_m'}{\partial x_l} p_{ln} \right] \\ & + 2 \langle \rho \rangle \{ \mu_{mn}^S - \beta \overline{v_m' v_n'} \} \end{aligned} \quad (71)$$

Fig. 6 Simulation (particle tracking) and KM predictions using Chapman–Enskog approximation, Eq. (72) for turbulent pipe flow

where μ_{mn}^S refers to the components of the symmetric part of $\mu = \beta \langle \mathbf{u}''(\mathbf{x}, t) \Delta \mathbf{v}(\mathbf{x}, t|0) \rangle$ and $\mathbf{v}(\mathbf{x}, t|0)$ is the change in velocity of all particles arriving at $\mathbf{x}, t$.

So referring to the terms on the RHS of Eq. (71)

(1) The first term is a third-order velocity moment of the particle pdf which we can refer to as the turbulent kinetic stress flux that for $m = n$ includes the turbulent kinetic energy flux and is a term that requires closure. In this case, one can use the methods developed in kinetic theory to approximate this term. In particular, applying the Chapman–Enskog (C–E) approximation gives the following relationship involving the gradients of the velocity covariance and the particle diffusion coefficients ε_{ij} , a result obtained by Swailes and Sergeev [28] among others:

$$\overline{v'_i v'_j v'_k} = -\varepsilon_{li} \frac{\partial}{\partial x_l} \overline{v'_j v'_k} - \varepsilon_{lj} \frac{\partial}{\partial x_l} \overline{v'_i v'_k} - \varepsilon_{lk} \frac{\partial}{\partial x_l} \overline{v'_i v'_j} \quad (72)$$

Compare their result with the form used for the third-order moment in single phase flow by Daly and Harlow [65]. How accurate and important it is to take it into account is illustrated by the two graphs in Fig. 6 giving a comparison with results from tracking many particles in a channel flow and then averaging. Figure 6(a) shows the particle tracking result for the triple moment in the normal streamwise direction compared with that obtained from the Chapman–Enskog (C–E) approximation and those based on an approximation derived from a transport equation for the triple moments where fourth order moments are closed assuming a Gaussian distribution, known as the quasi-normal approximation. The approximation does well but under predicts the maximum. The center of the channel is at $R = 1$ and the walls at $R = 0$. Figure 6(b) shows the contribution the triple correlation makes to the particle velocity covariance or kinetic stresses, clearly indicating they make a significant contribution near the walls.

(2) The second term in brackets represents “viscous”¹¹ losses from the action of surface forces $\mathbf{p}$ (as defined in Eq. (65)) in changing the shape and size of an elemental volume of the dispersed flow as it moves through the mean shear gradients of that flow. So this term acts as a source of production of turbulent kinetic energy for the suspended particles. We recall in the case of particle dispersion in a simple shear flow the particle rms velocity in the streamwise direction (in the direction of the straining) is greater than that in the cross-streamwise direction by an amount that is proportional to the strain rate, see Fig. 3(a).

(3) The third and fourth terms are net loss and production terms arising from an internal volume dissipative force $-\beta \mathbf{v}'$ (third term) and a driving force $\beta \mathbf{u}''(\mathbf{x}, t)$ (fourth term). Here $\mathbf{v}' = |\mathbf{v}'|$. We note that at equilibrium in homogeneous turbulence

$$\overline{v'^2} = \langle \mathbf{u}''(\mathbf{x}, t) \cdot \Delta \mathbf{v}(\mathbf{x}, t|0) \rangle \quad (73)$$

all other terms being zero. Using the appropriate form for $\Delta \mathbf{v}(\mathbf{x}, t|0)$ gives the correct analytic form in Eq. (46).

4.2.1 Form for the Kinetic Stresses for $St \ll 1$. The particle kinetic stresses depend explicitly on the shearing of the dispersed phase (the term in square brackets in Eq. (71)) and the shearing of the carrier flow (the terms involving $\langle u''_i(\mathbf{x}, t) \Delta v_n(\mathbf{x}, t|0) \rangle$ in Eq. (71)).

To illustrate this behavior still further let us refer to $\langle \mathbf{u}''(\mathbf{x}, t) \Delta \mathbf{v}(\mathbf{x}, t|0) \rangle$ by ζ and divide it into a homogeneous part $\zeta^{(0)}$ (as if the flow was uniform and independent of the shearing of the carrier flow) and a deviatoric part $\delta \zeta$ linear in the local shearing of the carrier flow. Likewise, we divide the particle kinetic stress

into similar components. Consider thus the case when the particle Stokes number $St = (\beta \tau_e)^{-1}$ is very small (almost fluid point motion). Only a balance of the terms of order St^{-1} are important in the kinetic stress equation so that we have

$$\begin{aligned} -2\delta \overline{v'_n v'_m} + \{\delta \zeta_{mn} + \delta \zeta_{nm}\} - \varepsilon_{mi} \frac{\partial \overline{v'_n}}{\partial x_i} - \varepsilon_{ni} \frac{\partial \overline{v'_m}}{\partial x_i} \\ = 2\overline{v'_n v'_m}^{(0)} - \{\zeta_{mn}^{(0)} + \zeta_{nm}^{(0)}\} \end{aligned} \quad (74)$$

The terms on the LHS contain all the deviatoric terms and the terms of the RHS are all the homogeneous terms. The whole equation must express the fact that in this limit, the particle velocity covariances are the same as the carrier flow covariances: this is consistent with the bracketed terms containing all the homogeneous forms and the deviatoric terms being both zero. The implication for the sum of the deviatoric terms being zero is that

$$\delta \overline{v'_n v'_m} = -\varepsilon_{mi} \frac{\partial}{\partial x_i} (\overline{v'_n} - \overline{u}_n) - \varepsilon_{ni} \frac{\partial}{\partial x_i} (\overline{v'_m} - \overline{u}_m) \quad \beta^{-1} \rightarrow 0 \quad (75)$$

that is the particle deviatoric kinetic stresses in the limit of very small particles are linear in the relative shearing between the carrier and dispersed phases. For the case of very large particles, the contribution from the interfacial momentum transfer term to the deviatoric particle Reynolds stresses drops to zero with hence no explicit dependence on the shearing of the carrier flow: the contribution is entirely viscous.

4.3 Constitutive relations Based on the Generalized Langevin Model. The closure expression in this case are transport equations for $\overline{u''}$ and $u'_k v'_j$ derived from the GLM pdf equation for $\langle P \rangle$ Eq. (38). Multiplying Eq. (38) by u_i and integrating overall $\mathbf{v}$ and $\mathbf{u}$ we have

$$\frac{\partial}{\partial t} \langle \rho u_i \rangle + \frac{\partial}{\partial x_j} \langle \rho v_j u_i \rangle = \left\{ \left\{ f_i(\mathbf{x}) - \alpha_{ij} \overline{u''_j} + (\overline{v'_k} - \overline{u}_k) \frac{\partial \langle u_i \rangle}{\partial x_k} \right\} \right\} \langle \rho \rangle$$

Recognizing that we can rewrite the LHS as

$$\frac{\partial}{\partial t} \langle \rho u_i \rangle + \frac{\partial}{\partial x_j} \langle \rho v_j u_i \rangle = \langle \rho \rangle \frac{D_p}{Dt} \langle u_i \rangle + \langle \rho \rangle \frac{D_p}{Dt} \overline{u''_i} + \frac{\partial}{\partial x_j} \overline{v'_j u''_i} \langle \rho \rangle \quad (76)$$

and that from Eqs. (34) and (17)

$$\left(\frac{\partial}{\partial t} + \overline{u}_j \frac{\partial}{\partial x_j} \right) \langle u_i \rangle = \frac{D_f}{Dt} + \overline{u''_j} \frac{\partial \langle u_i \rangle}{\partial x_j}$$

Using the relationship given in Eq. (33), gives finally the transport equation for $\overline{u''_i}$, namely,

$$\begin{aligned} \langle \rho \rangle \frac{D_p}{Dt} \overline{u''_i} = -\frac{\partial}{\partial x_j} \overline{v'_j u''_i} \langle \rho \rangle + \langle \rho \rangle \frac{\partial}{\partial x_j} \langle u''_j u''_i \rangle \\ - \left\{ \frac{\partial \langle u_i \rangle}{\partial x_j} + \alpha_{ij} \right\} \overline{u''_j} \langle \rho \rangle \end{aligned} \quad (77)$$

A transport equation can also be obtained for $\overline{u'_k v'_j}$ by transforming the GLM pdf equation into an equation for $P(\mathbf{v}', \mathbf{u}', \mathbf{x}, t)$, multiplying the resulting equation by $u'_i v'_j$ and then integrating over all $\mathbf{u}'$ and $\mathbf{v}'$. This gives

$$\begin{aligned} \langle \rho \rangle \frac{D_p}{Dt} \overline{u'_i v'_j} = -\frac{\partial}{\partial x_k} \langle \rho \rangle \overline{u'_i v'_j v'_k} - \langle \rho \rangle \overline{v'_j v'_k} \frac{\partial \overline{u''_i}}{\partial x_k} \\ - \left(\langle \rho \rangle \overline{u'_i v'_k} \frac{\partial \overline{v'_j}}{\partial x_k} + \overline{v'_j u'_k} \frac{\partial \overline{u''_i}}{\partial x_k} \right) \\ - \langle \rho \rangle \beta \left(\overline{u'_i v'_j} - \overline{u'_i u'_j} \right) \\ + \langle \rho \rangle \alpha_{ik} \overline{u'_k v'_j} \end{aligned} \quad (78)$$

¹¹Equivalent to viscous losses and increasing the temperature in flowing gas.

Fig. 7 Particle mean streamwise and rms velocity predictions of Simonin [13] using kinetic stress transport equations compared to experimental measurements in vertical channel flow [68] and turbulent round jet [69]

1153 Fluid-particle velocity correlation models
 1154 The general form of α in Pope's GLM is assumed to be linear
 1155 in the local strain rates of the carrier flow the form, i.e.,

$$\alpha_{ij} = \alpha_{ij}^{(0)} + \beta_2 \frac{\partial \bar{u}_i}{\partial x_j} \quad (79)$$

1156 where $\alpha_{ij}^{(0)}$ is the homogeneous (strain rate independent) compo-
 1157 nent and β_2 a constant whose value is obtained from measured
 1158 values of one-point statistics. In the case of the SDM model the
 1159 values of $\alpha_{ij}^{(0)}$ are dependent on the particle motion itself since
 1160 they refer to fluid timescales viewed by the particle. In particular,
 1161 the SDM model accounts for the influence of crossing trajectories
 1162 by choosing the following form for $\alpha_{ij}^{(0)}$:

$$\alpha_{ij}^{(0)} = \frac{\delta_{ij}}{\tau_{fp,\perp}} + \left[\frac{1}{\tau_{fp,\parallel}} - \frac{1}{\tau_{fp,\perp}} \right] \hat{n}_i \hat{n}_j$$

1163 where $\tau_{fp,\perp}$ and $\tau_{fp,\parallel}$ are the turbulent characteristic timescales of
 1164 the fluid velocity fluctuations viewed by the particles in the direc-
 1165 tions normal and parallel to the mean relative velocity vector $\bar{\mathbf{V}}_r$
 1166 between particle and carrier flow which has direction cosines $\hat{n}_i$.
 1167 Thus adopting the same approach as Csanady [60] for gravita-
 1168 tional settling, $\tau_{fp,\perp}$ and $\tau_{fp,\parallel}$ are given by

$$\tau_{fp,\parallel} = \tau_f (1 + C \zeta_r^2)^{-1/2}; \quad \tau_{fp,\perp} = \tau_f (1 + 4C \zeta_r^2)^{-1/2}$$

1172 where the closure of the transport equation for the fluid-particle
 1173 covariances in Eq. (78), we need finally a closed expression for
 1174 the particle-fluid covariance flux $\overline{\rho \mathbf{v}'_i \mathbf{v}'_k}$. In the case of the scalar
 1175 particle fluid covariance $\langle \mathbf{u}' \cdot \mathbf{v}' \rangle$ for which Simonin [66] has used
 1176 a Boussinesq approximation

$$\langle \rho \mathbf{u}' \cdot \mathbf{v}' \mathbf{v}'_i \rangle = -\langle \rho \rangle \nu'_{pf} \frac{\partial}{\partial x_i} \langle \mathbf{u}' \cdot \mathbf{v}' \rangle \quad (80)$$

1178 where ν'_{pf} is referred to as the fluid-particle turbulent viscosity
 1179 written in terms of the timescale of the fluid along a particle tra-
 1180 jectory τ_{pf} , namely,

$$\begin{aligned} \nu'_{pf} &= \frac{1}{3} \langle \mathbf{u}' \cdot \mathbf{v}' \rangle \tau_{pf} \\ \langle u'_i v'_j \rangle &= \frac{1}{3} \langle \mathbf{u}' \cdot \mathbf{v}' \rangle \delta_{ij} + \frac{\langle \mathbf{u}' \cdot \mathbf{v}' \rangle}{\langle u'^2 \rangle} \left[\langle u'_i u'_j \rangle - \frac{1}{3} \langle u'^2 \rangle \delta_{ij} \right] \\ &\quad - \frac{1}{2\beta \langle u'^2 \rangle} \left[\langle \mathbf{u}' \cdot \mathbf{v}' \rangle \left\{ \langle u'_i v'_k \rangle \frac{\partial \bar{y}}{\partial x_k} + (1 - \beta_2) \langle u'_i v'_k \rangle \frac{\partial \bar{u}_j}{\partial x_k} \right\} \right. \\ &\quad \left. - \langle u'_i v'_j \rangle \left\{ \langle u'_m v'_n \rangle \frac{\partial \bar{y}}{\partial x_n} + (1 - \beta_2) \langle v'_m u'_n \rangle \frac{\partial \bar{u}_m}{\partial x_n} \right\} \right] \end{aligned} \quad (81)$$

where $\langle u'^2 \rangle = \langle \mathbf{u}' \cdot \mathbf{u}' \rangle$. For practical application, this algebraic
 expression may be used with the transport equation of the fluid
 particle covariance $\langle \mathbf{u}' \cdot \mathbf{v}' \rangle$ obtained directly from Eq. (78). Fev-
 rier and Simonin [67] go further and derive an even simpler model
 than the algebraic model by assuming that the fluid-particle
 covariance tensor anisotropy is small, so that, for instance, certain
 ratios in the algebraic model equation can be replaced by their
 local quasi-homogeneous value. Thus

$$\frac{\langle \mathbf{u}' \cdot \mathbf{v}' \rangle}{\langle u'^2 \rangle} = \frac{\beta \tau_f}{1 + \beta \tau_f}$$

This sort of approximation gives a Boussinesq or eddy-viscosity
 model for the fluid-particle velocity covariance, namely,

$$\begin{aligned} \langle u'_i v'_j \rangle &= \frac{1}{3} \langle \mathbf{u}' \cdot \mathbf{v}' \rangle \delta_{ij} + \frac{\beta \tau_f}{1 + \beta \tau_f} \left\{ \langle u'_i u'_j \rangle - \frac{1}{3} \langle \mathbf{u}' \cdot \mathbf{v}' \rangle \right\} \\ &\quad - \frac{\nu'_{pf}}{1 + \beta \tau_f} \left\{ \frac{\partial \bar{y}}{\partial x_i} - \frac{1}{3} \nabla \cdot \bar{\mathbf{v}} + (1 - \beta_2) \left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\delta_{ij}}{3} \nabla \cdot \bar{\mathbf{u}} \right) \right\} \end{aligned} \quad (82)$$

4.4 Comparison of Predictions With Experimental Results
for Nonuniform Unbounded Flows. Here we briefly consider
 the application of the kinetic-pdf approach for predicting the con-
 centration, mean velocity, and velocity covariances of a dilute
 suspension of particles in nonuniform unbounded flows where
 near-wall behavior is not a feature. In particular, Fig. 7 shows the

Fig. 8 Turbulent round jet. Further GLM pdf predictions versus experimental measurements of the radial and axial particle rms velocities as a function of radial location for a range of axial distances (Simonin [13]).

1202 predictions of Simonin and Fevrier [13] using a particle kinetic
 1203 stress transport model for the particle mean and rms velocities in a
 1204 vertical channel flow and in a turbulent round jet compared with
 1205 the experimental measurements of Rogers and Eaton [68] for the
 1206 vertical channel flow and that of Hishida and Maeda [69] for
 1207 the round jet. The results show the significant difference between
 1208 the streamwise and normal streamwise rms particle velocities in
 1209 the case of channel flow and between the axial and radial rms
 1210 velocities for the round jet. You can see that the greatest differ-
 1211 ence near the walls in the vertical channel flow where the shear
 1212 stresses are greatest and also near the nozzle in the case of the
 1213 round jet. In both cases this is due to the work done by the kinetic
 1214 stresses as the mean shearing of the particles flow compresses or
 1215 dilates the particle flow in the direction in the streamwise or axial
 1216 direction (see the terms proportional to the mean shearing in
 1217 Eq. (62) which are responsible for the difference). Note that in the
 1218 case of the jet, the kinetic stress transport model gives slightly bet-
 1219 ter predictions for the radial rms velocities than the quasi-
 1220 homogeneous model due to the contribution of the gradients of
 1221 the triple correlation. This is one of many examples where a com-
 1222 parison between model predictions and experimental measure-
 1223 ments have been made.¹²

1224 Figure 8 shows the axial and radial particle rms velocities for
 1225 the turbulent round jet as a function of radial location for a range
 1226 of axial distances from the jet nozzle. Whilst showing the same
 1227 anisotropy in the axial and radial rms velocities as in Fig. 6, the
 1228 Figure also indicates the contribution of the particle fluid covar-
 1229 iances based on the algebraic model (Eq. (81)) and the eddy vis-
 1230 cosity model Eq. (82). Application of the algebraic model
 1231 accurately predicts the values in the particle velocity fluctuations
 1232 in both the axial and radial directions for all measured axial loca-
 1233 tions. The fluid-particle eddy viscosity model is reasonably

accurate in predicting the radial velocity fluctuations but clearly
 under predicts the axial values.

5 Particle–Wall Interactions and Transport in Turbulent Boundary Layers

Not only does this kinetic theory provide a formal way of deriv-
 ing the continuum equations and constitutive relations of the dis-
 persed particle phase but it also correctly deals with the near-wall
 behavior and particle–wall interactions that form the natural
 boundary conditions of the dispersed phase. Applying boundary
 conditions to the continuum equations themselves as is done for
 the continuous phase two-fluid modeling is inappropriate because
 such boundary conditions imposed are artificial. In reality, the nat-
 ural boundary conditions have to do with the particles' response
 to the surface molecular forces which for impacting particles at a
 solid surface express a relationship between the distribution of
 particle velocities before and after impact with possible deposi-
 tion/absorption and subsequent resuspension of the deposited par-
 ticles sometime later. So whilst the velocity distribution at the
 wall is an important feature of the boundary conditions, it is not
 known a priori but is an intrinsic part of the calculation.

In this section, we briefly review the work of Swailes et al.
 [70–73] on the application of the kinetic-pdf approach to near-
 wall behavior in a turbulent boundary and the influence of natural
 boundary conditions. We note that the steep change in the level of
 turbulence near the wall means that only for very small particles
 are the two-fluid equations (mass, momentum, and energy) likely
 to apply. That is the particle distribution of velocities at any posi-
 tion within the turbulent boundary layer will not be locally related
 to the turbulence: depending on its size, a particle will retain some
 memory of its behavior in the far wall or bulk flow. More pre-
 cisely this depends on the variation of the turbulence over a parti-
 cle mean free path defined as the distance a particle travels in a
 time equal to its correlation time ε/v' : the same sort of conditions
 apply in a gas at low pressure when the dimensions of the con-
 tainer are comparable to the molecular mean free path: under such

¹²See the series of Workshops on Two-Phase Flow predictions 1984- (organized by M. Sommerfeld) https://www-mvt.iw.uni-halle.de/events/14th_workshop_two-phase_flows/?lang=en

circumstances, so-called continuum theory no longer applies. It is to be noted that even without the steep change in turbulence, the boundary conditions at the wall are in themselves likely to cause a lack of validity of two fluid model equations simply because the particle wall distribution will be so very much different from the distribution away from the wall (one mean free path away) and far from the assumption that it is close to Gaussian.

However, to begin with we consider particles whose inertia is sufficiently large that their transport through the turbulent boundary layer is ballistic, i.e., they are unaffected by the turbulent boundary layer adjacent to the wall, and for which the effective mean free path of the particles is comparable to the dimensions of the containment. We consider first the interesting case of particles settling out under gravity with partial absorption and diffuse reflection at the wall with inelastic collisions for those particles that rebound. All this is a valuable precursor to a consideration of the way the kinetic approach deals with the most challenging case of transport of particles through a turbulent boundary layer where its rate limits the particle deposition at the wall. It's a case where inhomogeneity of the flow together with the nonlocal nature of the transport and the particle surface interactions (either through impact and absorption followed by resuspension) all play an equally important role

5.1 General Boundary Conditions at the Wall. Referring to Fig. 9, the general boundary conditions for a particle impacting at a wall at $\mathbf{x}$ with velocity $\mathbf{u}$ and rebounding with a range of possible velocities $\mathbf{v}$, is the flux condition

$$\mathbf{v}P(\mathbf{v}, \mathbf{x}, t) = \int_{\mathbf{u} \cdot \mathbf{n} \leq 0} \mathbf{u}P(\mathbf{u}, \mathbf{x}, t)\Theta(\mathbf{v}|\mathbf{u})d\mathbf{u} \quad (83)$$

where $\mathbf{n}$ is the direction normal to the wall at $\mathbf{x}$, and $\Theta(\mathbf{v}|\mathbf{u})$ is the transition or scattering probability density that a particle will rebound with a velocity $\mathbf{v}$ after impacting the surface with velocity $\mathbf{u}$. $\mathbf{u}$ and $\mathbf{v}$ are related deterministically (specular reflection) or stochastically (diffuse scattering as in the case of a microscopically rough surface). Swailes and his coworkers [70–73] have obtained solutions for the pdf equation for simple flows in both these cases. Both cases involve duct flow in which the turbulence is regarded as homogeneous with uniform mean velocity in the streamwise direction. In these cases therefore the particle's response time is sufficiently large that it does not respond to the spatial variations in the mean flow and the turbulence, especially near the wall. In these cases, it is the boundary conditions themselves that determine the near-wall behavior where the continuum equations are inappropriate and the behavior can be well approximated by a simple steady-state solution of the pdf equation in 1D in $\mathbf{x}$ and in $\mathbf{v}$. The conditions for particle response times are consistent with mean carrier flow normal to the wall being set to zero as is the body force due to inhomogeneity in the flow (20). In this case, then the kinetic equation can be normalized in a universal form under steady conditions as [71]

$$\left(\mathbf{v} \frac{\partial}{\partial \mathbf{y}} - \frac{\partial}{\partial \mathbf{v}} \mathbf{v} + \mathbf{g} \frac{\partial}{\partial \mathbf{v}} + \frac{\partial^2}{\partial \mathbf{v}^2} \right) \langle W(\mathbf{y}, \mathbf{v}, t) \rangle = 0 \quad (84)$$

where y is the normal distance from the wall ($y = 0$) and positive velocities are directed toward the wall, particles are acted upon by a gravitational force g directed toward the wall, and velocities and distances are normalized on the particle rms velocity at equilibrium (perfectly reflecting walls) and on the particle mean free path ε/v' .

In the simple flows considered by Swailes et al., the flow is divided into a far wall region which acts as a constant source of particles entering the near-wall region. The interface is set at some distance Y from the wall in particle mean free paths where the spatial distribution of the particles is uniform. It follows from Eq. (84) that this distribution will be Gaussian:

$$w(0, \mathbf{v}) = (2\pi)^{-1/2} \exp\left(-\frac{1}{2}\mathbf{v}^2\right) \text{ for } \mathbf{v} > 0 \quad (85)$$

5.1.1 Method of Solution. The pdf equation is solved numerically using a spectral expansion in terms of Hermite polynomials, looking for solutions in the form

$$w(\mathbf{y}, \mathbf{v}) \approx \sum_{n=0}^N \phi_n(\mathbf{y})\psi_n(\mathbf{v}) \quad (86)$$

where the ψ_n are orthonormal functions based on the Hermite polynomials H_n . They are

$$\psi_n(\mathbf{v}) = \left(\frac{b}{2^n n! \sqrt{\pi}} \right)^{1/2} \exp\left(-\frac{1}{2}(b\mathbf{v})^2\right) H_n(b\mathbf{v}) \quad (87)$$

The inclusion of the scaling factor b allows the placement of a set of collocation points $\mathbf{v}_j$ ($j = 0, 1, \dots, N$), to be optimized. At these collocation points, the approximation in Eq. (86) is exact. In this problem, the collocation points are taken to be the zeros of the function ψ_{N+1} which provide discrete orthonormal properties for $\psi_n(\mathbf{v}_s)$. Substituting the approximation Eqs. (86) into (84) and making it exact at these collocation points gives a system of first-order equations

$$\frac{d}{d\mathbf{y}} \mathbf{W} = \mathbf{A} \mathbf{W} \quad (88)$$

where $\mathbf{W}$ is a column vector whose elements are the values of the pdf at the collocation points and $\mathbf{A}$ is a matrix whose elements are functions of ψ_n^s .

The boundary conditions are given by Eqs. (83) and (85) are discretized at the points $\mathbf{v}_j$. If we define N^* to be the integer such that $\mathbf{v}_j < 0$ for $j < N^*$ and $\mathbf{v}_j \geq 0$ for $j \geq N^*$, then the boundary condition at the interface $y = Y$ can be written as

$$\sum_{n=0}^N \zeta_{jn} w_n = 1, \quad j \geq N^* \quad (89)$$

where $w_n = w(\mathbf{v}_n, Y)$ and

$$\zeta_{jn} = \delta_{jn} (2\pi)^{1/2} \exp\left(\frac{1}{2}\mathbf{v}_j^2\right) \quad j \geq N^* \quad (90)$$

The boundary condition at the wall $y = 0$ is

$$\sum_{n=0}^N \zeta_{jn} w_n = 0, \quad j < N^* \quad (91)$$

where

$$\zeta_{jn} = \delta_{jn} \mathbf{v}_n + h_n^{-1} \sum_{m=0}^N \psi_m^n I_m(\mathbf{v}_j) \quad j \geq N^* \quad (92)$$

with

Fig. 9 Particle impact and rebound velocities at a rough wall

Fig. 10 Velocity distribution $P(v)$ for particles settling under gravity in a homogeneous turbulent flow, impacting at a wall with partial absorption: $v_c = 5$, $v_g = 5$ (in normalized units); impact velocities are for $v \geq 0$

$$I_m(v_j) = \int_0^\infty \psi_m(u) u \Theta(v_j|u) du \quad (93)$$

The interface and wall boundary conditions represent standard two-point boundary conditions for the solutions of Eq. (88) and can be solved by a standard numerical method. Figures 10 and 11 show some of the results obtained by Swailes [70,71], for particle deposition at a wall with or without gravity for specific examples of the wall scattering function $\Theta(v_j|u)$. In each case, results are compared with those obtained from a random walk simulation which simulates the system precisely. In this case, it was assumed that upon impact there was an energy loss which was conveniently described by defining a critical impact velocity v_c below which a particle adhered upon impact but above which a particle rebounds with a prescribed rebound velocity $v = \Theta(u)$. Thus $\Theta(v|u)$ for specular reflection is

$$\Theta = \begin{cases} 0 & 0 < v \leq v_c \\ \delta(v - \theta(u)) & v > v_c \end{cases} \quad (94)$$

modeling the dependence of $v = \theta(u)$ from a constant energy loss upon impact, as

$$v = -\sqrt{u^2 - v_c^2} \quad \text{for } u > v_c \quad (95)$$

gives the simple form

$$\langle W(v, 0) \rangle = \langle W(u, 0) \rangle \quad \text{for } u > v_c \quad (96)$$

where v and u are related by Eq. (95).

We note that $v_c = 0$ (no absorption and no energy loss gives the perfect reflection boundary condition $\langle W(v, 0) \rangle = \langle W(-v, 0) \rangle$, while letting $v_c \rightarrow \infty$ gives the perfect absorption case $\langle W(v, 0) \rangle = 0, v < 0$. Results were obtained for a range of values of the gravitational settling velocity v_g and critical impact velocity v_c . Figure 10 shows the results of solving the kinetic Eq. (84) with those obtained from the simulation for the velocity distribution at the wall for the specific case of a partially absorbing wall with $v_c = 5$ and $v_g = 5$ (in normalized units). Note there are two peaks: one centered at $v = v_g$ and the other one with its center slightly displaced from the origin. The relative heights of these peaks depend upon the ratio of v_c/v_g : for $v_c/v_g = 0$ (zero absorption) the latter peak has a maximum value $v = 0$, with no contribution from the peak at $v = v_g$; in contrast the reverse is the case when $v_c/v_g \rightarrow \infty$

$$I_m(v_j) = \int_0^\infty \psi_m(u) u \Theta(v_j|u) du \quad (97)$$

5.1.2 Diffuse reflection With Deposition. As an illustration, we suppose that particles arriving at the surface are still reflected with a deterministic speed, but now the velocity vector is directed at some random angle α to the surface. Since we are concerned only with particle transport in the direction normal to the wall, we may consider the rebound velocity to be $v = -r \cos \alpha$ where, as in Eq. (95), the deterministic speed is $r = \sqrt{u^2 - v_c^2}$. If $u < v_c$ then the particle is considered to adhere.

A variety of distributions $\Theta(v|u)$ can be constructed depending on the prescribed distribution of α . For illustration, Darbyshire and Swailes [70] considered the simple case where the reflection angle α is uniformly distributed on $(-\gamma, \gamma)$ in which case

$$\Theta(v|u) = \begin{cases} \gamma^{-1} (u^2 - a^2)^{-1/2} & \text{for } a \leq u \leq c \\ 0 & \text{otherwise} \end{cases} \quad (98)$$

where $a(v) = \sqrt{v_c^2 + v^2}$ and $c(v) = \sqrt{v_c^2 + v^2 \sec^2 \gamma}$.

Fig. 11 Wall distribution of velocities for the scattering of particles of a rough surface: left-hand figure, specular reflection $\gamma = 0^\circ$, $v_c = 1$; right-hand figure diffuse reflection $\gamma = 75^\circ$, $v_c = 1$ from Swailes and Darbyshire [70]

Predictions for the velocity distribution at the wall compared with those obtained from random walk simulations are shown in Fig. 11 for $\gamma = 75$ deg. Compare this distribution with that for specular reflection with the same critical impact velocity shown in Fig. 11 which illustrates the essential effect of diffuse reflection, namely, the reduction near the wall of the normal component of the particle rms velocity, the effect becoming more pronounced with increasing γ . These features are accompanied by an increase in particle wall concentration as γ increases.

5.2 Particle Transport in Turbulent Boundary Layers.

There has been intensive research over the last 20 years on the near-wall behavior of particles suspended in a turbulent flow (see, e.g., the review by Li and Ahmadi [74]), in particular how particles interact with near-wall structures and how this transports and deposits them at the wall. In this regard DNS has been particularly useful in simulating the behavior of the fluid motion. Much of our understanding comes from particle tracking in these flows. Of particular note is the work of Soldati [75] in illuminating the transport mechanisms and in developing models for particle deposition which have been the major pre-occupation from a practical point of view. The problems here have been in formulating an appropriate transport equation to account for the influence of the severe changes in the turbulence intensity in the near-wall region which in general makes the particle transport entirely nonlocal, i.e., far from local equilibrium. In this regard, the kinetic-pdf approach has been particularly successful. Whilst the two-fluid equations are inappropriate near the wall, the solution of the pdf

equation itself still provides a valid description. Furthermore, the boundary conditions arising from the particle wall interactions are only expressible in terms of boundary conditions for a pdf equation since as we have said they involve changes in the velocity distribution at the wall. Traditional-fluid modeling is inappropriate because the boundary conditions (bc's) imposed are artificial. We note that advection diffusion models for deposition are implicit in the particle momentum equation derived from the pdf equations where the inertial term is ignored [76]

$$j = \langle \rho \rangle v_d - \varepsilon \cdot \frac{\partial \langle \rho \rangle}{\partial \mathbf{x}} \quad (99)$$

where

$$v_d = -\tau_p \frac{\partial}{\partial \mathbf{x}} \cdot \langle \mathbf{v} \mathbf{v} \rangle + \kappa - \frac{\partial}{\partial \mathbf{x}} \cdot \lambda \quad (100)$$

The drift velocity v_d is composed of essentially two terms that are of different origin. The first term arises from the gradients of the kinetic stress and reflects a balance between a drag force and the gradients of stress, whilst the remaining terms are derived from body forces that arise directly from spatial inhomogeneity in the flow. The first term has often been referred to as turbophoresis [22].

5.3 Particle Deposition in Turbulent Boundary Layers.

Deposition of particles in turbulent pipe flow has a huge literature

Fig. 12 Particle near-wall behavior as a function of distance from wall y^+ and particle response time τ^+ (both in wall units), van Dijk and Swailes [77] σ_{p2} is the local particle equilibrium rms velocity in the wall normal direction

Fig. 13 Particle deposition in turbulent pipe flow Zaichik [81]

from very large values where the motion is basically ballistic (no response at all to the near-wall turbulence). Figure 12(b) shows the ratio of the rms of the particle wall normal velocities, v_2 to the local rms velocity of the carrier flow u_2 as a function of distance from the wall, indicating that this ratio $\gg 1$ as you approach the wall because of the particles' inertia and the much higher velocities they have attained further away from the wall where the gradients of the turbulence are much less.

Figure 12(c) for the particle pdf $p(v_2, x_2)$ shows that particles enter the domain at $x_2 = 100$ for $v_2 < 0$, and subsequently move toward the wall via, mainly, a diffusive mechanism; the pdf remains close to the local equilibrium state over a large part of the spatial domain. Closer to the wall, at about $x_2 = 20$, the fluid rms velocity decreases rapidly. The effect of this is that the particles are no longer driven by diffusion, but start moving in free flight ballistically. Most of the heavy particles ($\tau^+ = 300$, see Fig. 12) have enough momentum to reach the wall, even those that have a relatively low speed. Only very slowly moving particles get trapped near the wall, and slowly drift towards adhesion at $x_2 = X_0$. This results in a small build-up near the wall of particles with low velocity. For lighter particles ($\tau^+ = 10$, Fig. 12(c)) only the fast particles reach the wall in free flight while most will be trapped. Hence the very sharp peak in the pdf around zero particle velocity. This feature would not be picked up in particle tracking because of the requirement of a very high resolution. This results in a strong build-up in concentration which is also clearly visible in Fig. 12(a), where the particle concentration, ρ , in the boundary layer is shown. In fact, recent work suggests that there is a threshold velocity of τ^+ below which particles are trapped in the region of almost stagnant fluid near the wall and never get deposited, see the recent analysis of Sikovsky [78]. Similar features have been observed in particle pair collisions in homogeneous isotropic turbulence [79,80]. The normalized particle velocity distribution, presented in Fig. 12(d), illustrates this process as well: the distribution for $\tau^+ = 300$ has a significant tail, while for $\tau^+ = 10$ the distribution is strongly localized near $v_2/\sigma_{p2} = 0$.

Finally, Fig. 13 shows the predictions of the particle deposition velocity (normalized on the friction velocity) j^+ as a function of particle response time τ^+ obtained by Zaichik [81] compared to a range of experimental and DNS results. In particular, Zaichik's predictions were obtained by solving a closed set of moment equations derived from the kinetic equation. The closure is based on a quasi-normal assumption for the fourth-order moments of particle velocity and local-equilibrium closure for third-order moments (neglecting their advection). The method of the solution has thus much in common with the RANS approach in CFD involving Reynolds stress transport equations. Given the experimental error is very large the pdf solutions predict the huge

Fig. 14 Removal of a particle from a surface by aerodynamic forces in a turbulent boundary layer. Note in the diagram on the left-hand side the deformation of the sphere in the region of contact with the surface is exaggerated.

changes in deposition velocity from 10^{-1} to 10^{-5} for a change in τ^+ from 10 to 10^{-1} which reflects the role of particle inertia on the deposition.

5.4 Particle Resuspension From Surfaces in a Turbulent Boundary Layer. Kinetic equations and their solutions play an important role in deriving a formula for the rate constant for the removal of particles from an adhering surface by near wall aerodynamic forces. The process is similar to the desorption of molecules from a surface and the rate constant for removal is very similar to the Arrhenius formula for the molecular desorption rate [82,83]. Because the near flow is turbulent it is necessary to take account of the contribution of the fluctuating removal forces as well as the mean forces. This means that the process is stochastic rather than a force balance between the adhesive forces holding the particles onto the surface and the aerodynamic removal forces. More particularly the removal process is described by a probability per unit time of a particle being removed from a surface or equivalently a rate constant. So if the rate constant for removal p , the fraction of particles $f_R(t)$ remaining on a surface at time t is given by

$$f_R(t) = \exp(-pt) \quad (101)$$

Figure 14 shows the aerodynamic removal forces acting on a spherical particle on a smooth surface in a turbulent boundary layer together with the van der Waals adhesive force holding the particle onto the surface. It shows the spherical particle to be deformed in the contact area between particle and surface (much exaggerated in Fig. 14 indicating the presence of elastic restoring forces that balance the adhesive force when the particle is sitting on a surface in static equilibrium (in the absence of external forces). We can represent the dependence of the surface forces (adhesive and elastic forces) and a mean removal lift force upon surface deformation by a surface potential well, a typical profile is shown in Fig. 14. This shows a position of stable equilibrium, A, where the adhesive force balances the repulsive elastic restoring force and a constant mean lift force, and a position of instability, B, where the attractive adhesive force balances the mean lift force. Increasing the mean lift force reduces both the width of the potential well and Q , the height of the potential barrier of B above A, that a particle has to overcome before it can be detached from the surface. We suppose that the number of particles on the surface is sufficient to form an ensemble of all realizable states of a single particle in a constant potential well. The fluctuating removal force will cause the particle-surface deformation $y(t)$ to oscillate randomly about the point of minimum potential at A until a particle derives enough energy from the fluctuating forces (the turbulence) to escape over the potential barrier at B and detached from the surface. The objective, therefore, is to use the pdf equation to calculate the flux of particles out of the well at B and this quantity divided by the number of particles in the well, is the probability per unit time of a particle escaping from the well, i.e., the resuspension rate constant.

In using the solution of kinetic equations to evaluate the rate constant, we recognize that the phase space dispersion coefficients μ and λ are functions of the particle surface deformation y . In the case of a harmonic potential, the displacement $\Delta y(t)$ in Eq. (27) determines the dispersion coefficients corresponding to the solution of a very stiff, lightly damped harmonic oscillator. Thus for a particle of mass m , the deformation displacement $\Delta y(t)$ at time t , about the point of minimum potential A, is obtained from the solution of a damped harmonic oscillator equation of motion of the form

$$\ddot{\Delta y}(t) + \beta \dot{\Delta y}(t) + \omega^2 \Delta y(t) = m^{-1} f_L(t) \quad (102)$$

where $f_L(t)$ is the random fluctuating component of zero mean associated with the total aerodynamic lift force

$$F_L = \langle F_L \rangle + f_L(t) \quad (103)$$

where $\langle F_L \rangle$ is the mean lift force which in this instance is assumed independent of time, ω is the natural frequency based on the harmonic approximation for small deformations about A, and β is the fluid and mechanical damping term. Reeks, Reed, and Hall [84] show that the rate constant p can be written as

$$p = \frac{\omega_0}{2\pi} \exp(-Q/\langle PE \rangle) \quad (104)$$

where $\langle PE \rangle$ is the average potential energy of the particles in the potential well and ω_0 a frequency for particle motion in the well. Both these quantities reflect a process of energy transfer from the turbulence to a particle in the potential well, the particle being resuspended when it has accumulated enough vibrational energy to detach itself from the surface. This is the basis of the kinetic model of Reeks, Reed, and Hall [84] which allows for the possibility of resonant energy transfer when the forcing frequency of the lift force fluctuations is not too different from the natural frequency of vibration of the particle-surface deformation. Under such circumstances, a particle is removed much easier from a surface than applying the same lift force quasi-statically (which is the basis of the simple force balance approach). It is a more general model than the so-called force balance model because it admits the possibility of resonant energy transfer. When this transfer is zero, then the formula for the resuspension rate constant reduces to the form appropriate to a force balance. That is the motion of the particle/surface deformation is approximated by a quasi-static balance between the instantaneous aerodynamic lift force and the adhesive force at each location/deformation in the adhesive surface potential well. This implies a functional relationship between the particle deformation and the removal force at each instant of time. Both resonant energy transfer and quasi-static removal are two extremes in the value of ω_0 and $\langle PE \rangle$ depending on the value forcing frequency $n = (\langle \dot{f}_L^2 \rangle / \langle f_L^2 \rangle)^{1/2}$, so for $n \ll \omega$, $\omega_0 \rightarrow n$, $n \rightarrow \omega$, $\omega_0 \rightarrow \omega$ with corresponding values for $\langle PE \rangle$ at these limiting frequencies.

The situation of smooth contact of a sphere with a surface represented in Fig. 14 is somewhat idealized. In reality, microscopic roughness significantly reduces the adhesion between particles and surface even in the case of particle contact with a polished surface. Contact with the surface is made by surface asperities so that the area of contact and hence adhesion is much reduced from that for perfectly smooth contact. In this case, experiments have shown that particles are removed from surfaces by rolling where the drag force plays a much more significant role than the lift force. Even so, the formula in Eq. (104) still applies if the potential energy is based on the rocking and rolling of particles about surface asperities and equivalent forces involving the drag force are used rather than lift forces normal to the surfaces as in Fig. 14(a). We refer to Reeks et al. [85–87] for the way these models have been developed and applied to the resuspension of monolayer and multilayer coverages of particles on a rough surface, where the decay in the resuspension rate decays in the long term inversely with time in contrast to a smooth surface where the decay is exponential [88].

6 Kinetic Equations for Particle Pair Mixing and Collisions

In this second part of this review, we examine and assess the way this kinetic theory has been used to describe the statistical motion of particle pairs in turbulent flows. In particular how it has been used to quantify interparticle collision rates and the influence they have on the continuum equations and constitutive relations for a particle suspension in a turbulent gas. There is an obvious similarity between colliding particles in a turbulent gas and colliding gas molecules, reflected in the form of the collision integrals in the kinetic and Maxwell–Boltzmann equations. However, we

shall see later there are important differences regarding the legitimacy of the molecular chaos assumption used for molecular collisions when applied to particles colliding in a turbulent gas.

We shall also consider how the kinetic approach can be used to quantify the demixing or segregation of particles at the small scales of turbulence through the calculation of the distribution of particle pairs as a function of their separation. The segregation influences the collision rates since it brings particle pairs closer together, to begin with and this, in turn, causes droplets to coalesce and solid particles to agglomerate. In the case of agglomeration, it is necessary to also consider whether particles stick or bounce upon collision or whether they detach from one another sometime later. There is an obvious parallel here with similar processes of deposition and resuspension of particles to surfaces in a turbulent boundary layer (Secs. 5.3 and 5.4).

The calculation of binary collision rates which interests us here and the issues that surround it necessitates the use of a two-particle/pair pdf $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2, t)$ where subscripts 1 and 2 refer to particles 1 and 2. The net collision rate of an individual particle with surrounding particles depends upon the relative velocities $\mathbf{v}_2 - \mathbf{v}_1$ between particle pairs and their concentration at their separation $\mathbf{x}_2 - \mathbf{x}_1$ upon collision. The influence of both on the collision rates is reflected in the value of the collision kernel which we will define and formulate in terms of the two particles pdf and discuss its dependence on the particle response to the small and large scales of the turbulence. As a matter of definition and convenience when dealing with a total of N particles suspended in a turbulent flow, we will normalize P_2 such that the integral of P_2 over all $\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2$ is $N(N-1)$ and the integral of P_2 over all $\mathbf{v}_2, \mathbf{x}_2$ is P_1 .

When considering a suspension of monodisperse particles there are essentially two mechanisms that influence and control the collision between individual particles. The first mechanism we will refer to as *the local equilibrium approach* and is due to the lack of correlation of the particle motion with the local fluid motion and is entirely dependent upon the particle inertia defined in terms of the Stokes number as the ratio of the particle response time to the large and inertial range of turbulent scales. For these particles, though they may partially or approximately follow the large scales of the turbulence of the suspending carrier flow they are ballistic on the scale of the small scale motion and the difference in velocities imposed by the shearing of the large scales is virtually zero. It is the influence of these particles whose stop distances (spatial correlation) are comparable to the integral length scale of the carrier flow that influences the mass, momentum, and energy equations of the dispersed phase and it is necessary to add an extra term to the kinetic equation to account for their collisions. This term is precisely analogous to the Boltzmann collision integral in the Maxwell-Boltzmann equation but accounting for the relative motion of particle and fluid. This feature highlights the invalidity of the molecular chaos assumption for particle collisions in turbulent flows except for very inert particles when particles and fluid motion are uncorrelated.

The second mechanism is due to the random shearing of the flow and is associated with the small dissipating eddies of the turbulence. This gives rise to a velocity difference for colliding particles arising from the difference in carrier turbulent velocities encountered by particle pairs at the point of collision (the separation of the centers of two colliding spheres being known as the collision radius). This difference in particle velocities will also depend upon the particle response to the shearing itself measured by the particle's Stokes number St_K defined as the ratio of the particle response time τ_p to the typical shear rate $\sim(\epsilon_f/\nu_f)^{1/2}$ where ϵ_f is the turbulent energy dissipation rate. The influence of particle inertia defined in terms of St_K is similar to that of particle inertia defined in terms of τ_p^+ for particles deposited at a wall in a turbulent boundary layer where the velocity of depositing particles and local concentration has more to do with the history of their motion than their response to the local fluid motion. So it is the same in this case with regard to the difference in fluid velocity

experienced by a particle pair as a function of separation as the particles approach collision with some memory of the greater separation of velocities from encounters with small scales at earlier times and greater separation. Accompanying this is the process of segregation or clustering observed at the small scales which leads to an increase in the particle concentration in the neighborhood of individual particles and enhances their collision rate with other particles. We refer to this process as the *nonlocal equilibrium approach* and shall discuss this process and how the kinetic approach can be used to capture and quantify both aspects of this mechanism in more detail later on.

In the Secs. 6–8 we discuss both these mechanisms in detail but we begin first with the formulation of the collision kernel in terms of the particle pair pdf.

6.1 The Particle Collision Kernel. The particle collision kernel $\Gamma(\mathbf{x})$ is $\bar{z}$, the net collision rate of an individual particle with surrounding particles normalized by their average number concentration of particles within a control volume. The number of particles remains constant in time (or more correctly the average concentration sufficiently far away from the individual particle at $\mathbf{x}_1$ that is constant).¹³ More precisely the collision rate is the integrated influx j^+ of surrounding particles colliding with an individual particle integrated over the total collision surface formed by the colliding particles. In terms of the particle pair distribution pdf $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2, t)$ for arbitrary shaped particles and size, $\bar{z}$ is therefore given by

$$\bar{z} = \bar{n}^{-1}(\mathbf{x}_1, t) \int_{dS \cdot (\mathbf{v}_2 - \mathbf{v}_1) \leq 1} P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_1 + \mathbf{r}_c, t) (\mathbf{v}_2 - \mathbf{v}_1) \cdot d\mathbf{S}(\mathbf{r}_c) d\mathbf{v}_1 d\mathbf{v}_2 \quad (105)$$

where $\bar{n}(\mathbf{x}_1, t)$ is the average number concentration of particles at $\mathbf{x}_1$ at time t , $\mathbf{r}_c$ defines the point of contact between an individual particle at $\mathbf{x}_1$ and a neighboring particle at $\mathbf{x}_1 + \mathbf{r}_c$ and $d\mathbf{S}(\mathbf{r}_c)$ is an elemental surface area whose normal is along the line of centers of the colliding particles at the point of contact. So $\mathbf{r}_c$ defines the location of the collision surface for all possible particle pair collisions. In the case of two small colliding spherical droplets of radii r_1 and r_2 , the collision surface is a sphere of radius $r_c = r_1 + r_2$ and for collisions in isotropic homogeneous turbulence, the distribution of relative velocities along the line of centers $\phi_r(w_r)$ is spherically symmetric (independent of ϕ, θ) and independent of $\mathbf{v}_1$ and $\mathbf{x}_1$. So if we consider collisions with a single particle

$$\bar{z} = 4\pi r_c^2 n(r_c) 1/2 \int |w_r| \phi(w_r) dw_r \quad (106)$$

where $n(r_c)$ is the number concentration of surrounding particles at r_c . The factor of $1/2$ reflects the condition on the velocities for a collision in Eq. (105) and to account for the fact that half the particles are moving toward a surface as are moving away, reflecting the fact that the surface is perfectly reflecting. So we write explicitly

$$\Gamma = \bar{z}/\bar{n} = 2\pi r_c^2 g(r_c) \langle |w_r| \rangle \quad (107)$$

where $g(r_c) = n(r_c)/\bar{n}$ is known as the radial distribution function [6] and accounts for the enhancement of collision rates due to clustering or segregation. $\bar{n}$ may also be interpreted more precisely as the value of $n(r)$ at a sufficiently large distance $r \gg r_c$ from an individual particle that the concentration of surrounding particles is effectively constant and equivalent to the fully mixed concentration. $\langle |w_r| \rangle$ is the net velocity toward any individual

¹³Compare this definition with that of that for the 'deposition velocity' of particles to a surface exposed to a turbulent flow.

particle of neighboring particles at the collision radius along their line of centers.

6.2 The Influence of the Particle–Fluid Velocity Correlation on Particle Collisions (the Equilibrium Mechanism). The way particle pairs close together to interact with a coherent carrier flow turbulent structure increases the correlation of the velocity of the particles to the local fluid velocity and in turn the correlation between them. In so doing it reduces the relative velocity between particle pairs and their collision rate over the lifetime of the coherent structure (see Zhou et al. [89] for a simple 1D model). This can easily be seen in the expression for the mean square relative velocity $\langle v_{12}^2 \rangle$ between particle pairs in terms of the covariances of the individual particle pair velocities $\mathbf{v}_1$ and $\mathbf{v}_2$, namely,

$$\langle v_{12}^2 \rangle = \langle v_1^2 \rangle + \langle v_2^2 \rangle - 2\langle \mathbf{v}_1 \cdot \mathbf{v}_2 \rangle \quad (108)$$

for which w_r is the resolved component of $\mathbf{v}_{12}$ along the line of centers. Following Lavieville [90,91], Simonin [13], and Zaichik [92], we can see the influence of the fluid–particle velocity correlation on the particle pair pdf, $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2, t)$ if we introduce the joint two point pdf of particle and fluid velocities $\mathbf{v}, \mathbf{u}$, respectively, namely, $P_2(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{u}_2, \mathbf{x}_2)$ and given in terms of conditional probabilities as

$$P_2(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{u}_2, \mathbf{x}_2) = P_1(\mathbf{v}_1, \mathbf{x}_1 | \mathbf{u}_1) P_1(\mathbf{v}_2, \mathbf{x}_2 | \mathbf{u}_2) P_2(\mathbf{u}_1, \mathbf{u}_2) \quad (109)$$

where $P_1(\mathbf{v}_1, \mathbf{x}_1 | \mathbf{u}_1)$ means the conditional probability density for a particle velocity $\mathbf{v}_1$ measured at $\mathbf{x}_1$ conditional upon there being a fluid velocity $\mathbf{u}_1$ at the same position $\mathbf{x}_1$ and $P_2(\mathbf{u}_1, \mathbf{u}_2)$ is the joint probability distribution of carrier flow velocities $\mathbf{u}_1$ and $\mathbf{u}_2$ encountered by particles 1 and 2 at $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively. We have

$$P_1(\mathbf{v}_1, \mathbf{x}_1 | \mathbf{u}_1) = P_1(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1) / P_1(\mathbf{u}_1) \quad (110)$$

and similarly $P_1(\mathbf{v}_2, \mathbf{x}_2 | \mathbf{u}_2)$ where $P_1(\mathbf{u}_1)$ is the probability distribution of carrier flow velocities observed by particle 1 at $\mathbf{x}_1$

From the two point particle–fluid velocity distribution $P_2(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{u}_2, \mathbf{x}_2)$ we can calculate $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2)$ from

$$P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2) = \int P_2(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{u}_2, \mathbf{x}_2) d\mathbf{u}_1 d\mathbf{u}_2 \quad (111)$$

using the relationship in Eq. (109) and assumed formulae for the conditional probabilities. Lavieville et al. [90] in the case of statistical stationary homogeneous isotropic turbulence, assumed a Gaussian for the conditional probabilities that involve ξ the particle–fluid velocity correlation coefficient based on the local equilibrium between particle and carrier flow at a fixed point in space, i.e., for an isotropic turbulent flow, namely,

$$\xi = \frac{\langle \mathbf{u} \cdot \mathbf{v} \rangle}{\langle v^2 \rangle^{1/2} \langle u^2 \rangle^{1/2}} \quad (112)$$

where, e.g., $\langle v^2 \rangle = \langle \mathbf{v} \cdot \mathbf{v} \rangle$. The implicit assumption is that this correlation is the same as the Lagrangian correlation which because of homogeneity, is independent of position, i.e.,

$$\langle \mathbf{v}(\mathbf{x}, t) \cdot \mathbf{u}(\mathbf{x}, t) \rangle = \langle \mathbf{v}(\mathbf{x}, 0 | t) \cdot \mathbf{u}(\mathbf{x}, 0 | t) \rangle_{t \rightarrow \infty} = \beta^{-1} \mu_\infty$$

For Stokes' drag assuming an exponential autocorrelation for the flow velocity along a particle trajectory

$$\xi = (\langle v^2 \rangle / \langle u^2 \rangle)^{1/2} = 1 / (1 + St_L)^{1/2} \quad (113)$$

where St_L is the particles Stokes number $1/\beta T_L$ where T_L is the Lagrangian integral timescale of the fluid motion (in the case of

Lavieville's model [90,93] T_L is associated with the large scale motion). The form for $P_2(\mathbf{u}_1, \mathbf{u}_2)$ in Eq. (109) used in the evaluation of $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2)$ in Eq. (111) is based on a two point particle joint Gaussian distribution for the components of $\mathbf{u}_1, \mathbf{u}_2$ involving the longitudinal and lateral velocity correlation $F(r)$ and $G(r)$, respectively, where r is the distance between the particle pair. This gives rise to a Gaussian distribution in the particle velocities $\mathbf{v}(\mathbf{x}_1), \mathbf{v}(\mathbf{x}_2)$ which when transformed to a distribution $P_1(\mathbf{w})$ for the relative velocities $\mathbf{w}$ between particle pairs implies a similar Gaussian distribution for the fluid velocities but with values for the radial and normal components velocity correlation $F(r)$ and $G(r)$ scaled by ξ^2 . Thus the radial distribution is given by

$$P_1(w_r) = (2\pi \langle w_r^2 \rangle)^{-1/2} \exp(-w_r^2 / 2 \langle w_r^2 \rangle) \quad (114)$$

where at the point of contact between colliding particle

$$\langle w_r^2 \rangle = 2 \langle v^2 \rangle (1 - F(r_c)) \quad (115)$$

and that with reference to the collision kernel Γ defined in Eq. (107)

$$\langle |w_r| \rangle = \left(\frac{2}{\pi} \langle w_r^2 \rangle \right)^{1/2} \quad (116)$$

So the formula in Eq. (115) accounts for both the effects of the induced correlation of particle motion with that of the local fluid for each member of the particle pair and the spatial correlation between particle pair velocities arising from the spatial correlation of fluid velocities themselves. Zaichik [94] has used these formulae to obtain expressions for Γ for the large scale, intermediate inertial subrange, and small scale viscous dissipating (Kolmogorov) range of scales, considering both the influence of particle pair separation and fluid-particle correlation and its dependence on particle inertia. In particular, substituting the formulae for $\langle w_r^2 \rangle$ and $\langle |w_r| \rangle$ into Eq. (107) for Γ and ignoring segregation, we have

$$\Gamma = 4\sqrt{\pi} r_c^2 \langle v^2 \rangle^{1/2} (1 - F(r_c))^{1/2} \quad (117)$$

Whilst the results reproduce the Saffman and Turner [95] result for the collision kernel of inertialess passive scalar particles in the small scale viscous dissipating range and the result of Abrahamson [96] for the large scale large inertia $St_L \gg 1$, the approach implicitly assumes a local equilibrium between particles and carrier flow which is inappropriate for collision at the small scale. The approach does not take account of the memory and history of the particle pair separation and the relative velocities the particles encounter throughout the entire particle pair history before they collide. It assumes furthermore that particles are fully mixed, that any particle sees a uniform concentration of particles surrounding it. The process we may see is precisely analogous to the way particles are transported through a turbulent boundary layer, where there is a concentration build-up near the wall and nonlocal particle velocities at the wall. A number of deposition models in a turbulent boundary exploit this memory through the concept of free flight to the wall and are missing from this local equilibrium approach. We shall see also that using a solution of the kinetic equation for relative particle motion this feature is accounted for in a way similar to the way the solution of the kinetic equation accounts for these features for particle transport in a turbulent boundary layer discussed in Sec. 5 and in particular the results of Swales and Van Dyke [77]

6.3 Contribution of Interparticle Collisions to the Dispersed Phase Continuum Equations. In this section, we consider the transport of particles in a turbulent flow and the influence interparticle collisions have on the continuum equations of the dispersed particle phase. We shall approach this in a similar

way to the approach we used to obtain the continuum equations due to the turbulence acting alone. That is we consider the way the collisions affect the kinetic equation for a single particle as an additional term that represents the rate of change $\partial P/\partial t$ due to particle collisions within and outside an elemental volume in particle phase space. Using the analogy of solid particle collisions with those of gas molecules, following the work of Lavieville, Simonin, Zaichik et al. [66,90,93,97] we evaluate the Boltzmann collision integral for the collision of inelastic solid spheres. As in kinetic theory, we assume that the particle suspension is sufficiently dilute that only binary collisions are significant. We are specifically interested in cases where the particles response time $\beta^{-1} \sim$ the integral time scale T , $St_L \sim 1$. We note that experiment and numerical simulations have indicated that inert particle collisions have a measurable influence on coarse particle transport properties in gas-solid turbulent flows, even for small values of the dispersed phase volume fraction, $\alpha \sim 10^{-2}$. Neglecting hydrodynamic interaction between colliding particles, hard sphere kinetic theory can be used to account for interparticle inelastic collisions in a kinetic-pdf approach to particle flows.

Thus referring to Fig. 15 for an inelastic collision between two identical spherical particles labeled 1 and 2

$$\begin{aligned} \mathbf{v}_1^* &= \mathbf{v}_1 + \frac{1}{2}(1 + e_c)(\mathbf{v}_{21} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} \\ \mathbf{v}_2^* &= \mathbf{v}_2 - \frac{1}{2}(1 + e_c)(\mathbf{v}_{21} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} \end{aligned} \quad (118)$$

where $\mathbf{v}_1^*$ and $\mathbf{v}_2^*$ the velocities of particles 1 and 2 after the collision related to the velocities $\mathbf{v}_1$ and $\mathbf{v}_2$ before the collision, involving the coefficient of restitution e_c , the unit vector $\hat{\mathbf{n}}$ directed from the center of the first colliding sphere to the center of the second at impact and $\mathbf{v}$ is the relative velocity of particle 2 with respect to that of particle 1 at impact. Note that there is no interparticle friction.

Whilst there are certain obvious similarities between molecular collisions and particle collisions in a turbulent flow, there are as we have pointed out earlier however fundamental differences, namely, that in the kinetic theory of dilute gases, the statistics of binary collisions are derived by assuming that the velocities and positions of any two particles are independent of each other (the molecular chaos assumption). Whereas, in gas-solid flow, the probable positions and velocities of colliding particles will definitely be correlated through their interaction with the same

surrounding turbulent flow. In this section, we describe the original approach due to Simonin [98] which ignores this correlation, and then the approach first proposed by Laviéville et al. [90] and developed extensively by Simonin and Zaichik et al. which attempts to take it into account.

6.3.1 The Boltzmann Collision Integral for a Suspension of Particles in a Turbulent Flow. If particle-to-particle interactions in which more than two particles take place are assumed to be negligible in number and effect, the collision pdf rate of change may be written in terms of the particle-particle pair probability distribution function $P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2, t)$ for particle 1 with velocity $\mathbf{v}_1$ at position $\mathbf{x}_1$ and particle 2 with velocity $\mathbf{v}_2$ at position $\mathbf{x}_2$ for which special closure assumptions are needed. The net rate of change of the number of particles within an elemental volume of phase space $d\mathbf{v}_1 d\mathbf{x}_1$ at $\mathbf{v}_1, \mathbf{x}_1$ due to collisions with particles at $\mathbf{x}_1 + d_p \hat{\mathbf{n}}$ is made up of two contributions: first a rate of loss directly due to collisions of particles within the phase space volume $d\mathbf{v}_1 d\mathbf{x}_1$ with particles at $\mathbf{x}_1 + d_p \hat{\mathbf{n}}$ over the collision surface for all particles with relative velocities directed toward the collision surface. Referring to Fig. 15, we can write this explicitly as

$$\begin{aligned} \partial P^-(\mathbf{v}_1, \mathbf{x}_1, t)/\partial t &= -d_p^2 \int \int_{\mathbf{v}_{21} \cdot \hat{\mathbf{n}} > 0} \hat{\mathbf{n}} \cdot \mathbf{v}_{21} \\ &P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_1 + d_p \hat{\mathbf{n}}, t) d\hat{\mathbf{n}} d\mathbf{v}_2 \end{aligned} \quad (119)$$

The second contribution is a positive increase arising from the collision of particles within the phase space volume $d\mathbf{v}_1^+ d\mathbf{x}_1$ at $\mathbf{v}_1^+, \mathbf{x}_1$ with particles with velocities $\mathbf{v}_2^+$ at $\mathbf{x}_1 + d_p \hat{\mathbf{n}}$ and ending up after collision in the elemental phase space volumes $d\mathbf{v}_1 d\mathbf{x}_1$ at $\mathbf{v}_1, \mathbf{x}_1$ and $d\mathbf{v}_2 d\mathbf{x}_1$ at $\mathbf{x}_1 + d_p \hat{\mathbf{n}}$. The total collision rate is then an integration of the collision 'arrival' flux over the collision surface and over all $\mathbf{v}_2^+$ similar to that in the expression for the rate of loss in Eq. (119), namely,

$$\begin{aligned} d\mathbf{v}_1^+ d\mathbf{x}_1 \partial P^+(\mathbf{v}_1^+, \mathbf{x}_1, t)/\partial t &= d\mathbf{v}_1^+ d\mathbf{x}_1 d_p^2 \int \int_{\mathbf{v}_{21} \cdot \hat{\mathbf{n}} > 0} \\ &\hat{\mathbf{n}} \cdot \mathbf{v}_{12}^+ P(\mathbf{v}_1^+, \mathbf{x}_1; \mathbf{v}_2^+, \mathbf{x}_1 + d_p \hat{\mathbf{n}}, t) d\hat{\mathbf{n}} d\mathbf{v}_2^+ \end{aligned} \quad (120)$$

For $\mathbf{v}_1^+, \mathbf{v}_2^+ \rightarrow \mathbf{v}_1, \mathbf{v}_2$ after collision

$$\mathbf{v}_1^+ = \mathbf{v}_1 + \frac{1 + e_c}{2e_c}(\mathbf{v}_{21} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} \quad \mathbf{v}_2^+ = \mathbf{v}_2 - \frac{1 + e_c}{2e_c}(\mathbf{v}_{21} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} \quad (121)$$

which implies that

$$\left| \frac{\partial(\mathbf{v}_1^+, \mathbf{v}_2^+)}{\partial(\mathbf{v}_1, \mathbf{v}_2)} \right| = \frac{1}{e_c}; \quad \mathbf{v}_{12}^+ = \frac{1}{e_c} \mathbf{v}_{12}$$

and using both these relations in Eq. (120)

$$\begin{aligned} \left(\frac{\partial P(\mathbf{v}_1, \mathbf{x}_1, t)}{\partial t} \right)_{\text{collisions}} &= \partial P^+(\mathbf{v}_1^+, \mathbf{x}_1, t)/\partial t + \partial P^-(\mathbf{v}_1, \mathbf{x}_1, t)/\partial t \\ &= d_p^2 \int \int_{\mathbf{v}_{21} \cdot \hat{\mathbf{n}} > 0} d\hat{\mathbf{n}} d\mathbf{v}_2 \hat{\mathbf{n}} \cdot \mathbf{v} \Delta P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_1 + d_p \hat{\mathbf{n}}, t) \end{aligned} \quad (122)$$

where

$$\Delta P_2 = e_c^{-2} P_2(\mathbf{v}_1^+, \mathbf{x}_1; \mathbf{v}_2^+, \mathbf{x}_1 + d_p \hat{\mathbf{n}}, t) - P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_1 + d_p \hat{\mathbf{n}}, t) \quad (123)$$

The mean collision rate of change $C(\psi)$ for some property ψ , e.g., kinetic energy, is the integral over all possible binary collisions of the change in ψ in a particular collision multiplied by the probable frequency of such a collision and can be written

Fig. 15 The inelastic collision of two spherical particles labeled 1 and 2 with velocities $\mathbf{v}_1, \mathbf{v}_2$ before impact and $\mathbf{v}_1^*, \mathbf{v}_2^*$ after impact

$$C(\psi) = d_p^2 \int \int_{\mathbf{v}_{21} \cdot \hat{\mathbf{n}} > 0} (\psi_2^* - \psi_2) P_2(\mathbf{v}_1, \mathbf{x}; \mathbf{v}_2, \mathbf{x} + d_p \hat{\mathbf{n}}, t) \mathbf{v}_{21} \cdot \hat{\mathbf{n}} d\mathbf{n} d\mathbf{v}_1 \quad (124)$$

1963 where $\psi_2 = \psi_2(\mathbf{v}_1, \mathbf{v}_2)$ and $\psi_2^* = \psi_2(\mathbf{v}_1^*, \mathbf{v}_2^*)$

1964 **6.3.2 Collision Models.** Using the molecular chaos approach
1965 adopted in kinetic theory, the pair distribution functions in the col-
1966 lision integral is simply written in terms of the single distribution
1967 function, assuming that the velocities of colliding particles are
1968 completely independent, namely,

$$P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_1 + \hat{\mathbf{n}} d_p, t) = P_1(\mathbf{v}_1, \mathbf{x}_1, t) P_1(\mathbf{v}_2, \mathbf{x}_2 + d_p \hat{\mathbf{n}}, t) \quad \tau_p \gg \tau_e \text{ (eddy lifetime)} \quad (125)$$

1960 The above assumption has been retained in the derivation of
1971 the collision integral used by Simonin [99] and is referred to as
1972 the random collision model. This is also the assumption used
1973 implicitly by Oesterlé and Petjean [100] and Sommerfeld [101].
1974 However, the molecular chaos assumption is valid only when the
1975 particle response time is much larger than the eddy-particle inter-
1976 action time, i.e., when the particle motion is ballistic. However, as
1977 we pointed out in Sec. 6.2 that when the particle response time is
1978 of the same order or smaller than this interaction time, the
1979 approaching particle velocities will be correlated through interac-
1980 tion with the same eddy and this needs to be taken into account.

1981 **6.3.3 Particle-Fluid Correlated Collision Model.** We refer to
1982 Eq. (109) and the particle pair probability density involving the
1983 particle position, velocity, and flow velocity encountered by
1984 the particle $P_2(\mathbf{v}_1, \mathbf{u}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{u}_2, \mathbf{x}_2)$. For two colliding particles,
1985 the collision radius is so small compared to the length scale of the
1986 energy containing eddies that we may safely assume that both par-
1987 ticles encounter the same fluid velocities $\mathbf{u}$ so we may write this
1988 probability density as

$$P_1(\mathbf{v}_1, \mathbf{x}_1 | \mathbf{u}, \mathbf{x}_1) P_1(\mathbf{v}_2, \mathbf{x}_1 + \hat{\mathbf{n}} d_p | \mathbf{u}, \mathbf{x}) P_1(\mathbf{u}_1, \mathbf{x}_1) = P_1(\mathbf{v}_1, \mathbf{u}, \mathbf{x}_1) P_1(\mathbf{v}_2, \mathbf{u}, \mathbf{x}_1 + \hat{\mathbf{n}} d_p) / P_1(\mathbf{u}, \mathbf{x}_1) \quad (126)$$

1990 where we have assumed that since the colliding particles are
1991 separated by a distance $\ll$ integral length scale, that $P_1(\mathbf{u}, \mathbf{x}_1)$
1992 $\cong P_1(\mathbf{u}, \mathbf{x}_1 + d_p \hat{\mathbf{n}})$

$$P_1(\mathbf{u}, \mathbf{x}_1) \cong P_1(\mathbf{u}, \mathbf{x}_1 + d_p \hat{\mathbf{n}}) \\ P_2(\mathbf{v}_1, \mathbf{x}_1; \mathbf{v}_2, \mathbf{x}_2 + d_p \hat{\mathbf{n}}) = \int d\mathbf{u} P_1(\mathbf{v}_1, \mathbf{u}, \mathbf{x}_1) P_1(\mathbf{v}_2, \mathbf{u}, \mathbf{x}_1 + \hat{\mathbf{n}} d_p) / P_1(\mathbf{u}, \mathbf{x}_1) \quad (127)$$

1993 **6.3.4 Third-Order Moment Expansion (Grad's Theory).** Fol-
1994 lowing Grad's theory of rarefied gases [102], the distribution func-
1995 tion in the collision term may be approximated by its third-order
1996 expansion in Hermite polynomials:
1997

$$P(\mathbf{v}, \mathbf{x}, t) = \left[1 + \frac{a_{ij}}{2T^2} v'_i v'_j + \frac{a_{ijk}}{6T^3} v'_i v'_j v'_k - \frac{a_{ijj}}{2T^2} v'_i \right] P^0(\mathbf{v}, \mathbf{x}) \quad (128)$$

1999 where using q^2 to denote the mean the particle kinetic energy per
2000 unit particle mass

$$T = \frac{2}{3} q^2; \quad a_{ij} = \overline{v'_i v'_j} - \frac{2}{3} q^2 \delta_{ij}; \quad a_{ijk} = \overline{v'_i v'_j v'_k} \quad (129)$$

2002 We recall that $\overline{(\dots)}$ denotes a particle density weighted aver-
2003 age.¹⁴ $P^0(\mathbf{v}, \mathbf{x})$ is the equilibrium pdf given by a

¹⁴ T is referred to as the granular temperature in granular flows.

Maxwell-Boltzmann (Gaussian) distribution for the particle
velocities, that is,

$$P^0(\mathbf{v}, \mathbf{x}) = v'_i v'_j (4\pi q^2/3)^{-3/2} \exp\left(-\frac{v'^2}{4q^2/3}\right) \quad (130)$$

Using the hard sphere collision model, Jenkins and Richmann
[103] derived the following collision terms $C(mv'_i v'_j v'_k \dots)$ in the
transport equations for the particle mass (m), momentum (mv_i)
and kinetic stresses ($\frac{1}{2}mv^2$) and kinetic energy flux, respectively
($mv'_i v'_j v'_k$):

$$C(m) = 0 \quad (131)$$

$$C(mv) = 0 \quad (132)$$

$$C(mv'_i v'_j) = -\alpha_p \rho_p \frac{\sigma_c}{\tau_c} \left(\langle v'_i v'_j \rangle - \frac{1}{3} \left\{ 1 - \frac{1}{3} (1 - e_c^2) \right\} \langle v'^2 \rangle \delta_{ij} \right) \quad (133)$$

$$C(mv'_i v'_j v'_k) = -\frac{5}{12} \alpha_p \rho_p \frac{\xi_c}{\tau_c} (9a_{ijk} - a_{ill} \delta_{jk} - a_{jll} \delta_{ik} - a_{mll} \delta_{ij}) \quad (134)$$

where ρ_p is the particle mass density, α_p the local volume fraction
of the particle phase, τ_c is the time between particle collisions,
 $\sigma_c = (1 + e_c)(3 - e_c)/5$ and $\xi_c = (1 + e_c)(49 - 3e_c)/100$ where
 e_c is the coefficient of restitution for particle collisions. The colli-
sion term in the kinetic stress transport equation is written as a
return to isotropy term analogous to the Rotta term in the Reyn-
olds stress transport turbulence modeling approach. Elastic colli-
sions ($e_c = 1$) lead to a destruction of the off-diagonal correlations
and redistribution of energy among the various normal stresses
without modifying the total kinetic energy. The extension to
inelastic collisions leads to a linear dissipation rate in the kinetic
stress transport equations proportional to the collision frequency
and a function of e_c .

Extending the approach of Jenkins and Richmann [103], Lavié-
ville [93], and more recently Zaichik [94,104], used Grad's theo-
retical approach for particle-fluid correlated collisions by
performing a Hermite polynomial expansion on the fluid-particle
joint particle pdf. This eventually leads to a generalized form for
the collision source term in the kinetic stress transport equation

$$C(mv'_i v'_j) = -\rho_p \frac{\sigma_c}{\tau_c} (a_{p,ij} + \xi^4 a_{f,ij} - \xi^2 a_{fp,ij}) \quad (135)$$

where

$$a_{p,ij} = \overline{v'_i v'_j} - \frac{1}{3} \overline{v'^2} \left\{ 1 - \frac{1}{3} (1 - e_c^2) \right\} \delta_{ij} \\ a_{f,ij} = \overline{u'_i u'_j} - \frac{1}{3} \overline{u'^2} \delta_{ij} \\ a_{fp,ij} = \overline{u'_i v'_j} - \frac{1}{3} \xi^2 \overline{u'^2} \delta_{ij} \quad (136)$$

and ξ is the particle fluid velocity correlation defined in Eq. (112),
 τ_c the interparticle collision time and $\overline{u'_i v'_j}^S$ the symmetric part of
 $\overline{u'_i v'_j}$. We note that when $\xi = 0$, the collision terms reduce to the
forms given by Jenkins and Richmann [103].

Following a similar approach, Zaichik [94] evaluated the colli-
sion terms for the third-order moment C_{ijk} as in Eq. (134) as:

$$C_{ijk} = -\frac{3(1 - \xi^2)}{\tau_c} \overline{v'_i v'_j v'_k}; \quad \tau_{c2} = \frac{180\tau_c}{(1 + e_c)(49 - 33e_c)} \quad (137)$$

so that the influence on the Chapman Enskog approximation for the third-order moment given in Eq. (72) becomes

$$\overline{v'_i v'_j v'_k} = \frac{\left(1 + (1 - \xi^2) \tau_p / \tau_{c2}\right)^{-1}}{3} \times \left(\varepsilon_{li} \frac{\partial}{\partial x_l} \overline{v'_j v'_k} - \varepsilon_{lj} \frac{\partial}{\partial x_l} \overline{v'_i v'_k} - \varepsilon_{lk} \frac{\partial}{\partial x_l} \overline{v'_i v'_j} \right) \quad (138)$$

6.3.5 Interparticle Collision Time. Referring to the definition of collision rate in terms of the collision kernel and using the form of the collision kernel defined in Eq. (117) with no segregation and $F(r_c) = 1$, we can write

$$\tau_c = \tau_c^k (1 - \xi^2)^{-1/2} \quad (139)$$

where τ_c^k is the standard kinetic theory interparticle collision time based on the molecular chaos assumption and given explicitly by

$$(\tau_c^k)^{-1} = n_p \pi d_p^2 \sqrt{\frac{32}{12\pi}} \langle v^2 \rangle^{1/2} \quad (140)$$

where n_p is the particle number density.

The above equations show that the effective interparticle collision rate based on the correlated collision model is always smaller than the one given by standard kinetic theory and decreases with respect to the ratio of the eddy-particle interaction time to particle relaxation time as a result of the increase of correlation coefficient ξ_{12} . This behavior was observed by Laviéville et al. [91] in LES/Lagrangian simulations in homogeneous isotropic turbulent flows showing that neighboring particles have correlated turbulent velocities. The inclusion of interparticle collisions and the coupling with carrier flow turbulence; how they affect the continuum equations and the constitutive relations; the influence of collisions on particles kinetics stresses and isotropy.

6.4 The Effect of Particle Collisions on Turbulent Stresses in a Homogeneous Shear Flow. As an important validation of the correlated collision model, we present the results of Moreau et al. [105,106] who considered perfectly elastic collisions (in the absence of gravity) of spherical particles suspended in an evolving uniform shear flow whose turbulent characteristics were been obtained by Lagrangian simulation of individual particle trajectories based on a Langevin based equation for the carrier phase

using data obtained from LES. The initial flow conditions corresponded to isotropic turbulence and the particle volume fraction $\sim 1.25 \times 10^{-2}$. Figure 16 shows the time evolution of normal turbulent stresses in the disperse phase under the action of the rate of shear, the carrier, and dispersed phases evolving from an isotropic equilibrium state. The results were obtained by solving the momentum and kinetic stress equations with and without the collision terms given in Eqs. (135)–(137) are shown in Fig. 16. The data obtained by DPS in the presence and the absence of particle collisions are depicted by solid and open symbols, respectively. Turbulent kinetic stresses of the disperse phase are normalized by the initial kinetic energy of particles and the correlations of the velocity of the continuous and disperse phases by the initial kinetic energy of this correlation.

Figure 16 reveals a strong anisotropy of particle velocity fluctuations in the absence of collisions. This anisotropy manifests itself in a significantly higher intensity of the longitudinal component as compared to the transverse components. There are in this case two mechanisms responsible for the generation of the longitudinal component of velocity of the disperse phase: via the average velocity gradient and via the interaction of particles with the turbulent eddies of the continuum. On the other hand, fluctuations in the transverse directions are generated only via the interaction of particles with the turbulent fluid. Collisions tend to equalize the intensities of particle fluctuations in different directions, decreasing the intensity of the longitudinal component of velocity fluctuations and increasing the intensities of the transverse components; in other words, the net effect of collisions is the isotropization of the turbulent characteristics of the disperse phase. As one can see from Fig. 17 the theoretical model with collisions based on particle–fluid velocity correlations concurs with the numerical simulation data predicting an increase of $\overline{u'_i v'_j}$ due to collisions. The effect of collisions on $\overline{u'_i v'_j}$ manifests itself through the dependence of the duration of particle interactions with the turbulence on the time interval τ_c . A comparison of model predictions with the data obtained by Moreau et al. [106] shows that the above-described model reproduces all the essential features of the dependence of the character of dispersed phases velocity fluctuations as well as correlations of velocity between the two phases on particle collisions between particle collisions.

Figure 18 shows the model predictions for the collision times based on Eq. (139) and the computation of the particle fluid velocity correlation ξ from the moment equations. Also shown for comparison are the average particle relaxation time and the Stokes relaxation time together with the eddy particle interaction time.

Fig. 16 Time development of particle kinetic stresses in a developing simple turbulent shear flow showing the influence of particle collisions. S_p and S_f are the mean shear rates for the particle and fluid, respectively, at time t . On the left comparison of model predictions (lines) against Lagrangian tracking with correlated collisions (filled symbols); without collisions (open symbols) and decorrelated collisions (dashed symbols). On the right the results based on DPS with an LES of the shear flow, symbols as for the left side. Taken from Moreau et al. [106].

Fig. 17 Evolution of the fluid–particle velocity correlation. S_p and S_f are the mean shear rates for the particle and fluid, respectively, at time t . On the left, comparison between Monte Carlo simulation results and model predictions based on the solution of the moment equations particle with collision terms (lines). Without collisions (empty symbols), with decorrelated collisions (dashed symbols), with correlated collisions (filled symbols). On the right, DPS/LES results without collision effect (empty symbols) and with collision effect (filled symbols); streamwise components $\langle u_1' v_1' \rangle$: circles; transverse components: $\langle u_2' v_2' \rangle$: squares and $\langle u_3' v_3' \rangle$: triangles up and $\langle u_2' v_1' \rangle$: triangles inverted. Taken from Moreau et al. [106].

2114 7 Particle Segregation and Demixing: The Nonlocal 2115 Equilibrium Mechanism)

2116 It is by now well known that turbulence, contrary to tradition-
2117 ally held views, can demix a suspension of particles (see, e.g.,
2118 Fessler et al. [107]). The process of demixing often referred to as
2119 particle segregation, clustering or preferential concentration
2120 depends upon the ratio of the particle response time to the time-
2121 scale of the turbulent structures in the flow (i.e., the Stokes num-
2122 ber, St). Early experiments and simulations (e.g., Crowe et al.
2123 [108]) have shown that the demixing reaches a maximum when
2124 the particle response time is approximately equal to the timescale
2125 of the turbulent structures (i.e., the particle Stokes number $St \sim 1$)
2126 and in particular, those associated with the highest strain rate in
2127 the flow, the suspended particles being observed to segregate into
2128 regions of high strain rate in between the regions of high vorticity.
2129 This feature is best illustrated graphically in Fig. 19 which shows
2130 the segregation patterns arising from an initially fully mixed sus-
2131 pension of particles diffusing in a 2D random array of counter
2132 rotating vortices. The figure shows the segregation pattern at a
2133 given value of time $t = 20$ (in units of the integral time scale)
2134 from the initial fully mixed state for three values of the particle
2135 Stokes number $St = 0.05, 0.5, 5$. It is clear that maximum segre-
2136 gation occurs in the case of $St = 0.5$. What this figure doesn't
2137 show however is the fact that the segregation evolves contin-
2138 uously in time, the patterns becoming more and more filamental as
2139 time progresses. Whatever their Stokes number, all particles will
2140 segregate, it is just that the greater the Stokes number, the longer
2141 the process takes to achieve a given level of segregation. This is
2142 contrary to what many have thought that segregation reaches an
2143 equilibrium state. Particles will continue to segregate until they
2144 touch. In fact, what happens is the segregation forms a network of
2145 filamental caustics similar to the patterns of light obtained at the
2146 bottom of swimming pools as shown in Fig. 19(d) where within
2147 these filamental networks it is observed that the light beams cross
2148 one another. Similarly, in the case of particle segregation in a tur-
2149 bulent flow within the filamental caustics, particle trajectories are
2150 observed to cross also. The formation of caustics in particle dem-
2151 ixing processes was first recognized by Wilkinson and Mehlig [7]
2152 and this crossing of trajectories within a caustic is intimately
2153 related to the occurrence of RUM in flow fields that are spatially
2154 random but smoothly varying [8,109].

2155 In recent years, the process of segregation of inertial particles
2156 has been studied from different viewpoints when the Stokes

number is relatively small. On the one hand, Chen et al. [110] 2157
demonstrated a strong correlation between the positions of small 2158
inertial particles and the locations of zero-acceleration points in 2159
the carrier flow. On the other hand, Balkovsky et al. [111] carried 2160
out a theoretical analysis based on the assumption that the velocity 2161
of inertial particles can be directly related to the carrier flow 2162
velocity. By doing so, they were able to show that the segregation 2163
of particles continues indefinitely in the course of time, and they 2164
showed that the concentration of inertial particles in a turbulent 2165
flow is highly intermittent, so the particles are distributed far from 2166
uniformly over space. A similar approach was chosen by Chun 2167
et al. [112] who demonstrated that the time-converged solution of 2168
the radial distribution function $g(r) \sim r^{-\chi}$, where χ is proportional 2169
to St_K^2 where St_K is the particle Stokes number measured in terms 2170
of the particle response to the small dissipating scales of the turbu- 2171
lence. In addition, they confirmed this by showing results from a 2172
DNS of statistically stationary homogeneous isotropic turbulence. 2173

Fig. 18 Time development of the particle relaxation time and the collision time in homogeneous turbulent shear flow with particle–particle collision influence. Symbols are the stochastic simulation results: mean particle relaxation time τ_{fp}^F (filled triangles), collision time (cross), eddy particle interaction time τ_{fp}^I (circle), Stokes relaxation time (empty triangles), and the lines are predictions from the moment method. Taken from Moreau et al. [105].

Most importantly here is that the KM has been used by Zaichik [32,113] to obtain a similar result. We shall discuss these features in more detail in Sec. 7.2 on segregation when we consider the application of two particles pdfs for calculating segregation using the kinetic equation for particle pair dispersion derived by Zaichik and his coworkers. However, before doing so we shall first consider in more detail the mesoscopic Eulerian particle velocity fields (MEPVF) and RUM components associated with the particle velocity field and how these components depend upon the particle Stokes number.

7.1 Formulation of Random Uncorrelated Motion and Mesoscopic Eulerian Particle Velocity Fields. Segregation and RUM are related to the occurrence of interparticle collisions as follows from the seminal work of Sundaram and Collins [6] and Wang and Wexler [89] in which they demonstrate: (a) segregation enhances the particle concentration of certain regions of the flow; (b) RUM, i.e., the decorrelation of velocity between particles and local fluid, causes two nearby particles to collide and possibly to agglomerate. Segregation is well-known to manifest itself especially for $St_K \sim 1$, whereas the effect of RUM is almost invisible for all particles becoming increasingly important for larger St_K . Since the interplay between these two effects determines the collision rate in a turbulent flow, it is essential to quantify segregation and RUM as accurately as possible as a function of the Stokes number and some typical flow properties to correctly predict the rate of interparticle collision rates.

Fevrier et al. [8] observed that the velocity of suspended particles subject to Stokes drag in a DNS of homogeneous isotropic turbulence consisted of two components: a passive scalar component resulting from transport in a smoothly continuously varying carrier flow velocity field that accounts for all particle–particle and fluid–particle two point spatial correlations which they referred to as the MEPVF; and a spatially uncorrelated component which is referred to as RUM (the component of random uncorrelated motion) whose contribution to the particle kinetic energy increases as the particle inertia increases. Fevrier, Simonin, and Squires (FSS) attribute this feature to the ability of the particles with inertia to retain the memory of their interaction with very distant, and statistically independent eddies in the flow field. This feature had also been observed by Falkovich et al. [109] which they referred to as the *sling effect*.

The presence of RUM in a particle laden turbulent flow is illustrated in Fig. 20(a) taken from FSS [8] which shows the instantaneous velocity vectors of particles and carrier flow suspended in an isotropic turbulent flow. You can see that a majority of the particle velocity vectors are correlated with a smooth vortex pattern associated with the underlying carrier flow field at that instant of time. But you will notice there are a number of particles whose vectors are randomly oriented and not part of the smooth vortex pattern. It is the motion of these particles that constitute RUM or random uncorrelated motion.

More precisely FSS quantified the contributions of MEPVF and RUM to the velocity $\mathbf{v}_p^m(t)$ of a single particle m by partitioning it

Fig. 19 (a)–(c) Positions of 10^4 particles after time $t=20$ in a nonisotropic random straining flow, for $St=0.05$ (a), $St=0.5$ (b) and $St=5$ (c). (d) caustic patterns observed at the bottom of a swimming pool.

into a mesoscopic component derived from the MEPVF contribution to the instantaneous particle velocity $\tilde{\mathbf{v}}_p(\mathbf{x}, t, \mathcal{H}_f)$ (where $\mathbf{x}$ is the position in the flow field) and a residual velocity RUM component $\delta\mathbf{v}_p^m(t)$ by

$$\mathbf{v}_p^m(t) = \tilde{\mathbf{v}}_p(\mathbf{x}^m(t), t, \mathcal{H}_f) + \delta\mathbf{v}_p^m(t) \quad (141)$$

where $\mathcal{H}_f$ refers to a single realization of the continuously varying carrier flow velocity field. They pointed out that the MEPVF is defined in an Eulerian frame of reference and therefore may be considered as a velocity field shared by all particles of the dispersed system. In contrast, the total particle velocity $\mathbf{v}_p(t)$, as well as the residual component $\delta\mathbf{v}_p(t)$ are Lagrangian quantities defined along trajectories of individual particles $\mathbf{x}_p(t)$. The decomposition of the particle velocity given by Eq. (141) is unique, decomposing the particle velocity into contributions that take into account the spatial structure of the particle velocity field in the first MEPVF term and the spatially uncorrelated motion in the second RUM term (FSS referred to this originally as the quasi-Brownian velocity distribution).

Figure 20(b) shows the contribution of the MEPVF and RUM to the turbulent particle kinetic energy k_p as a function of St_K the particle Stokes number defined in terms of the Kolmogorov length scale η_K associated with the viscous dissipating length scales of the turbulence for the DNS isotropic homogeneous turbulent flow from which the particle and fluid velocity vectors shown in Fig. 20(a) have been extracted.

Thus

$$k_p = \tilde{k}_p + \delta k_p \quad (142)$$

where $\tilde{k}_p$ and δk_p are, respectively, the MEPVF and RUM components of the particle turbulent kinetic energy k_p . Figure 20 shows the RUM part starting at zero for zero Stokes number St_K and reaching 100% for $St_K \gg 1$, when the particle motion is ballistic (with random velocities in any small volume of the particles). The reverse is the case for the mesoscopic part as a function of St_K .

Fevrier, Simonin, and Squires used the statistics of the particle velocity distribution to evaluate the Lagrangian temporal correlation and the Eulerian two-point (spatial) correlation which in this case involves contributions from the MEPVF and RUM. The Lagrangian velocity correlations are defined classically along particle trajectories as

$$R_L^p(\tau) = 1/3 \langle \mathbf{v}(t) \cdot \mathbf{v}(t + \tau) \rangle \quad (143)$$

and obtained by averaging over all realizations of the flow for any given particle. This is shown in Fig. 21(a) as a function of time t normalized on the fluid Lagrangian integral timescale T_L for a range of values of the particle Stokes numbers τ_p/T_L . It shows the well-known effect of particles becoming less correlated with their initial velocity with increasing time but becoming more persistent with increasing particle inertia.

The two-point velocity correlations of any two (separate) particles labeled m and n of the system are defined in terms of the particle-pair pdf and expressed as

$$R_{ij}^{pp}(\mathbf{x}, \mathbf{x} + \mathbf{r}, t) = \langle \mathbf{v}_i^{(m)}(t) \mathbf{v}_j^{(n)}(t) | \mathbf{x} = \mathbf{x}^{(m)}(t); \mathbf{x} + \mathbf{r} = \mathbf{x}^{(n)}(t) \rangle \quad (144)$$

The dependence on the separation r normalized on the longitudinal integral length scale L_F^l of the carrier flow turbulence is shown in Fig. 21(b) for the same values of the particle inertia as in Fig. 21(a). An important result revealed in this spatial correlation is that in the limit $r/L_F^l \rightarrow 0$ this correlation does not $\rightarrow 1$, indicating that there is a portion of the particle velocity distribution which is not correlated in time or space, i.e., the RUM component and analogous to the molecular distribution in the kinetic theory of dilute gases. FSS note that if particle motion was completely analogous to molecular motion in a dilute system, the particle positions (in addition to the velocities) would be uncorrelated and the velocity distribution would be Gaussian. For a dilute particle-laden turbulent flow this component satisfies the molecular chaos assumption.

In the seminal paper of FSS and the subsequent work of Masi and coworkers [114–117], a mesoscopic Eulerian formalism (MEF) involving contributions from the MEPVF and RUM has been developed and applied to dispersed flows in more complex turbulent shear flows with heat transfer. In particular, the transport equations that describe the evolution of the MEPVF and RUM components have been derived and used to shed light on the properties of the particle velocity and temperature fields. In this regard, MEF has much in keeping with LES where the filtered equations for the large scale and residual small scale turbulent motion in LES is analogous to the MEPVF and RUM components in MEF. So, for instance, the momentum equations for the MEPVF contain a contribution from the RUM component of the kinetic stress tensor. This tensor represents diffusion and pressure corresponding to the important physical characteristic that within any volume Ω (with dimensions comparable to or smaller than the smallest length scales of the turbulence) separate particles will possess

Fig. 20 RUM: (a) instantaneous fluid and particle velocity vectors from a single plane of a direct numerical simulation of forced isotropic turbulence with Lagrangian particle tracking and (b) RUM and MEPVF contribution to the particle kinetic energy as functions of Stokes no. St_K (taken from Fevrier et al. [8]).

different velocities because of the separate fluid interaction histories. This is the case shown in Fig. 20(a).

7.2 The Kinetic Equation and Its Solutions for Particle Pair Dispersion. In this section we show the way the kinetic equation and its solution for particle pair dispersion quantifies segregation and RUM and provides a method for calculating the particle collision kernel of colliding particles, reflecting the contribution of both processes to the collision rate. We recall the formula in Eq. (117) which provides an analytic expression for the collision kernel which in principles can be used over the entire range of the scales of turbulence from the large scale to the small scale Kolmogorov dissipating scales. We recall however that it assumes the particles are fully mixed (zero segregation) and that particle velocities are dependent on particle-fluid velocity correlations based on a local equilibrium between particle and fluid at the same location. So while this approach is quite valid for the large scales where there is an absence of shear, in the small scales where the shearing of the flow is greatest, the memory of encounters with fluid elements at higher separation and hence higher relative velocities makes a significant contribution to the collision rate. It is of course encounters of this sort for particles transported in a turbulent boundary layer that gives rise to a buildup of particle concentration near the wall and higher wall impact velocities, the combination of both having a profound influence on particle-wall collision rates.

So we consider a kinetic equation for particle pairs pdf $P_1(\mathbf{r}, \mathbf{w}, t)$ where $\mathbf{w}$ is the relative velocity between identical particle pairs a distance $\mathbf{r}$ apart for which the corresponding relative fluid velocity experienced by the particle pair is $\Delta\mathbf{u}(\mathbf{r}, t)$. The statistical properties of $\Delta\mathbf{u}(\mathbf{r}, t)$ are expressed in terms of its statistical moments which for the small scales of turbulence have spherical symmetry (independent of (θ, ϕ)) dependent only the distance of separation $\mathbf{r}$. These, therefore, are the structure functions of which the most relevant here are the second-order structure functions $\langle \Delta u_r^2(r) \rangle, \langle \Delta u_\theta^2(r) \rangle \sim (r/\eta_K)^2$ for $r/\eta_K \ll 1$. The equation of motion for $\mathbf{w}(t), \mathbf{r}(t)$ for identical particle pairs is exactly the same as that for the individual particles so the kinetic equation is identical to Eq. (18) with $\mathbf{w}, \mathbf{r}, \Delta\mathbf{u}$ replacing $\mathbf{v}, \mathbf{x}, \mathbf{u}$. Thus

$$\left(\frac{\partial}{\partial t} + \mathbf{w} \cdot \frac{\partial}{\partial \mathbf{r}} - \beta \frac{\partial}{\partial \mathbf{w}} \cdot \mathbf{w} \right) P_1(\mathbf{w}, \mathbf{r}, t) = -\beta \frac{\partial}{\partial \mathbf{w}} \cdot \Delta\mathbf{u} P_1 \quad (145)$$

Using the LHDI or Furutsu–Novikov-based closures we have similar to Eq. (20)

$$\beta \Delta\mathbf{u} P_1(\mathbf{r}, \mathbf{w}, t) = - \left(\frac{\partial}{\partial \mathbf{r}} \lambda + \frac{\partial}{\partial \mathbf{w}} \cdot \mu - \kappa \right) P_1(\mathbf{r}, \mathbf{w}, t) \quad (146)$$

with similar expressions for λ , μ and κ as those given in Eq. (21) (Furutsu–Novikov closure) or Eq. (26) (LHDI) (with velocities and displacements replaced by relative velocities and displacements and the fluctuating force $\mathbf{f}$ replaced by $\beta \Delta\mathbf{u}(\mathbf{r}, t)$, noting that for the small scale turbulence $\langle \Delta\mathbf{u}(\mathbf{r}, t) \rangle = 0$. To consider the kinetic equation used by Zaichik we can write Eq. (146) alternatively as

$$\beta \Delta\mathbf{u} P_1(\mathbf{r}, \mathbf{w}, t) = \left(-\lambda^\dagger \cdot \frac{\partial}{\partial \mathbf{r}} - \mu^\dagger \cdot \frac{\partial}{\partial \mathbf{w}} + \kappa - \nabla \cdot \lambda \right) P_1(\mathbf{r}, \mathbf{w}, t)$$

In the analysis of Zaichik and a subsequent paper, Zaichik assumes that

$$\kappa - \nabla \cdot \lambda = 0 \quad (147)$$

which is only true in homogeneous turbulence without external body forces like gravity. It ignores therefore the extra drift that arises because of particle segregation in inhomogeneous flows. However, bearing this in mind we shall consider the results Zaichik obtained from specific solutions of the moment equations obtained from Eqs. (145) using (146) with the drift term set equal to zero and using specific forms for $\langle \Delta u_r^2(r) \rangle, \langle \Delta u_\theta^2(r) \rangle$. The momentum equations are similar to those in the 1D case (appropriate for the turbulent boundary layer) except that now with spherical symmetry (θ, ϕ) independence, there is a contribution from centrifugal forces. Thus at equilibrium and for an isotropic stationary flow

$$-(S_2^p + \lambda^\dagger) \cdot \nabla \langle \rho \rangle - \langle \rho \rangle \nabla \cdot S_2^p = 0 \quad (148)$$

where we have used Zaichik's assumption in Eq. (147) and used $S_2^p(\mathbf{r})$ as shorthand for $\overline{\mathbf{w}(\mathbf{r}, t) \mathbf{w}(\mathbf{r}, t)}$, i.e., the pair density weighted relative velocity covariance at a separation $\mathbf{r}$. $S_2^p(\mathbf{r})$ we shall refer to as the second-order particle–structure function. Again if we multiply this equation by β^{-1} , the resulting equation can be interpreted as an equation representing a balance between diffusion

Fig. 21 Influence of particle inertia on (a) Lagrangian particle velocity correlations (b) the particle longitudinal spatial correlation function of particles suspended in isotropic turbulence. o, $\tau_p/T_L = 0.05$; +, $\tau_p/T_L = 0.3$; $\square$, $\tau_p/T_L = 1.47$; $\triangle$, $\tau_p/T_L = 3.4$; *, $\tau_p/T_L = 4.83$; τ_p is the particle response time for Stokes drag (taken from Fevrier et al. [8]).

Fig. 22 Influence of particle inertia St_K on the mean relative velocity magnitude $\langle |w_r| \rangle$ in units of $(v_{tef})^{1/4}$ for $r/\eta_K = 1$: 1–3; predictions with $r_c/\eta_K = 0$; 4–6, predictions with $r_c/\eta_K = 1$; 7–9, DNS [119]; 1, 4, 7, $Re_\lambda = 45$; 2, 5, 8, $Re_\lambda = 58$; 3, 6, 9, $Re_\lambda = 75$. See also Bragg and Collins [118] Fig. 2.

If we define $\langle \rho(r) \rangle = 1$ for $r \rightarrow \infty$ then $\langle \rho(r) \rangle$ becomes the radial distribution $g(r)$. Separate equations for $S_{2,||}^p$ and $S_{2,nn}^p$ based on Eq. (149) and using the Chapman–Enskog approximation for S_3^p (see Eq. (72)) combined with the longitudinal momentum balance Eq. (150) gives finally a set of closed equations for $g(r)$, $S_{||}^p(r)$, S_{nn}^p (see Zaichik [92,113]). These equations can then be solved subject to appropriate boundary conditions using measured forms for the longitudinal and transverse structure functions and values of the integral time scales. These equations in principle encompass both the large and small scales of turbulence. The empirical forms used by Zaichik cover both the dissipating and subinertial range with pair separation scaling as the Kolmogorov length scale η_K and timescales as the Kolmogorov timescales τ_K . β^{-1} then becomes the Stokes number $St_K = (\beta\tau_K)^{-1}$. Interestingly Bragg and Collins [118] show that ignoring the influence of the divergence terms in Eq. (149) with $S_2^p = \frac{1}{\beta}\mu^S$ gives a +ve value for $\overline{w_r}$ indicating that the inward –ve drift responsible for clustering and segregation arises entirely from the divergence term associated with the third-order moment in Eq. (149). Furthermore, a +ve drift would suggest that the net inward radial pressure gradient is outweighed by the centrifugal force.

Figure 22 illustrates the influence of particle inertia measured by the value of Stokes number St_K (associated with the small scale turbulence) on the mean absolute relative velocity $\langle |w_r| \rangle$ over a wide range of Stokes numbers St_K , $\langle |w_r| \rangle$ being defined in terms of the particle longitudinal structure function using the formula (151)

$$\langle |w_r| \rangle = \left(\frac{2}{\pi} \langle w_r^2 \rangle \right)^{1/2} = \left(\frac{2}{\pi} S_{||}^p \right)^{1/2} \quad (151)$$

which assumes a Gaussian distribution for w_r . As is clear, both the predictions and the numerical simulations follow the same trend and indicate a pronounced maximum of $\langle |w_r| \rangle$ as a function of St_K . The initial rise in $\langle |w_r| \rangle$ is attributable to a decrease in the correlation of particle velocities with St_K manifest as RUM. The subsequent decay of $\langle |w_r| \rangle$ beyond the maximum results from a decrease in the particle fluctuating velocities, since the particles become more sluggish and less responsive to the fluid turbulence. Note the similarity to the deposition velocities j^+ as a function of τ^+ for particle deposition in turbulent pipe flow. From Fig. 22, it is also seen that the predictions with $r_c/\eta_K = 1$ overestimate the DNS data at small Stokes numbers. The predictions that correspond to ghost particles lead to slightly smaller values of mean relative velocities at small St_K . However, a difference in the mean relative velocities of zero-size and finite size particles takes place only for relatively small Stokes numbers and vanishes at large St_K .

$$\overline{w_r} = \beta^{-1} \left(\frac{2(S_{2,nn}^p - S_{2,||}^p)}{r} - \frac{dS_{2,||}^p}{dr} \right)$$

which combining this term with the radial component of the first term in Eq. (148) gives

$$\frac{2(S_{2,nn}^p - S_{2,||}^p)}{r} - \frac{dS_{2,||}^p}{dr} - (\lambda_{||} + S_{2,||}^p) \frac{d \ln \langle \rho \rangle}{dr} = 0 \quad (150)$$

Fig. 23 (a) RDF, $g(r)$ as a function of St_K for $r_c/\eta_K = 1$: 1–4, predictions; 5–8, DNS [119]; 1, 5, $Re_\lambda = 24$; 2, 6, $Re_\lambda = 45$; 3, 7, $Re_\lambda = 58$; 4, 8, $Re_\lambda = 75$. (b) RDF $g(\bar{r})$ as a function of particle pair separation $\bar{r} = r/\eta_K$: 1–3, predictions; 4–6, DNS [120]; 7–9, experiments [120]; 1, 4, 7, $St_K = 0.21$, $Re_\lambda = 108$; 2, 5, 8, $St_K = 0.4$, $Re_\lambda = 134$; 1, 4, 9, $St_K = 0.6$, $Re_\lambda = 147$.

Figure 23(a) shows the influence of Stokes number St_K on the radial distribution function $g(\bar{r})$ for the separation $\bar{r} = r/\eta_K$ and Reynolds numbers Re_λ , corresponding to the DNS measurements of Wang et al. [119]. As expected, in the limiting cases of zero-inertia and high-inertia particles, the concentration field is statistically uniform, and so $g(r) = 1$. In accord with the computations, the predicted RDF $g(r_c)$ passes through a peak as St_K increases. Thus, there exists a critical St_K that results in a maximum preferential concentration as the numerical simulations demonstrate (see Fig. 19). The value of this critical $St_K \sim 1$, that is, the clustering is more considerable when tuning the particle parameters to the flow Kolmogorov scales. Figure 23(a) shows a qualitative agreement between the predicted and simulated at particle contact, although the predicted effect of Re_λ is not as strong as it was in simulations and the maxima of $g(\bar{r})$ with St_K are slightly shifted toward particles with larger inertia.

7.3 Analytic Forms for $S_{2,il}^p$ for Inertial Particles $St_K \leq 1$.

Figure 23(b) shows good agreement of Zaichik and Alipchenkovs' [113] (Z&A) predictions of the RDF finite size particles with low inertia $St_K \leq 1$, with both the experimental measurements and DNS calculations of Salazar et al. [120]. In addition (Z&A) [113] have obtained analytic expressions for the particle second-order structure functions $S_{2,il}^p(\bar{r})$, $S_{2,nn}^p(\bar{r})$ and the RDF $g(\bar{r})$ as a function of St_K for low inertia particles $St_K \leq 1$ with $\bar{r} = r_c/\eta_K \ll 1$ as solutions of the closed set of equations for the momentum and kinetic stresses for the relative motion of particle pairs. In this case, the set of equations for ghost particles (overlapping spherical particle pairs) in the vicinity of the origin $\bar{r} = 0$ are solved without regard for boundary conditions and the solutions expressed in the form

$$S_{2,il}^p = \alpha_l \bar{r}; \quad S_{2,nn}^p = \alpha_n \bar{r}; \quad g(\bar{r}) = C_g \bar{r}^\chi \quad (152)$$

in which the $S_{2,il}^p$, $S_{2,nn}^p$ coefficients α_l and α_n , as well as the exponent χ are functions St_K and Re_λ . However, the dependence on Re_λ turns out to be very weak, and α_l , χ and C_g are well approximated by

$$\begin{aligned} \alpha_l &= \frac{1}{15} + 0.16St_K - 0.21St_K^2 + 0.18St_K^3 \\ \chi &= -6St_K^2 + 9.8St_K^3 - 6.2St_K^4 \\ C_g &= 1 + 12St_K^2 \end{aligned} \quad (153)$$

Figure 24 compares the exponent χ given by the formula for χ in Eq. (153) with DNS and experimental values for a range of values of Re_λ .¹⁵ Also shown are the values of χ obtained as solutions to momentum and kinetic stresses Eq. (150) confirming the weak dependence of χ on the value of Re_λ . As can be seen, the values of χ are well approximated by the formula in Eq. (153) if $St_K < 0.6$ and $Re_\lambda > 30$ and are in excellent agreement with the DNS results [112], but they markedly overestimate those values reported by Salazar et al. [120] and underestimates those given in Falkovich and Pumir [121] for relatively large Stokes numbers.

Shown in Fig. 24 is the theoretical approximation derived by Chun et al. [112] for $St_K \ll 1$, namely,

$$\chi = -6.56St_K^2 \quad (154)$$

and the approximation obtained by Derevyanko et al. [122] using the DNS data of Falkovich and Pumir [121,123], namely,

$$\chi = -0.75St_K^2/(0.1 + St_K^3) \quad (155)$$

As can be observed, the predictions of Eqs. (154) and (155) correlate quite well with the predictions given by Eq. (153) at $St_K < 0.1$ but overestimate the experimental and DNS values of Salazar et al. [120] when $St_K > 0.1$.

It is worth commenting on the agreement between the model predictions of Chun et al. [112] in Eq. (154) and that of Z&A's pdf results based on Eq. (152) since the two approaches are seemingly very different and in the past have been the source of some controversy [12,118]. Only until recently has this agreement and lack of similarity in approach been properly explained [118]. The probabilistic approach of Chun et al. is strictly limited to $St \ll 1$ which in essence treats the particles as passive scalars transported by their own velocity field $\mathbf{v}(\mathbf{r}, t)$ (in the case of particle pair dispersion, it is the relative particle velocity field between particles distance $\mathbf{r}$ apart). The collision flux is modeled as the sum of two parts, namely, a "shear" diffusion flux $\mathbf{q}_D$ which depends on the mean concentration gradient of the satellite particles surrounding a target primary particle and a drift flux $\mathbf{q}_d$ that depends upon the local mean concentration of satellite particles and the compressibility of the relative particle velocity field. Explicitly for small Stokes numbers, where the concentration gradient is a small perturbation on the uniform concentration for passive tracers, and the components of $\mathbf{q}_D$

$$q_{Di} = -D_{ij} \frac{\partial \langle \rho \rangle}{\partial r_j}; \quad D_{ij} = \int_{-\infty}^t \langle \mathbf{v}_i(\mathbf{r}, t) \mathbf{v}_j(\mathbf{r}, t') \rangle dt'$$

where $\mathbf{v}(\mathbf{r}, t|t')$ is the velocity of a particle at the time t' arriving at $\mathbf{r}$ at time t and D_{ij} is the dispersion coefficient for relative dispersion; and

$$\mathbf{q}_d = -\langle \rho \rangle \int_{-\infty}^t \langle \mathbf{v}(\mathbf{r}, t) \nabla \cdot \mathbf{v}(\mathbf{r}_p(\mathbf{r}, t|t'), t') \rangle dt' \quad (156)$$

which explicitly involves the divergence $\nabla \cdot \mathbf{v}(\mathbf{r}_p(\mathbf{r}, t))$ (the compressibility) of the relative particle velocity field along a particle trajectory $\mathbf{r}_p(\mathbf{r}, t|t')$ which arrives at time t . We note that the form for the drift flux is the same as the form proposed by Maxey [124] for the enhancement of drift due to gravity and the form derived by Reeks [125] for particle dispersion in an inhomogeneous compressible flow field. In cases where $St_K \ll 1$ the particle pair equation of motion can be used to approximate $\mathbf{w}$ by

$$\mathbf{w} = \Delta \mathbf{u} - St_K \tau_K \mathbf{w} \cdot \nabla \mathbf{w} \quad (157)$$

Fig. 24 The effect of the Stokes number St_K on the power-law exponent χ of the RDF, Eq. (152): 1 and 2, solutions to momentum and kinetic stresses Eq. (150) etc. (for $Re_\lambda = 30$ and ∞); 3 χ Approximations: Eq. (152) Zaichik and Alipchenkov [113], 4 Chun et al. [112], 5 Derevyanko et al. [122]; 6 DNS Chun et al. [112]; 7 DNS Falkovich and Pumir [121]; 8 Experiment Salazar et al. [120]; 9 DNS Salazar et al. [120].

¹⁵As Z&A points out, of great interest is the derivation of analytical solutions to the problem of preferential concentration of low-inertia particles at large Reynolds numbers as these exist in atmospheric conditions and to date, it is not possible to reach the atmospheric Reynolds number using DNS. Furthermore, the values of St_K and the particle size related to the Kolmogorov length scale for typical atmospheric aerosols and rain droplets are less than those realizable in both direct simulations and laboratory experiments.

which on substituting in Eq. (156) gives

$$\mathbf{w}_T = -\frac{1}{3} \text{St}_K \tau_K \mathbf{r} \langle S^2(\mathbf{x}(t), t) - R^2(\mathbf{r}_p(t), t) \rangle \quad (158)$$

where $S(\mathbf{x}(t), t)$ is the symmetric strain rate tensor along a particle trajectory and S^2 is shorthand for $S : S$, and similarly R^2 for $R : R$ where R is the rotation tensor. From the force balance equation of Zaichik we have

$$\mathbf{w}_T = -\text{St}_\eta \tau_\eta \langle \rho \rangle \nabla \cdot \mathbf{S}_2^p$$

Bragg and Collins [118] have shown that using the energy equation for S_2^p and associated closure for S_3^p as Zaichik and Alipchenkov [113] have done, leads to the same expression as in Eq. (158).

7.4 Collision kernel Predictions. We recall the formula for the collision kernel given in Eq. (107) indicating the dependence upon two multiplicative factors, the value of $g(r)$ (due to segregation/preferential concentration) and the collision speed $\langle |w_r| \rangle$ (due to inertial impaction at the collision surface), both of which are enhanced by the dependence on particle Stokes number St_K from their fluid tracer values and showing a peaking around $\text{St}_K \sim 1$. Assuming a Gaussian distribution of velocities w_r at the collision radius r_c and substituting the formulae given in Eqs. (152) and (153) for S_{ll}^p and $g(r_c)$ into Eq. (107) we obtain

$$\Gamma = (8\pi\alpha_l)^{1/2} C_g \cdot \bar{r}_c^{-\chi+3} \left(\frac{\eta_K^3}{\tau_K} \right); \bar{r}_c = r_c / \eta_K \quad (159)$$

Figure 25 shows the behavior of the collision rate prediction using the formula for Γ in Eq. (159) as a function of the Stokes number $\text{St}_K < 0.6$ and normalized collision radius $\bar{r}_c = r_c / \eta_K$; in each case $\Gamma(\text{St}_K)$ rises monotonically from the Saffman and Turner value [95] at $\text{St} = 0$ for a passive scalar. The Z&A predictions compare favorably with the DNS results of Wang et al. [126] for low-inertia particles. Figure 25 also shows the collision rate of Derevyanko et al. [122] based on the power law indices χ in Pumir and Falkovich [121] which accounts for segregation and singularities in the particle concentrations (referred to as sling effects).

7.5 Particle Pair Dispersion, Random Uncorrelated Motion, and Caustics. In this section, we examine in more detail the relationship between caustics and RUM and the way they have been quantified. In this regard, we refer specifically to the recent work of Bragg and Collins [127] who compared the kinetic model of Zaichik and a more recent kinetic model of Gustavsson and Mehlig [128] with DNS results in a Stokes number regime where the formation of caustics and the presence of RUM made a

Fig. 25 Effect of the Stokes number on the collision kernel Γ for low-inertia particles: 1, 2, Eq. (159); 3, Saffman and Turner [95]; 4, 5, Derevyanko et al. [122]; 1, 4, 6, 8, 10, $r_c/\eta_K = 1$; 2, 5, 7, 9, 11, $r_c/\eta_K = 0.5$; 6, 11, DNS, Zhou et al. [89]; 6, 7, $\text{Re}_\lambda = 45$; 8, 9, $\text{Re}_\lambda = 59$; 10, 11, $\text{Re}_\lambda = 75$. Particle diameter $d_p = r_c$.

significant contribution to the particle pair structure function $S_{ll}^p(\bar{r})$. We recall in Sec. 7.1 we described the observation first made by Fevrier et al. [8] that the particle velocity field associated with a suspension of inertial particles in a turbulent flow could be split into two parts: a smoothly varying component (MEPVF) that was responsible for the finite spatial and temporal correlations of the particle motion and a totally random part (RUM). The extent to which these components contributed to the overall particle motion and in particular to the particles' kinetic energy depends upon the particles Stokes number St_K : for $\text{St}_K = 0$ the particle velocity is all derived from the MEPVF and for $\text{St} \rightarrow \infty$ it is all composed of RUM. It means that particle velocity at any one point in the field is not singled value, that particle trajectories can cross. Zaichik and Simonin [97] recognized that these features could be explained quite easily by a two-point statistical kinetic-pdf approach. Thus in a frame of reference of a moving particle, the RUM component represented the distribution of velocities that existed at a point ignoring the fact that particles have a finite radius and could overlap (such particles being referred to as ghost particles). It is this RUM component that is responsible for particle collisions. We recall from Eq. (142) that the total kinetic energy of the particulate phase k_p is represented as the sum of the mesoscopic-correlated and random-uncorrelated energy components, $\bar{k}_p$ and δk_p , respectively. These two parts of the particle kinetic energy are expressed in terms of the second-order longitudinal particle-structure function S_{ll}^p as

$$\bar{k}_p = \frac{S_{ll}^p(0) - S_{ll}^p(\infty)}{4} \quad \delta k_p = \frac{S_{ll}^p(0)}{4} \quad (160)$$

Figure 26 shows the influence of St_K on the correlated (MEPVF) and uncorrelated (RUM) energy components as fractions of the total particle kinetic energy. As is clear, the model predictions obtained from the formulae in Eq. (160) are in good agreement with the results of numerical simulations and follow the predicted asymptotic behavior with St_K . Compare these results with those shown earlier in Fig. 20.

We recall that RUM and the formation of caustics are intimately related. As an illustration, we refer back specifically to the filamental network of caustics shown in Fig. 19 where we remarked that within a caustic envelope particle trajectories cross one another. It happens because in any caustic there is a folding over of the particle phase space $\mathbf{v}, \mathbf{x}$ manifold so that particle trajectories double back on themselves, retracing their paths but in opposite directions similar to the motion of many particles distributed uniformly in a simple harmonic potential where at any one point there exist at least two velocities arising from particles traveling in opposite directions along the same trajectory. This feature is illustrated explicitly in Fig. 27, the left-hand figure showing a

Fig. 26 Effect of particle inertia on the MEPVF (1–3, 7–9) and random-uncorrelated components of the particle kinetic energy (4–6, 10–12): 1–6, predictions; 7–12, DNS [8]; 1, 4, 7, 10 $\text{Re}_\lambda = 52$; 2, 5, 8, 11, $\text{Re}_\lambda = 67$; 3, 6, 9, 12, $\text{Re}_\lambda = 134$. Figure taken from Zaichik and Simonin [97].

Fig. 27 Left: multivalued velocities of particles suspended in a 2D random flow with finite St_K . The orientation of the velocity is that of the arrow. All arrows have the same length, the magnitudes of the velocities are not shown. The blue line delineates the position of the caustics in the x - y -plane. The region of multivalued velocities ends in a cusp that is only approximately resolved. Right: corresponding particle-density in the x - y -plane, showing significantly enhanced particle-number density in the vicinity of the caustic line. Black corresponds to high density and white to low density. Figure taken from Gustavsson et al. [161]

2D caustic within which the particle velocities at any one point are multivalued. Outside of the caustic, the particle flow field is single valued corresponding to the smoothly varying mesoscopic velocity field (MEPVF) of Fevrier et al. [8]. The boundary between the single and multivalued flow field defines the caustic envelope. The particle velocities within any one particular caustic are not random but are related to one another. It is only because the caustics themselves are randomly distributed in space and time that the particle motion associated with the caustics becomes random and uncorrelated at any point fixed in space, i.e., RUM. The right-hand figure in Fig. 27 shows the corresponding concentration of particles within the caustic where in the vicinity of the caustic envelope it is significantly enhanced. Indeed the caustic envelope is a line of singularities in the particle concentration being the points at which the particle trajectories are at their extremities and turn back on themselves. The particle trajectories in these circumstances are nonlocal, the particles possessing memory of their history of previous encounters with turbulent eddies. Bragg and Collins [127] refer to this as *scale breaking*, the particle motion being more associated with the scaling of the inertial sub-range and to dependence on Re_λ rather than the dissipating scales in the vicinity of the collision surface. It is this feature that greatly enhances the possibility of particles colliding with one another.

Further insights into the occurrence of caustics and the way their behavior depends on St_K can be inferred from the form of the particle-structure function $S_{2,II}^p(r)$ as a function of separation based on Bragg and Collins predictions using Zaichik's kinetic equation-based model shown in Fig. 28 for four different Stokes' numbers St_K including $St_K = 0$. We note that for each value of St_K $S_{2,II}^p \geq S_{2,II}^f$ (the fluid structure functions corresponding to $St_K = 0$) for $r/\eta_K \leq 10$ which is entirely due to nonlocal effects of the particle pair relative motion arising from the contribution of the gradient of the third-order energy flux moment in Eq. (149). In the case of $St_K = 1.5$ there are clearly two distinct regions for $S_{2,II}^p$, a power-law region for $r/\eta_K > 0.3$ followed by a plateau region at smaller separations resulting in a nonzero intercept for $S_{2,II}^p$ in the limit $r \rightarrow 0$. This is similar to the behavior of depositing particles in a turbulent boundary layer where we recall that particles may start out in local equilibrium far away from the wall but their inability to follow the steep changes in the fluid velocity means that at any point the particles have some memory of their previous history—their velocity has more to do with where they came from than what is happening to the fluid motion locally (see Fig. 12).

The region over which $S_{2,II}^p(r)$ is roughly constant and significantly different from its local value is known as the free flight to the wall region in the particle wall deposition models. At larger separations, $S_{2,II}^p \leq S_{2,II}^f$, implying the particle relative motion is growing increasingly local with increasing separation, the form of Δu becoming statistically independent of separation at the integral scales of the turbulence. Moreover, at large separations, the particles become independent of each other, causing the structure function to approach twice the kinetic energy of the particles, a decreasing function of the particle Stokes number due to the filtering effect of particle inertia [29,30]. Note that all of these trends qualitatively match those found in the DNS study of Salazar and Collins [129]

Bragg and Collins have compared their DNS results with Zaichik's kinetic equation predictions and those of Gustavsson and Mehlig's (G&M) model [128] which focuses on the existence of caustics and the link they have with RUM and the mesoscopic smoothly varying component to the particle-structure function. They use a kinetic equation for the particle pair separation and

Fig. 28 Bragg and Collins [127] predictions of Zaichik's kinetic model predictions of the particle velocity structure function

relative velocity; however Δu is approximated so that the kinetic equation they derive is a classical Fokker–Planck equation ($\lambda = 0$, in the kinetic equation of Zaichik) and therefore only strictly valid for $St_K \gg 1$. From this, they construct approximate analytical expressions for the moments of the pdf in the dissipation range of the form

$$m_N = f_N(r/\eta_K)^{N+D_2-1} + g_N(r/\eta_K)^{d-1} \quad (161)$$

where the subscript N refers to the order of the moment, D_2 is the phase-space correlation dimension, and d is the physical space dimension (i.e., $d = 3$ for a 3D flow). The first term on the right-hand side of Eq. (161) describes the smooth part of the relative velocity moment and the second term describes the caustic (RUM) contribution, i.e., that associated with the nonlocal particle dynamics. The theory is unclosed since $f_N(St_K)$ and $g(St_K)$ are unknown functions (as is D_2), although they state that their numerical results imply that $g_N(St_K)$ is of an activated form (i.e., modeled using an Arrhenius rate expression, in which the Stokes number plays the role of temperature in the classical expression). The influence of Re_λ in the G&M theory would be contained in its effect upon the unspecified variables f_N , g_N , and D_2 . The particle second-order structure function is found from Eq. (161) by $S_{2,II}^p = m_2/m_0$ and for small r/η_K , $m_0(r) \propto r^{d_2}$ where $d_2 = \min[D_2, d]$ is the configuration space correlation dimension, which then gives

$$S_{2,II}^p = \frac{f_2}{f_0} (r/\eta_K)^2 + \frac{g_2}{f_2} (r/\eta_K)^{d-d_2} \quad (162)$$

In comparing the two theories for caustics and clustering, the case for $St_K = 1$ is revealing. Results in Biferale et al. [130] (for $d = 3$) show that d_2 (for $St_K = 1$) ≈ 2.3 , which implies that for $St_K = 1$ both contributions in Eq. (162) tend to zero as $r \rightarrow 0$. In other words, this does not allow for the simultaneous existence of small scale clustering and finite relative velocities at $r/\eta_K = 0$. This is in contrast to Zaichik's KM and the DNS results [129]. In light of this, Zaichik's model can be considered to describe $S_{2,II}^p(r/\eta_K)$ in three regions, with separate and distinct scaling upon St_K . The first two regions are qualitatively similar to those in the G&M theory: a region of large separation where the effect of inertia is perturbative and locally dependent on $\Delta u(r/\eta_K)$ so that $S_{2,II}^p/S_{2,II}$ is independent of r , then at smaller separations, a smooth transition to a nonsmooth region with $S_{2,II}^p(r/\eta_K) \propto (r/\eta_K)^{-2}$. However, the Zaichik kinetic theory, unlike the G&M theory, predicts that at sufficiently small r/η_K a third region exists in which the particle motions are entirely ballistic and $S_{2,II}^p \approx \text{constant}$ (this is the region that gives rise to the scale break). Bragg and Collins suggest that a possible explanation for this difference between the theories is that in the derivation of the G&M theory equation an a priori assumption is made that the clustering is always fractal, thus ruling out the possibility of a scale break at small r/η_K by definition. In fact, it is possible to show that the Zaichik kinetic theory gives the same scaling predictions as the G&M theory under a priori assumption that $g(r) \propto r^{d_2-d}$ [127].

7.6 Diffusive and Convective Flux Contributions to the Total Mass Flux in Inhomogeneous Turbulence. In our consideration of particle pair separation and clustering of monodisperse particles, the focus was on the particle pair kinetic equation Eq. (145) and its solution for the particle pair concentration (RDF) and second-order structure function Eqs. (148) and (149); how, for instance, they depended upon the particle pair separation and particle Stokes number St_K . The comparison was made with the near-wall buildup of particle concentration and the variation in particle rms velocity with wall distance y^+ for particle transport in a turbulent boundary layer: how they depended equivalently on τ^+ the equivalent of the Stokes number St_K (see Sec. 5.3 and Fig. 12). Both this and particle pair dispersion contain the same features that are properties of transport in inhomogeneous

Fig. 29 Mean square fluctuating flow velocity profile as a function of separation r /distance from stagnation point. Taken from Stafford [132].

turbulence in general and the way they are accounted for in the particle kinetic equation. We referred to Eq. (67) where the particle momentum equation has been interpreted at equilibrium (zero particle mass flux) as a balance of convective and diffusive fluxes or equivalently a balance of net forces in which the net force due to the turbulence is represented by a body force $\bar{\kappa}$ and the spatial gradient of a stress tensor $\bar{\lambda}$ which adds to the divergence of the kinetic stress contribution $\bar{v}'v'$. Both these stress tensors give rise to a diffusive flux $-\tau_p(\bar{\lambda} + \bar{v}'v')\partial_r\langle\rho\rangle$ and a convective flux $\langle\rho\rangle\nabla \cdot (\bar{\lambda} + \bar{v}'v')$ (where the kinetic contribution is commonly referred to as turbophoresis [131]). In the kinetic equation Eq. (145) used by Zaichik the convective flux $(\bar{\kappa} - \nabla \cdot \bar{\lambda})\langle\rho\rangle$ was ignored.

Recently Stafford and Swailes [132,133] computed the magnitude and relative contribution of the diffusive and convective fluxes represented in Eq. (67) for the case of particle transport in an inhomogeneous Gaussian turbulent velocity field. This field was created from the particle pair relative motion in a KS generated homogeneous flow field by considering the velocities and positions of particles in the frame of reference of a moving particle driven by the flow in the KS generated Gaussian flow field.

Fig. 30 Ratio of diffusive flux contributions as a function of separation distance r for monodisperse particles in inhomogeneous turbulence (see Fig. 29 for mean sq. velocity profile); LHA = local homogeneous approximation; KS = measured from kinematically simulated flow field. Taken from Stafford [132].

The kinetic equation based on FN/LHDI closures describing the motion of the particles in this frame of reference is exact because the flow field as with the underlying KS flow field is also Gaussian. The variation of the carrier flow mean square velocity fluctuation as a function of radial distance from the stagnation point is shown in Fig. 29.

Numerical assessment of the different terms within the particle mass flux expression using the KS velocity field reveals that the dominant contribution to both the diffusive and convective fluxes is determined principally by the value of the Stokes number St_E with the turbulence intensity u' playing a lesser role and only affecting the magnitude of the resultant fluxes. For the diffusive fluxes, the diffusive component $\tau_p \lambda_{rr}$ is dominant over the kinetic contribution $\tau_p \bar{\mathbf{v}} \bar{\mathbf{v}}_{rr}$ for small St_E , whereas the reverse is the case for large St_E , see Fig. 30.

For the convective fluxes, $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}})_r$ is the dominant contribution for small St_E , whilst the turbophoretic term $\nabla \cdot \bar{\mathbf{v}} \bar{\mathbf{v}}'$ dominates for large St_E . Furthermore, the direction in which $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}})_r$ acts varies, depending upon u' , becoming negative for large u' , see Fig. 31. Since the two contributions to the net convective flux act to oppose to each other within the expression for the particle mass flux, the highest buildup of particle concentration is accordingly seen for small St_E and large u' for which $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}})_r$ becomes negative, as the individual contributions that $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}})_r$ and $\nabla \cdot \bar{\mathbf{v}} \bar{\mathbf{v}}'$ make to the particle mass flux are then in the same direction, see Fig. 32.

This is notable in the context of developing closure models, as Zaichik's model $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}}) = 0$ has been used as the basis for forming closures in previous work on the premise that this expression only makes a negligible contribution to the convective flux. However, the findings of Stafford and Swailes [132] presented here indicate that there are no solid grounds for making such an approximation uniformly across all cases of St_E and u' , thereby providing the motive for developing improved closures for the expression $(\bar{\mathbf{K}} - \nabla \cdot \bar{\boldsymbol{\lambda}})$ in future work.

7.7 The Influence of Turbulence on Gravitational Settling:

The Maxey Effect. An interesting aspect of the motion of particles in turbulent flows related to particle segregation and clustering is the influence of turbulence on the gravitational settling of particles in homogeneous turbulence. This feature is distinctly different from the drift in a turbulent boundary layer that is on average inhomogeneous but more to do with the inherent instantaneous inhomogeneity in the turbulence, to the eddying motion of the turbulence and the way particles respond to the spatial structure. It's also related to the way a body force like gravity imposes a biasing of the motion of the particles enveloped by these structures. In their numerical simulations of particle settling in homogeneous turbulence and cellular flow fields, Maxey and his coworkers have shown, for instance, that turbulence can enhance the settling of small particles [124,134,135]. In particular, Maxey [124] showed that in situations of weak particle inertia (i.e., particle relaxation times $\ll$ the typical time scale of the turbulent structures in the flow) the net settling velocity $\mathbf{v}_g$ of an ensemble of particles in a homogeneous flow field was related to its value $\mathbf{v}_g^0$ in quiescent flow by the relationship

$$\mathbf{v}_g = \mathbf{v}_g^0 - \int_0^t \langle \mathbf{u}(\mathbf{x}, t) \nabla \cdot \mathbf{v}_p(\mathbf{x}_p(\mathbf{x}, t|s), s) \rangle ds \quad (163)$$

where $\langle \dots \rangle$ is an ensemble average; $\mathbf{u}(\mathbf{x}, t)$ is the carrier flow turbulent velocity field at position $\mathbf{x}$ for times $t \gg$ integral time scale of the turbulent motion; $\nabla \cdot \mathbf{v}_p(\mathbf{x}_p(\mathbf{x}, t|s), s)$ is the divergence of the particle velocity field $\mathbf{v}_p(\mathbf{y}, s)$ with respect to the spatial position $\mathbf{y}$ measured at $\mathbf{y} = \mathbf{x}_p(\mathbf{x}, t|s)$ at time s where $\mathbf{x}_p(\mathbf{x}, t|s)$ is the position of a particle at time s which arrives at $\mathbf{x}$ at time t . The particle velocity field $\mathbf{v}_p(\mathbf{y}, t)$ is defined as the particle velocity field arising from one realization of the flow field $\mathbf{u}(\mathbf{y}, t)$ with a prescribed set of initial conditions at $s=0$ for the particles which are the same in each realization of the flow field.

Fig. 31 Kinetic and turbulent convective fluxes for particles in inhomogeneous turbulence (see Fig. 29) derived from KS isotropic homogeneous stationary flow field. Taken from Stafford [132].

The divergence of the particle velocity field is a measure of the local compressibility of the particle flow. The presence of gravity means that the particles move in a preferential direction which in turn means that the correlation of the fluid velocity with the “local” divergence of the particle flow field is nonzero. For the case when the particles almost followed the flow, Maxey related the local compressibility of the particle flow field to the local straining of the underlying carrier flow and showed that the value

Fig. 32 Radial normalized steady-state particle number concentration $\hat{\rho}$. Taken from Stafford [132].

of the correlation would lead to an enhancement of the gravitational settling. Subsequently, Wang and Maxey [135] explained this result in more detail by looking at the way particles move around the edges of vortices; in particular, their results could be explained by the streaming of particles between vortices which always lead to an accumulation of particles on the down flow side of vortices (i.e., in the direction of gravity). They referred to this process as *preferential sweeping*. See Fig. 33. This however is not a unique result. For instance, depending upon the particle Froude number, D'Avila and Hunt [136] have shown it is possible for the opposite to occur.

From the particle equation of motion, we can write

$$D\mathbf{v}_p/Dt = \beta(\mathbf{u} - \mathbf{v}_p) \quad (164)$$

Under these circumstances for an incompressible carrier flow and weakly inert particles

$$\nabla \cdot \mathbf{v}_p \approx \beta^{-1} \left(\frac{\partial u_k}{\partial x_j} \right) \left(\frac{\partial u_j}{\partial x_k} \right) \quad (165)$$

and substituting this expression in Eq. (166) gives the expression given by Maxey [124] for the enhancement of the settling velocity due to gravity in homogeneous stationary turbulence for low inertial particles, namely,

$$\bar{\mathbf{v}}_g - \mathbf{v}_g^0 \approx \int_0^t \left\langle \mathbf{u}(\mathbf{x}, t) \left(\frac{\partial u_k}{\partial x_j} \right) \left(\frac{\partial u_j}{\partial x_k} \right) (\mathbf{x}_p(\mathbf{x}, t|s), s) \right\rangle ds \quad (166)$$

Such investigations of the influence of the turbulence are entirely appropriate due to the structure that is inherent within the dispersion tensors κ , λ and μ which emerge from the kinetic-pdf approach; the particle response tensor $\mathcal{G}$ in Eq. (23) contains information about the path history of particles, and in particular, the sampling of the fluid velocity gradient along particle trajectories, whilst the correlation tensor $\mathbf{R}$ describes the spatiotemporal structures within the flow field that particles interact with. The full unclosed form of the particle dispersion tensors consists of a conditional average that describes exactly the interaction between these two quantities, and which is capable of capturing the small-

scale physical effects that are characteristic of turbulent flows. In particular, for particles settling in homogeneous turbulence, the enhancement of the settling velocity is entirely described by its dependence on the nonzero component of the body force $\bar{\kappa}_i$ in the direction of gravity, namely,

$$\bar{\kappa}_i = \int_0^t \left\langle \mathcal{G}_{jk}^p(\mathbf{x}, t|s) \frac{\partial}{\partial x_j} R_{ki}(\mathbf{x}_p(t|s), s; \mathbf{x}, t) \right\rangle ds \quad (167)$$

where $\bar{\mathbf{x}}_p$ means an average over all particle velocities arriving at $\mathbf{x}$ and subscript p is meant to imply not only the explicit dependence of $\mathcal{G}$ on the particle response time to changes in the flow but also on trajectories of the particles arriving at $(\mathbf{x}, t)$, i.e., on the particle inertial dependence of $\mathbf{x}_p(t|s)$.

We refer here to the work of Swailes and Stafford [133] who recently compared the value of the body force κ in Eq. (21) with the measured enhanced settling velocity $\mathbf{v}_g$ as a function of the particle inertial response time to the turbulence. The particles settled under a constant applied gravitational force in KS incompressible statistically stationary Gaussian turbulent carrier flow. The simulation was carried out over a range of particle sizes and corresponding settling velocities $\mathbf{v}_g$. Predictions and measurements were plotted as a function of Stokes numbers St_E based on the Eulerian integral timescales and the particle response time for linear drag. Under such circumstances, there should be an exact agreement of the body force predictions based on the Furutsu–Novikov closure in Eq. (21) with the measured enhanced settling velocities. Swailes and Stafford (S&S) note that other closures do not capture this effect because they do not satisfy the fully mixed condition [26]. What differences are shown in Fig. 34 can be attributed to numerical error [132]. They then carried out further simulations to identify what aspect of the form for $\bar{\kappa}$ determine the enhancement by highlighting the correlation between $\mathcal{G}_{jk}^p(\mathbf{x}, t|s)$ and $\frac{\partial}{\partial x_j} R_{ki}$. To show this they separated out $\bar{\kappa}$ into distinct averages of the response tensor $\mathcal{G}$ and spatial gradients of $\mathbf{R}$ using an expansion in the cumulants $\mathbf{K}^n$ for the joint distribution $\phi(\mathcal{G}, \Delta \mathbf{x})$ where we recall $\Delta \mathbf{x} = \mathbf{x}_p(s) - \mathbf{x}$. S&S noted that previous work has produced both local [25,50,76] and nonlocal [50] closures for the dispersion tensors that arise in the kinetic-pdf model, however, all take the common approach of simply decoupling the conditional average which constitutes the integrand of κ_i as in Eq. (21) into the separate averages of the response $\mathcal{G}$ and correlation $\mathbf{R}$ tensors, respectively. Whilst such an approach is able to retrieve the characteristic particle behavior in nonzero mean flows, it is insufficient to extract the finer behavior of particles exhibited by homogeneous isotropic turbulence. What is revealing

Fig. 33 Reproduction of Wang and Maxey's sketch [135] showing the preferential sweeping mechanism for a heavy particle interacting with local flow vortical structures under its inertia and body force

Fig. 34 Variation of $|\bar{\kappa}_2|/\beta u'$ and $\langle u_{p2} \rangle/u'$ with particle Stokes number St_E and settling velocity ratio v_g/u' in a 2D fluid velocity field. Error bars represent the standard deviation from the time averaging. $-\cdot-\cdot-$ $v_g/u' = 0.1$, $- - -$ $v_g/u' = 0.3$, $- \cdot - \cdot -$ $v_g/u' = 1.0$; $\cdots$ $v_g/u' = 1.5$. St_E based on the Eulerian integral timescales and the particle response time for linear drag.

Fig. 35 Individual contribution from cumulants $\mathbf{K}^n$ to $\langle \mathcal{G}_{ij}(t|t') \partial_k R_{j2}(\Delta \mathbf{x}(t|t')) \rangle$ for $n \leq 4$. This is the case for $St_E = 0.1, v_g/u' = 1$ (the value at which the maximum settling enhancement occurs).

is that what emerges from the cumulant expansion is that it is the correlation $\langle \mathbf{u}(\mathbf{x}_p(\mathbf{x}, t|s), s) \cdot \nabla \mathbf{u}(\mathbf{x}_p(\mathbf{x}, t|s), s) \rangle$ which is responsible for the increase in particle settling velocity as in Eq. (163). The various contributions to the settling velocities from the cumulant $\mathbf{K}^n$, $n \leq 4$ are shown in Fig. 35. The first cumulant $\mathbf{K}^1$, which is only sufficient for including the mean trajectory history dependence, makes a negligible contribution to the enhancement. In contrast, the $\mathbf{K}^2$ contribution involves the covariance of the response tensor and separation along trajectories $\Delta \mathbf{x}$ which is consistent with the form required to capture preferential concentration of particles, and thereby the key to capturing the increase in particle settling velocity. Furthermore, $\mathbf{K}^3$ and $\mathbf{K}^4$ are seen to be of the same order as $\mathbf{K}^1$ and of negligible contribution.

8 The Transport and Collisions of Bidisperse Particles

We conclude this section on particle pair mixing and collisions with a brief account of the work of Zaichik [31,137] and Simonin and Fede et al. [138,139] in extending this kinetic theory for gas particle flows to cover the case of inelastic collisions of spherical particles of different sizes (bidisperse particles) using largely the DNS studies of Zhou et al. [126] as a source of validation. A theory for bidisperse particle collisions is especially important because it can easily be extended to include the transport and collisions of polydisperse particles. As with monodisperse particles two approaches can be employed. We have referred to the first approach as the *local equilibrium approach* because the relative velocities between particle pairs depend upon the correlation of the particle velocities with their local fluid velocities and the spatial correlation of the fluid velocities at the particle pair separation Eq. (115). As with monodisperse particles, collisions are based on a joint pdf of fluid and particle velocities, which is given a priori in the form of a correlated Gaussian distribution and utilizes Grad's method [102] to take into account the anisotropy of particle velocity fluctuations. It is the influence of these particles whose stop distances (spatial correlation) are comparable to the integral length scale of the carrier flow that influences the mass, momentum, and kinetic stress equations of the dispersed phase and it is necessary to add an extra term to the kinetic equation to account for their collisions. The second approach is based on the kinetic equations for the particle pair pdf and generalizes the kinetic model presented in Eq. (145) for the case of bidisperse particles. We referred to this approach as the *nonlocal equilibrium approach*. Thus the collision rate Σ_{12} of particles of type 1 with particles of type 2 per unit time is given by

$$\Sigma_{12} = \bar{z}_{21} \bar{n}_1 = \bar{z}_{12} \bar{n}_2 = \Gamma \bar{n}_1 \bar{n}_2, \quad \Gamma = 2\pi r_c^2 \langle |w_r(r_c)| \rangle \quad (168)$$

where $\bar{z}_{ij}$ is the collision frequency of a test particle of type i with particles of type j with $i, j = 1, 2$; r_c as before is the radius of the

collision sphere equal to the sum of radii of the two particles. It is illuminating to see how these two approaches for bidisperse particles both arise under various assumptions for the kinetic equation for the pdf distribution $P_2(\mathbf{x}_1, \mathbf{v}_1; \mathbf{x}_2, \mathbf{v}_2; t)$ of particles of type 1 and type 2 with particle inverse response times β_1 and β_2 , respectively, as an extension of the kinetic equation for a single particle given in Eq. (18) using the closure approximation given in Eq. (20). Thus we have

$$\frac{\partial P_2}{\partial t} + \mathbf{v}_i \cdot \frac{\partial P_2}{\partial \mathbf{x}_i} + \frac{\partial}{\partial \mathbf{v}_i} \cdot \{ \bar{\mathbf{f}}_i + \beta_i \langle \mathbf{u}(\mathbf{x}_i) \rangle - \mathbf{v}_i \} P_2 = 0 \quad (169)$$

where $\bar{\mathbf{f}}_i = \beta_i \mathbf{u}''(\mathbf{x}_i, t)$, $i = 1, 2$. $\bar{\mathbf{f}}_i$ is the aerodynamic drag force experienced by a particle of type $i = 1, 2$ at $\mathbf{x}_i$ conditional upon particle i having velocity $\mathbf{v}_i$ at time t . So

$$\bar{\mathbf{f}}_i P_2 = \left(\frac{\partial}{\partial \mathbf{x}_j} \cdot \boldsymbol{\lambda}^{(j,i)} + \frac{\partial}{\partial \mathbf{v}_j} \cdot \boldsymbol{\mu}^{(j,i)} \right) P_2 \quad (170)$$

$i, j = 1, 2$ with repeated indices summed

with $\boldsymbol{\mu}^{(j,i)}$ and $\boldsymbol{\lambda}^{(j,i)}$ given by

$$\begin{aligned} \boldsymbol{\lambda}^{(j,i)} &= \beta_i \langle \Delta \mathbf{x}(\mathbf{x}_j, \mathbf{v}_j, t|0) \mathbf{u}''(\mathbf{x}_i, t) \rangle \\ \boldsymbol{\mu}^{(j,i)} &= \beta_i \langle \Delta \mathbf{v}(\mathbf{x}_j, \mathbf{v}_j, t|0) \mathbf{u}''(\mathbf{x}_i, t) \rangle \end{aligned} \quad (171)$$

In the case of dispersion in a statistically homogeneous and stationary turbulent flow using an exponential decay for the autocorrelation of fluid velocities along a particle trajectory Derevich [140] gives

$$\boldsymbol{\lambda}^{(j,i)} = (\beta_i St_j)^{-1} \boldsymbol{\mu}^{(j,i)}; \quad \boldsymbol{\mu}^{(j,i)} = \beta_i \frac{\langle \mathbf{u}''(\mathbf{x}_j, t) \mathbf{u}''(\mathbf{x}_i, t) \rangle}{(St_j + 1)}$$

For Stokes drag, the mean square relative velocity along the line of centers $\langle w_r^2 \rangle$ is given in Derevich [140]

$$\langle w_r^2 \rangle / \langle u^2 \rangle = \left(1 - \frac{2\beta_2 F(r_c)}{\beta_1 + \beta_2} \right) \xi_1^2 + \left(1 - \frac{2\beta_1 F(r_c)}{\beta_1 + \beta_2} \right) \xi_2^2 \quad (172)$$

where we recall ξ_i is the particle–fluid velocity correlation for particle $i = 1, 2$, Eq. (112). Contrast this formula with the much simpler formula given by Zaichik et al. [141]

$$\langle w_r^2 \rangle / \langle u^2 \rangle = \xi_1^2 + \xi_2^2 - 2\xi_1 \xi_2 F(r) \quad (173)$$

Fig. 36 Rms relative velocity between particle pairs as a function of separation: comparison of predictions based on Derevich's formula Eq. (172) and Zaichik's formula Eq. (173); r is the separation distance normalized on the integral length scale; $\tau_{p2}/\tau_{p1} = \beta_1/\beta_2$ in Eq. (172), $St = St_1$, $St_2 = St_1 \times (\tau_{p2}/\tau_{p1})$

A comparison of the predictions of both formulae for homogeneous isotropic turbulence using an exponential decay for the spatial longitudinal correlation of the fluid velocity fluctuation is shown in Fig. 36 indicating a noticeable difference for small separation r . Using the formula of Derevich in Eq. (172) (for dilute flows where the collision rate does not influence the particle kinetic equation) the collision kernel, Γ is given by

$$\Gamma = \left\{ \left(1 - \frac{2\beta_2 F(r_c)}{\beta_1 + \beta_2} \right) \xi_1^2 + \left(1 - \frac{2\beta_1 F(r_c)}{\beta_1 + \beta_2} \right) \xi_2^2 \right\}^{1/2} \sqrt{8\pi r_c^2 \langle u^2 \rangle}^{1/2} \quad (174)$$

In Zaichik [63] (as with the monodisperse case) use is made of the spatial correlation $F(r)$ associated with the inertial subrange, namely,

$$F(r_c) = 1 - \frac{r_c^2}{\sqrt{60} \text{Re}_\lambda} \quad (175)$$

We note that when $\beta_1/\beta_2 = 1$, the degenerate monodisperse case the 2 formulae are identical. Note also that in this case $\langle w_r^2 \rangle / \langle u^2 \rangle = 0$ at zero separation in contrast to the finite value for $\beta_1/\beta_2 \neq 1$.

Figure 37 shows a comparison of the DNS measurements of Zhou et al. with the predictions of Zaichik based on the formula $\xi_{12} = \xi_1 \xi_2 F(r)$ for the radial velocity covariance of two particles with relaxation times τ_{p1}/T_e and τ_{p2}/T_e using a bi-exponential autocorrelation function for the Lagrangian autocorrelation of the longitudinal fluid velocities and the form for $F(r)$ in Eq. (175). T_e is the microscale time scale $\varepsilon_f / \langle u^2 \rangle$.

We see that in Fig. 37 everywhere except for a narrow range of values τ_{p2}/T_e , Zaichik's simple formula describes the variation of ξ_{12} with acceptable accuracy, predicting a monotonic decrease with an increase of both τ_{p1} and τ_{p2} . Such behavior we would expect from a decreasing correlation of each particle with the local fluid as the inertia increases. However, it shows that the formula fails to reproduce the small spike in the correlation coefficient at small values of τ_{p2}/T_e and exaggerates the actual drop of the correlation coefficient at large values of τ_{p2}/T_e .

8.1 Collisions of Bidisperse Particles With Gravitational Settling. An important consideration for bidisperse flows is the collision rate when the particles have different mean velocities as in the case of gravitational settling and with it the combined influence of the relative settling velocities and turbulence. In extending the formula for Γ in Eq. (174) to include a relative settling velocity W between two different types of particles, we can write Γ more generally as

$$\Gamma = \pi r_c^2 F_0(z) W \quad (176)$$

where

$$F_0(z) = \frac{e^{-z}}{\sqrt{\pi z}} + \left(1 + \frac{1}{2z} \right) \text{erf}(\sqrt{z}) \quad (177)$$

and z is a parameter characterizing the interrelation between the effects of gravity and turbulence on the collision kernel and given by the ratio $W^2/2\langle w'^2 \rangle$ where W is the relative settling velocity between the two types of particle, i.e., $|\tau_{p1} - \tau_{p2}|g$. At small values of z , the expression for Γ in Eq. (176) coincides with the solution obtained by Saffman and Turner [95] when the effect of gravity is weak, namely,

$$\Gamma = \Gamma_t \left(1 + \frac{1}{3} z \right) \quad (178)$$

where Γ_t is the turbulent component of the collision kernel (see Eq. (174). For $z \rightarrow \infty$ Γ in Eq. (176) reduces to the well-known expression for the collision kernel due to gravitational settling alone, namely,

$$\Gamma = \pi r_c^2 W_g \quad (179)$$

The formula in Eq. (176) was first obtained by Abrahamson [96] and later reproduced by Gourdel et al. [142], Alipchenkov and Zaichik [143], and Dodin and Elperin [144]. Figure 38 compares the time intervals between particle collisions in a binary mixture based on the formula in Eq. (176) with the results of a Lagrangian trajectory simulation of particle motion in a turbulent flow field using the LES method of Gourdel et al. [142]. The particles were of two types having the same radius of $325 \mu\text{m}$ but different material densities of $\rho_{p1} = 117.5 \text{ kg/m}^3$ and $\rho_{p2} = 235 \text{ kg/m}^3$. The volume concentration of particles of type 1 is 1.3×10^{-2} while the volume concentration of particles of type 2 varied. The time intervals between collisions of particles 1 with particles 2 and particles 2 with particles 1 are, respectively, equal to

$$\tau_{12} = (\Gamma n_2)^{-1} \quad \tau_{21} = (\Gamma n_1)^{-1} \quad (180)$$

where n_1 and n_2 are the number density of particles 1 and 2. In the formula for the collision kernel in Eq. (179) the particles under consideration were highly inertial so that any correlation of their motion via the underlying turbulence and their interactions with small-scale turbulence did not play a significant role. In this case, one can use Abrahamson's formula for Γ_t

Fig. 37 The particle velocity correlation coefficient between colliding particles $\bar{r}_c = 1$ for $\text{Re}_\lambda = 45$; 1–4—Zaichik formula; 5–8—DNS by Zhou et al. [148]; 1,5— $\tau_{p1}/T_e = 0.1$; 2, 6— $\tau_{p1}/T_e = 0.4$; 3, 7— $\tau_{p1}/T_e = 1$; 4, 8— $\tau_{p1}/T_e = 2$

Fig. 38 Time intervals between particle collisions in a binary mixture: 1, 2, 3, 7— τ_{12} ; 4, 5, 6, 8— τ_{21} ; 1, 4—Eq. (176); 2, 5—Eq. (181); 3, 6—Eq. (179); 7, 8—Gourdel et al. [142] Φ_2 = marker fraction of type 2 particles. Volume fraction of type 1 particles $\Phi_1 = 1.3 \times 10^{-2}$.

$$\Gamma_t = \sqrt{8\pi r_c^2 (\langle v_1^2 \rangle + \langle v_2^2 \rangle)^{1/2}} \quad (181)$$

Also shown in Fig. 38 are the time intervals between collisions calculated using the Abrahamson formula Eq. (181) that describes the effect of turbulence while neglecting the relative drift and by the formula in Eq. (179) that considers the force of gravity while neglecting the contribution of turbulence. One can see that both formulae overestimate τ_{12} and τ_{21} compared to the values calculated by Gourdel et al. [142]; this is especially true for Eq. (181) at small volume fractions and Eq. (179) at large values of the volume fraction. We also note that as the volume fraction grows, the increased collision frequency results in a smaller difference between the average velocities of particles 1 and 2, that is, in a smaller relative drift velocity W_g . Therefore, τ_{12} and τ_{21} are better described by Eq. (179) at small volume fraction and by Eq. (181) at large volume fractions. The formula in Eq. (176) which includes both of these two effects—turbulence and gravity—ensures good agreement with the data obtained by Gourdel et al. [142].

8.2 Influence of Bidisperse Particle Collisions on the Transport of Mass, Momentum, and Kinetic Stresses. In considering the influence of collisions in a suspension of bidisperse particles on the continuum equations of the bidisperse phase, Eq. (118) for the velocities before and after a collision for two colliding particles of mass m_1 and m_2 become

$$\begin{aligned} \mathbf{v}_1^* &= \mathbf{v}_1 + \frac{m_1}{m_1 + m_2} (1 + e_c) (\mathbf{v}_{21} \cdot \hat{\mathbf{n}}) \hat{\mathbf{n}} \\ \mathbf{v}_2^* &= \mathbf{v}_2 - \frac{m_1}{m_1 + m_2} (1 + e_c) (\mathbf{v}_{21} \cdot \hat{\mathbf{n}}) \hat{\mathbf{n}} \end{aligned} \quad (182)$$

where we recall e_c is the coefficient of restitution. Collisions do not change the volume concentration of particles. But collisions with particles of different size and mass contribute to the momentum equation through terms $C_i^{(1)}$ and $C_i^{(2)}$ added to the particle momentum equation for type 1 and type 2 particles, respectively. In the transport equation for the kinetic stresses including the kinetic energy we add collision terms $C_{ij}^{(1,1)}$, $C_{ij}^{(2,1)}$, $C_{ij}^{(1,2)}$ characterizing the contribution of particles of one and the same type and of particles of different types. To close the set of mass, momentum, and kinetic stress equation, we only need to determine $C_i^{(p)}$ and $C_{ij}^{(p,q)}$, since the quantity $C_{ij}^{(p,p)}$, $p, q = 1, 2$ is already given in Sec. 6.3.2 by Eq. (135). To find the collision terms, it is necessary to know the pdf of velocities of particle pairs. As in Sec. 6.3.2 Grad's method is used to represent the two-point particle velocity pdf as an expansion

$$P(\mathbf{v}_1, \mathbf{v}_2) = P^{(0)}(\mathbf{v}_1, \mathbf{v}_2) + P^{(1)}(\mathbf{v}_1, \mathbf{v}_2) \quad (183)$$

$P^{(0)}(\mathbf{v}_1, \mathbf{v}_2)$ is based on an isotropic Gaussian distribution in which the particle velocity correlation between $\mathbf{v}_1$ and $\mathbf{v}_2$ are related to that at of the local fluid velocities at their corresponding location which in turn are spatially correlated with lateral and longitudinal correlations $G(r)$ and $F(r)$ where r is the separation distance. We refer to Zaichik [63,141] for the precise details of evaluation of $P^{(1)}$ from the equilibrium distribution $P^{(0)}$. The two types of particles will have different mean velocities and a mean relative velocity W as in the case considered with particles of different settling velocities in Sec. 8.1. In evaluating the relative velocities between the two particle types, W and $\langle w^2 \rangle$ will play a part reflected in the parameter $z = W/\langle w^2 \rangle^{1/2}$ contributing to both the zeroth-order component $\langle |w_r| \rangle^{(0)}$ arising from the equilibrium distribution $P^{(0)}$ and $\langle |w_r| \rangle^{(1)}$ arising from $P^{(1)}$

$$\langle |w_r| \rangle^{(0)} = \frac{W}{2} F_0(z) \quad (184)$$

$$\langle |w_r| \rangle^{(1)} = B_{ij} W_i W_j W F_1(z) \quad (185)$$

where we recall $z = W^2/2\langle w^2 \rangle$, with $F_0(z)$ given by Eq. (177) and $F_1(z)$ given by

$$F_1(z) = \frac{3 \exp(-z)}{4\pi^{1/2} z^{5/2}} + \left(\frac{3}{8z^3} - \frac{1}{4z^2} \right) \text{erf}(\sqrt{z}) \quad (186)$$

where $W_i = V_{1i} - V_{2i}$ and $W = (W_i W_i)^{1/2}$, V_1, V_2 being the mean velocity of type 1 and 2 particles, respectively.

Making use of the binary particles' collision velocities before and after collision in Eq. (182) Zaichik obtained the following expression for the collision terms $C_i^{(p)}$ in the momentum equation for type $p = 1, 2$ particles defined as:

$$C_i^{(p)} = C_i^{(p,0)} + C_i^{(p,1)} \quad (187)$$

where $C_i^{(p,0)}$ and $C_i^{(p,1)}$ are derived from $P^{(0)}$ and $P^{(1)}$, respectively,

$$C_i^{(p,0)} = \frac{\pi r_c^2 N_q m_q (1 + e_c) W}{2(m_p + m_q)} W_i F_1(z) p \neq q; p, q = 1, 2 \quad (188)$$

where N_q is the number concentration of particles of species q

$$\begin{aligned} C_i^{(p,1)} &= \frac{\pi r_c^2 N_q m_q (1 + e_c) \langle w^2 \rangle^2}{(m_1 + m_2)} \\ &\times \left[B_{ik} \left(\frac{W_k}{W} \right) F_2(z) - \frac{B_{jk} W_i W_j W_k}{2W^3} F_3(z) \right] \end{aligned} \quad (189)$$

where

$$F_2(z) = \left(\frac{3}{8z^3} - \frac{1}{4z^2} \right) \text{erf}(\sqrt{z}) - \frac{3 \exp(-z)}{4\sqrt{\pi} z^{5/2}} \quad (190)$$

$$F_3(z) = 4F_0(z) - 3F_1(z) - \frac{2F_2(z)}{z} \quad (191)$$

We note that when there is zero correlation between particle velocities, $C^{(p,0)}$ is the same expression given in Eq. (179) for the collision kernel with relative gravitational settling. In the limiting case of small and large values of z , it follows from Eqs. (187)–(191) that

$$\lim_{z \rightarrow 0} \frac{C_i^{(p,1)}}{C_i^{(p,0)}} = \mathcal{O}(1) \quad \lim_{z \rightarrow \infty} \frac{C_i^{(p,1)}}{C_i^{(p,0)}} = \mathcal{O}(z) \quad (192)$$

So the contribution of anisotropy of particle velocity fluctuations to $C_i^{(p)}$ is more important in the case of small values of the drift parameter z .

In the evaluation of the collision terms $C_{ij}^{(p,q)}$ in the transport equations for the particle kinetic stresses Eq. (135) Zaichik, Simonin & Fede again split these terms into the zeroth-order and first-order contributions, namely,

$$C_{ij}^{(p,q)} = C_{ij}^{(p,q,0)} + C_{ij}^{(p,q,1)} \quad (193)$$

We need only deal with the case when $p \neq q$. As for $C_i^{(p)}$, both components depend upon the drift parameter z . The expressions, in this case, are very complicated involving both the correlation between the particle velocities with the underlying carrier flow, ξ_p as well as the drift factor z and we refer to Zaichik [63] Eqs. (6.39) and (6.40) for the specific formulae of both components. We note that as with $C_i^{(p)}$ that as the drift parameter $z \rightarrow \infty$, the ratio $C_{ij}^{(p,q,1)}/C_{ij}^{(p,q,0)} = \mathcal{O}(z^{-1})$ so that asymmetries in the collision

Fig. 39 Particle kinetic energy transfer rates versus the volumetric fraction of type q particles. Symbols are simulation results, solid lines are the model results based on the molecular chaos assumption and the dashed lines are the model results which take into account the velocity correlation of colliding particles. Model predictions are computed with particle kinetic energies measured in the simulations [138].

terms introduced by asymmetries in the flow are only significant when z is small. We also note that when the particles are of the same type the collision terms reduce to the forms for the total collision rate given in Eq. (135).

More instructive and more revealing is the contribution of the various dissipative energy loss mechanisms and energy transfer rates arising from collisions to the source terms in the kinetic energy equations for each component kinetic energy k_1 . These have been calculated by Fede and Simonin [138] for a binary mixture undergoing inelastic collisions with no settling. They divided the contribution to the sources $C^{(1,1)}$ and $C^{(1,2)}$ into two basic contributions

$$C^{(p,p)} = \varepsilon^{(p,p)} \quad (194)$$

$$C^{(p,q)} = \chi^{(p,q)} + \varepsilon^{(p,q)} \quad p, q = 1, 2, p \neq q \quad (195)$$

Fig. 40 Particle kinetic energies k^α and k^γ of species α and γ versus the volumetric fraction of species γ particles. Symbols are simulation results, solid lines model predictions using molecular chaos assumption, dashed lines model predictions using the correlated closure and dotted lines are predictions based on molecular chaos assumption [138].

where $\varepsilon^{(p,p)}$ and $\varepsilon^{(p,q)}$ are the dissipative parts due to the nonelasticity of the particles and $\chi^{(p,q)}$ corresponds to kinetic energy transfer between particles of species p and species q satisfying the relationship: $\chi^{(p,q)} = \chi^{(q,p)}$. Eq. (30) in Fede and Simonin [138] for the kinetic energy transfer rate shows clearly that $\chi^{(p,q)}$ is a return-to-equilibrium term driving the separate particle kinetic energy $k^{(p)} p = 1, 2$ toward their thermal equilibrium values with $m_1 k^{(1)} = m_2 k^{(2)}$. This is also true of the collision energy transfer term based on the molecular chaos assumption also but toward different equilibrium values. Figure 39 shows the comparison between the model predictions of the particles' kinetic energy transfer term and simulation results. The correlation between the colliding particle velocities decreases not only the collision frequency but also the mean kinetic energy transfer in each collision. In contrast with the molecular chaos assumption, the correlated colliding particle closure accounts for both these phenomena. Figure 40 shows the particle kinetic energy dependence on the volumetric fraction ϕ_γ of particles of species γ . The dotted lines represent the particles' kinetic energies assuming "thermal equilibrium". In gas-solid turbulent flows with a nonsettling binary mixture of particles, two mechanisms compete. On the one hand, particles suspended in a turbulent fluid will move toward a stationary state given by the classical result of Tchen's theory (see Eq. (46)). Following this theory, the particle kinetic energies are driven toward the fluid-particle covariance which is linked with the fluid kinetic energy through the fluid integral time scale to particle relaxation time ratio. On the other hand, particle-particle interactions drive the particles toward thermal equilibrium. Figures 39 and 40 show that the model predictions based on molecular chaos assumption overestimate this return-to-equilibrium term, hence the particle kinetic energies deviate slightly from the measured ones toward thermal equilibrium. This effect is found to increase when the collision frequency is increasing. At the opposite end, the model derived using the correlated colliding particle closure is in good agreement with the simulation results. In this study, the particle kinetic energies are not strongly modified by collisions because the dominant effect is the particle interaction with the carrier flow turbulence.

8.3 Clustering and Relative Velocities of Bidisperse Particle Pairs at Small Separation. Here we follow a similar but more complex approach of Zaichik et al. [137] for bidisperse particles as was used for monodisperse particles. More complex because unlike monodisperse particles, the separation of position and separation of velocity for bidisperse particles cannot be divorced from the motion of the center of mass of the particle pair. It is therefore necessary to deal explicitly with the pdf of the individual particle positions and velocities of the particle pair explicitly in the kinetic equation as given in Eq. (169).

This equation as before for single point particle transport can be used to generate equations for the velocity moments of the individual bidisperse particles. Thus the zeroth-order moment equation gives the equation for the net number density $\langle n_{12} \rangle$ of particle pairs composed of type 1 and 2 particles separated by a distance $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$ and is given by

$$\frac{\partial \langle n_{12} \rangle}{\partial t} + \frac{\partial \cdot \bar{\mathbf{v}}_1 \langle n_{12} \rangle}{\partial \mathbf{x}_1} + \frac{\partial \cdot \bar{\mathbf{v}}_2 \langle n_{12} \rangle}{\partial \mathbf{x}_2} = 0 \quad (196)$$

with the bidisperse particle mean velocities of each component 1 and 2 given by

$$\bar{\mathbf{v}}_1 = \langle n_{12} \rangle^{-1} \int \mathbf{v}_1 P_2 d\mathbf{v}_2 d\mathbf{v}_1, \quad 1 = 1, 2 \quad (197)$$

for which the equation for the momentum transport for type 1 given by

$$\begin{aligned}
& (\partial/\partial t + \bar{\mathbf{v}}_1 \cdot \partial/\partial \mathbf{x}_1 + \bar{\mathbf{v}}_2 \cdot \partial/\partial \mathbf{x}_2) \bar{\mathbf{v}}_1 \\
& = -\beta_1 (\langle \mathbf{u} \rangle - \bar{\mathbf{v}}_1) - \partial \cdot \bar{\mathbf{v}}_1 \bar{\mathbf{v}}_1 / \partial \mathbf{x}_1 \\
& - \partial \cdot \bar{\mathbf{v}}_1 \bar{\mathbf{v}}_2 / \partial \mathbf{x}_2 - \beta_1 \varepsilon_1 \cdot \partial \ln \langle n_{12} \rangle / \partial \mathbf{x}_1 - \beta_1 \varepsilon_{12} \cdot \partial \ln \langle n_{12} \rangle / \partial \mathbf{x}_2
\end{aligned} \quad (198)$$

$$\text{with } \varepsilon_1 = \beta_1^{-1} (\bar{\mathbf{v}}_1 \bar{\mathbf{v}}_1 + \lambda^{(1,1)}) \quad \varepsilon_{12} = \beta_1^{-1} \bar{\mathbf{v}}_1 \bar{\mathbf{v}}_2 + \beta_2^{-1} \lambda^{(1,2)\dagger} \quad (199)$$

with similar equations for the momentum transport of type 2 particles with subscripts 1 and 2 interchangeable in Eqs. (198) and (199) (recall $\dagger$ as in Eq. (65) denotes the transpose components). We note the comparison with the transport equation for the density weighted mean velocity of monodisperse single particles given in Eq. (61) using the closed form for $\beta \mathbf{u}''$ in Eq. (63) with $\kappa = 0$. We recall that in Sec. 4.1 the momentum equation was interpreted as an advection-diffusion equation with a diffusion coefficient given by Eq. (66) and the same as ε_1 in Eq. (199). However, in the momentum Eq. (198) for bidisperse particles, there is an additional contribution involving an extra diffusion coefficient ε_{12} which determines the contribution to the momentum equation of particles of type 1 arising from gradients of the particle pair concentration $\langle n_{12} \rangle$ in $\mathbf{x}_2$ of particles of type 2. We recall $\lambda^{(1,2)}$ defined in Eq. (170) and associated with the driving force $\beta_1 \mathbf{u}''(\mathbf{x}_1, t)$ for a particle of type 1 at position $\mathbf{x}_1$ initially separated from a particle of type 2 by a distance r . So for their long term values

$$\lambda^{(1,2)} = \beta_1 \int_0^\infty g_2(\tau) \mathbf{B}_{L2}(r, \tau) d\tau \quad (200)$$

where $\mathbf{B}_{L2}(r, \tau) = \langle \mathbf{u}''(\mathbf{R}_2(r, 0|\tau), \tau) \mathbf{u}''(0, 0) \rangle$ is the fluid velocity correlation measured at position $\mathbf{R}_2$ at time τ along a particle trajectory of type 2 initially separated by a distance r from the fluid velocity at the origin at time $\tau = 0$; g_2 is the response function for small changes δx_2 arising from small changes in fluid velocity along a particle trajectory of type 2. In homogeneous turbulence $g_2(\tau)$ is independent of direction and given by $g_2(\tau) = (1 - e^{-\beta_2 \tau})$, based on the deterministic response function Eq. (25) ($\lambda^{(2,2)}$ corresponds to the value $\lambda^{(2,1)}$ for identical particles of zero separation, i.e., using $\mathbf{B}_{L2}(0, \tau)$ in Eq. (200).

Following Zaichik [145], $\mathbf{B}_{Lp}(r, \tau)$ can be written approximately as:

$$\mathbf{B}_{Lp}(r, \tau) = \langle \mathbf{u}'' \mathbf{u}'' \rangle \Psi_{Lp}(\tau) - 1/2 \mathbf{S}_2(r) \Psi_{Lpr}(r|\tau), \quad p = 1, 2 \quad (201)$$

where $\Psi_{Lp}(\tau)$ is the Lagrangian autocorrelation coefficient of fluid velocity fluctuations measured along the trajectory of particle $p = 1, 2$ at time τ , and $\mathbf{S}_2(r)$ is the Eulerian fluid point pair second-order structure function tensor at a separation r .

To exemplify the composition of $\lambda^{(1,2)}$ reflected in the composition of $\mathbf{B}_{L1}(r, \tau)$, Zaichik et al. [137] write

$$\begin{aligned}
\lambda^{(1,2)} &= \beta_1 (1 - f_{u2}) \langle \mathbf{u}'' \mathbf{u}'' \rangle - 1/2 (1 - f_{r2}) \mathbf{S}_2(r) \quad \text{with} \\
f_{u2} &= \beta_1 \int_0^\infty \Psi_{L2}(\tau) e^{-\beta_2 \tau} d\tau; \\
f_{r2} &= \beta_1 \int_0^\infty \Psi_{Lr2}(r|\tau) e^{-\beta_2 \tau} d\tau
\end{aligned} \quad (202)$$

with subscripts 1, 2 interchangeable

Zaichik et al. [141,146] have then evaluated $\lambda^{(1,2)}$ using the autocorrelation function provided by Sawford [147].

They then change the spatial and velocity variables in these transport equations to consider directly the relative motion of particle pairs. This is achieved by introducing new variables, which describe, respectively, the motion of a bidisperse system as a

whole (i.e., its center of mass) and the relative motion of two groups of particles, namely,

$$\begin{aligned}
\mathbf{x} &= 1/2(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{v} = (\mathbf{v}_1 + \mathbf{v}_2) \\
\mathbf{r} &= (\mathbf{x}_1 - \mathbf{x}_2), \quad \mathbf{w} = (\mathbf{v}_1 - \mathbf{v}_2)
\end{aligned} \quad (203)$$

In terms of these new transformed variables ignoring the derivatives with respect to $\mathbf{x}$ due to the homogeneity of the turbulence

$$\begin{aligned}
\frac{\partial \langle n_{12} \rangle}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \langle n_{12} \rangle \bar{\mathbf{w}} &= 0; \\
\frac{D_{\mathbf{w}}}{Dt} \bar{\mathbf{v}}_i &= \beta_i (\langle \mathbf{u} \rangle - \bar{\mathbf{v}}_i) - (-1)^i \frac{\partial}{\partial \mathbf{r}} \cdot (\bar{\mathbf{v}}_i \bar{\mathbf{v}}_i - \bar{\mathbf{v}}_i \bar{\mathbf{v}}_j)
\end{aligned} \quad (204)$$

$$-(-1)^i \beta_i (\varepsilon_i - \varepsilon_{ij}) \cdot \frac{\partial \ln \langle n_{12} \rangle}{\partial \mathbf{r}} \quad i, j = 1, 2 \quad (205)$$

As in the case of monodisperse particles we consider the case at equilibrium when

$$\langle \mathbf{u} \rangle = \bar{\mathbf{v}}_i = \bar{\mathbf{w}}_i = 0, \quad i = 1, 2 \quad (206)$$

in which case Eq. (205) can be written in terms of the particle radial distribution function $g_{12}(r)$

$$g_{12}(r) = \langle n_{12} \rangle / \langle n_1 \rangle \langle n_2 \rangle \quad (207)$$

and the Eulerian second-order particle-structure function tensor $\mathbf{S}_2^p$ is given by

$$\mathbf{S}_2^p = \langle \mathbf{w} \mathbf{w} \rangle = \langle \mathbf{v}_1 \mathbf{v}_1 \rangle + \langle \mathbf{v}_2 \mathbf{v}_2 \rangle - \langle \mathbf{v}_1 \mathbf{v}_2 \rangle - \langle \mathbf{v}_2 \mathbf{v}_1 \rangle \quad (208)$$

$$\text{so } \partial \cdot \mathbf{S}_2^p / \partial \mathbf{r} + \beta_p^{-1} \varepsilon_p \cdot \partial \ln g_{12} / \partial \mathbf{r} = 0 \quad (209)$$

where $\beta_p = \frac{1}{2}(\beta_1 + \beta_2)$, and ε_p is the bidisperse pair diffusivity tensor for pair separation and given by

$$\varepsilon_p = \beta_p^{-1} \{ \beta_1 (\varepsilon_1 - \varepsilon_{12}) + \beta_2 (\varepsilon_2 - \varepsilon_{21}) \} \quad (210)$$

8.4 Collision model for Bidisperse Particles. As with the momentum equation for monodisperse particles at equilibrium (with zero inertial convective D/Dt terms) Eq. (205) for bidisperse particles similarly represents a balance between the turbophoretic drift and gradient diffusion with a particle diffusion coefficient which is a weighted sum of the relative diffusion coefficients associated with each collision model for bidisperse particles.

When considering collisions in isotropic homogeneous turbulence we can assume spherical symmetry and obtain a similar equation for the radial momentum balance as given in Eq. (150) for monodisperse particles but involving radial (longitudinal) components $\varepsilon_{p,ll}$ of the bidisperse diffusion coefficient tensor ε_p , namely,

$$\frac{2(S_{2,nn}^p - S_{2,ll}^p)}{r} - \frac{dS_{2,ll}^p}{dr} - \beta_p \varepsilon_{p,ll} \frac{d \ln g_{12}(r)}{dr} = 0 \quad (211)$$

where $\varepsilon_{p,ll}(r)$ refers to the longitudinal component of particle pair diffusivity tensor ε_p along the line of centers of the particle pair, Eq. (210) and similarly the longitudinal and normal components of the bidisperse particle-structure function tensor $\mathbf{S}_2^p(r)$. This radial momentum equation with the corresponding momentum equation for the lateral (normal) component are solved with appropriate reflecting boundary conditions as a closed set of coupled equations with solutions for $S_{2,ll}^p$ and $S_{2,nn}^p$ derived from their transport equations. These involve the gradients of the third-order moments $\mathbf{S}_3^p$ based on closed expressions similar to that for the monodisperse in Eq. (72). We note these equations involve

3286 Eulerian structure functions $S_{2,nn}$ and $S_{2,ll}$ and the Lagrangian
 3287 autocorrelation coefficient for fluid velocity difference (see Eq.
 3288 (201)). Values of the collision kernel Γ are obtained from the
 3289 formula

$$\Gamma = \{8\pi S_{2,ll}^p(r_c)\}^{1/2} r_c^2 g_{12}(r_c) \quad (212)$$

3290 inserting the values of $S_{2,ll}^p$ computed from the solution of the set
 3292 of coupled equations Eq. (211). In the case of zero inertia particles
 3293 of type 2, the forms for $S_{2,ll}^p(r_c)$ can be written explicitly as

$$\bar{S}_{2,ll}^p(r) = \frac{(1 - f_{u1})\text{Re}_\lambda}{15^{1/2}} + f_{r1} \bar{S}_{2,ll}(r) \quad (213)$$

3295 where the overbar means velocities are normalized by the Kolmo-
 3296 gorov velocity scale $u_k = (\nu_f \varepsilon_f)^{1/4}$ and Re_λ is the Taylor Reyn-
 3297 olds number based on the Taylor microscale. Substitution of the
 3298 formula in Eqs. (213) into (212) gives

$$\Gamma = (8\pi)^{1/2} r_c^2 \langle u'^2 \rangle^{1/2} \left(1 - f_{u1} + \frac{f_{r1} \bar{r}_c^2}{15^{1/2}} \right) \text{ where } \bar{r}_c = r/\eta_k \quad (214)$$

3300 If particles of type 1 are also inertialess then Γ reverts to the Saff-
 3301 man and Turner formula

$$\Gamma_{ST} = \left(\frac{8\pi \varepsilon_f}{15\nu_f} \right)^{1/2} r_c^3 \quad (215)$$

In the case where particles of type 2 are highly inert, $\beta_2 \rightarrow 0$ and 3303

$$\bar{S}_{2,ll}^p \rightarrow \frac{f_{r1} \text{Re}_\lambda}{15^{1/2}} \quad (216)$$

We recall f_{u1} and f_{r1} given in Eq. (202). 3305

In Fig. 41, solutions of the closed set of equations for $S_{2,ll}^p$, $S_{2,nn}^p$ 3306
 and g_{12} (Eq. (211) etc. based on the *nonlocal equilibrium* 3307
approach are compared with those based on the *local equilibrium* 3308
approach and the DNS computations of Zhou et al. [148] for 3309
 $r_c/\eta_k = 1$ as a function of the particle response time τ_{p2} of parti-
 cle 2 for fixed values of τ_{p1} of particle of type 1. As is seen, the 3310
 overall agreement between the predicted and simulated profiles of 3311
 the mean radial relative velocity for the *nonlocal equilibrium* 3312
approach is generally very good, especially at small values of 3313
 τ_{p1}/T_e and τ_{p2}/T_e . According to the formula for $S_{2,ll}^p$ in Eq. (173),
 $\langle |w'_r| \rangle / \langle u'^2 \rangle^{1/2}$ increases monotonically with increasing τ_{p2}/T_e
 due to a decrease in the correlation of particle pair velocities. In 3314
 contrast, the difference in inertia of particles from different groups 3315
 enhances the relative velocity between pairs. Conversely accord- 3316
 ing to Eq. (216), at large τ_{p2}/T_e , $\langle |w'_r| \rangle / \langle u'^2 \rangle^{1/2}$ monotonically 3317
 decreases with increasing τ_{p1}/T_e since the particle response to the 3318
 fluid turbulence decreases. Figure 41 shows that the relative 3319
 velocity first drops with increasing τ_{p2}/T_e , passes through a mini- 3320
 mum, and then increases, approaching the constant value corre- 3321
 sponding to the value given by the formula in Eq. (216). This 3322
 minimum is especially pronounced at small τ_{p1}/T_e . As indicated 3323
 in Zhou et al. [148], in comparison with the monodisperse results, 3324

Fig. 41 The mean radial relative velocity of colliding particles for $\text{Re}_\lambda = 45$; 1, 2, 4: bidisperse system; 3: monodisperse system; 1: *local equilibrium approach*; 2, 3: *nonlocal equilibrium approach*; 4: DNS by Zhou et al. [148]; (a): $\tau_{p1}/T_e = 0.1$; (b): $\tau_{p1}/T_e = 0.2$; (c): $\tau_{p1}/T_e = 1$; (d): $\tau_{p1}/T_e = 2$; turbulence microscale $T_e = \varepsilon_f/u'^2$; τ_{p1} , τ_{p2} = particle response times of particles 1, 2, taken from Zaichik et al. [137]

the difference in particle inertia between particle component pairs is to increase the radial relative velocity. Therefore, the values of $\langle |w_r| \rangle / \langle u^2 \rangle^{1/2}$ in a bidisperse system are always more than those in a monodisperse case with $\tau_{p1} = \tau_{p2}$, so that the minima of the relative velocity correspond to the values for which $\tau_{p1} = \tau_{p2}$. In other words, the relative velocities of particles with different inertia are bounded from below by those of identical particles, namely, curves 3 in Fig. 41. The relative velocities predicted for low-inertia particles $St_1, St_2 \leq 1$ are found to be almost coincident with those from DNS. However, the agreement between the predicted and simulated relative velocities of high-inertia particles is not as good. Zaichik [137] notes that this discrepancy between the predicted and simulated results may be due to the effect of particle inertia on the eddy-particle interaction time scales. Thus, from the comparisons presented in Fig. 41, it can be concluded that the model considered properly captures the main special features of the behavior of particle relative velocities in a bidisperse system. Figure 42 shows Zaichik et al.'s [137] predictions and comparison with simulations of the RDF $g_{12}(r_c)$ at the contact radius $r_c/\eta_K = 1$ as a function of the Stokes number St_2 of particle 2 while St_1 of particle 1 is fixed for each curve. As follows from Eq. (213) and Eq. (216), in the limiting cases of low-inertia and high-inertia particles from particles to type 1 or 2, the RDF of particles from different groups is uniform and hence $g_{12} = 1$. In accordance with the DNS data [148] the RDF as predicted goes through a peak as St_2 increases, although compared with the DNS result, this peak is noticeably shifted toward particles with noticeably higher inertia. The RDF attains a maximum when the response times of particles from both groups are equal, namely, $St_1 = St_2$. Also shown in Fig. 42 is the RDF of a monodisperse system, which corresponds to the maxima of g_{12} . Hence, the RDF of particles with different inertia is bounded from above by that of identical particles. Thus the phenomenon of clustering is most pronounced in monodisperse suspensions and becomes less tangible when the difference between particle inertia increases.

9 Concluding Remarks: Insights, Challenges, and Future Prospects

In these concluding remarks, it is useful to reflect on some of the important issues that have been raised in this review, to elaborate on the insights and understanding this kinetic theory has provided, and to highlight some of the long standing problems in the modeling of dispersed flows this approach has resolved. It's important also to mention the obvious computational advantages of using this approach especially for bidisperse and polydisperse particles (by implication) together with its accuracy and reliability compared to other traditional methods and approaches. In conclusion, future prospects are briefly discussed: how, for instance, the

Fig. 42 The radial distribution function $g_{12}(r_c)$ for $Re_k = 45$. 1–6: predictions; 7–12: DNS of Zhou et al. [148]; 1,7: $St_1 = 0.5$; 2,8: $St_1 = 1.0$; 3,9: $St_1 = 1.17$; 4,10: $St_1 = 2.34$; 5,11: $St_1 = 11.7$; 6,12: monodisperse system, taken from Zaichik et al. [137]

two kinetic approaches KM, and GLM referred to in this review can be used to support one another in practice, together with their advantages and disadvantages and where improvements can be made to broaden the scope and application to different flows, to the behavior of nonspherical particles and situations other than that of gas-particle flows.

9.1 Advantages of a Kinetic Theory. There are a number of very positive advantages of using a “kinetic” approach over the more traditional approaches and in particular of using a kinetic equation for the transport of particles in phase space. In KM the instantaneous phase space density underlies the treatment of particle velocity and position as random variables whilst in the GLM, it involves the carrier flow velocity at the particle position and velocity as an extra phase space variable. In both KM and GLM the corresponding transport equation for the particle phase space density is a linear partial differential equation, in contrast to the particle momentum equation in real space which is a highly nonlinear partial differential equation. It means that, as Kraichnan first observed [46], the use of simple closure approximations, questionable for closure of a nonlinear equation, may have a sporting chance of success. As a corollary, simple gradient transport in phase space does not necessarily imply simple gradient transport in real space. Equally important is a single closure approximation in phase space implies closure forms for both the particle fluid velocity correlations and the net turbulent driving force in the particle momentum equation: in contrast it is necessary, in the traditional approach of Reynolds averaging of the momentum equations, to make separate and independent approximations for both these terms.

But perhaps most important of all, is the use of a kinetic phase space approach in resolving a long standing problem of boundary conditions which are more naturally prescribed in phase space than in real space. As an example, the impact of particles at a surface naturally involves some prescribed change in the particle velocity at impact and therefore imposes some constraint on the form of the particle velocity distribution at the surface. This information cannot be fed directly into the two-fluid momentum equations except in some artificial way through constraints on the spatial density and the average momentum. This is an inherent weakness in conventional two-fluid modeling noted before, and can only be properly resolved by a fully kinetic treatment close to the surface. See Sec. 5 for the near-wall concentration and velocity for absorbing and partially absorbing surface boundaries.

9.2 Closure of Kinetic Equations. Closure of the kinetic equations in both GLM and KM has been pivotal to the successful development and application of both approaches.

9.2.1 GLM Closure. The GLM follows the approach taken by Pope et al. [14,15,149] which uses a Langevin equation involving a white noise generated function describing the fluid velocity acceleration associated with the fluctuations of the small scales of the carrier flow turbulence. The kinetic equation for the particle phase space density involving the extra carrier flow velocity is described appropriately by a Fokker–Planck equation. However, the equation belies a hidden closure problem associated with the addition of an extra term necessary to account for the fluid acceleration encountered by particles and not by the fluid elements as in Pope’s GLM equation. See Eq. (35) for the difference between the particle and carrier flow accelerations involving the coupling of the particle–fluid relative velocity with the local shearing of the carrier flow velocity which requires additional closure. SDM in their particle-related version of GLM, absorbed these terms into the white noise components of the Langevin equation thus associating them with the influence of the small scales of the turbulence. In so doing they cleverly circumvented the necessity of closure but the problem remains as to the contribution this term makes. This problem will be returned later on when the differences between GLM and KM approaches are discussed.

9.2.2 *KM Closure.* Closure of the KM kinetic equation involves finding closed expressions for the net turbulent aerodynamic driving force $\bar{f}$, Eq. (20) and is more challenging than the closure of the GLM kinetic equation. This is essential because it deals with the role of the large and small scale turbulent structures on the dispersion and mixing of the suspended particles as well as the Lagrangian nature of the particle and fluid velocity correlations involved. In the construction and implementation of suitable closure approximations, self-consistency and preservation of invariance principles were key guidelines.

The focus has been on *legitimate* closure methods¹⁶ and in particular FN and LHDI methods chosen for their random Galilean transformation (RGT) invariance and realizability. As a consequence both closure formulations represent the net force due to the turbulence as linear contributions of spatial and velocity gradients of the net phase space density together with a body force (per unit mass) dependent on the particle response to the spatial and temporal inhomogeneity of the turbulence, see Eq. (20) in Sec. 2.2.1. The combination and contribution are crucial to obtaining the correct form for the particle equation of state that defines the relationship at equilibrium between the particle pressure and the local particle diffusion coefficient in homogeneous (statistically stationary) turbulence. Both FN and LHDI closures involve correlations of the aerodynamic driving force that are Lagrangian. However, in FN, it is the value of the Eulerian spatial/time correlation where the separation is measured along a particle trajectory. In contrast in LHDI, it is the Lagrangian correlation of the aerodynamic force itself measured along a particle trajectory. What, however, is important to appreciate is that the spatial and velocity gradients operate on $\mu\langle W \rangle$ and $\lambda\langle W \rangle$ not on $\langle W \rangle$ exclusively, as $\partial_v \cdot \mu\langle W \rangle + \partial_v \cdot \lambda\langle W \rangle$. This is not a trivial observation: it means that μ and λ behave as stress tensors in velocity and real space, not as dispersion tensors. It means in the end that the contribution of the μ and λ gradient terms is not entirely diffusive. So, for instance, in the expression for the particle mass flux there is a contribution from simple gradient diffusion as $\tau_p \bar{\lambda} \cdot \partial_x \langle \rho \rangle$ but also from convection as $\langle \rho \rangle \nabla \cdot \bar{\lambda}$ which adds to the convection from the body force $\bar{\kappa} \langle \rho \rangle$. It has, for instance, lead to valuable insights into the relationship between diffusion and convection embodied in the particle momentum equation in inhomogeneous turbulence reflected in particle transport and deposition in turbulent boundary layers. In homogeneous turbulence in the absence of gravitational settling these convective terms disappear. It is only in inhomogeneous turbulence that these terms make a measurable and significant contribution. The contribution these extra convective terms make to the particle mass flux has only recently been properly recognized and measured along with the turbophoretic flux [132,133] $-\langle \rho \rangle \tau_p \nabla \cdot \bar{v}' \bar{v}'$ due to the kinetic stresses. In Zaichik's equation for both single particles and for mono and bidisperse particles, only the dispersive part of the turbulent driving force has been accounted for Eq. (147).

9.2.3 *Gaussian Versus Non-Gaussian Processes.* The closure term $-(\partial_v \cdot \mu + \partial_x \cdot \lambda - \kappa)\langle W \rangle$ is an exact closure for a Gaussian process ensuring realizability and well posedness and has formed the basis of the kinetic theory presented here [23,52]. The closure has been extended to non-Gaussian processes involving an expansion in the cumulants $K^n\{\}$ with RGT satisfied at every order of the expansion (see Eq. (31)). For a Gaussian process all terms in the expansions are zero except the first term given by $-(\partial_v \cdot \mu + \partial_x \cdot \lambda - \kappa)\langle W \rangle$. Unfortunately the expansion is not uniformly convergent; furthermore, it is well 'known' [46] that realizable solutions for $\langle W \rangle$ can only be achieved by truncating the expansion after the first term or including all the terms in the expansion.

¹⁶Legitimate in the sense that they are formally related to the underlying equations of motion of both fluid elements and particles, and preserve realizability. The averaged equations have thus a much sounder theoretical basis, the only constants involved being those of the particle equations of motion and statistics of the carrier flow itself.

9.3 *Dispersion for High Stokes Number Particles $St \gg 1$ with Nonlinear Drag.* For high inertia particles with Stokes number $St \gg 1$, the kinetic equation contracts to a Fokker Planck equation [23]. In this case, analytic expression for the long-term particle diffusion coefficient and mean square velocity in homogeneous stationary turbulence have been obtained for nonlinear drag (see Eqs. (55) and (56) which show how they depend on particle Stokes number St and particle Reynolds number Re_p defined in terms of the turbulence intensity u_0 . Most surprisingly results show very little dependence of the diffusion coefficient on Re_p varying by $\sim 2\%$ with the value for Stokes drag for $Re_p = 0$. As with the case of Stokes drag, there is no implicit dependence on St . In contrast the value of the mean square particle-carrier flow velocity ratio $\langle v^2 \rangle / u_0^2 \propto St^{-1}$ and increases with increasing Re_p .

9.4 *Influence of Turbulence on Gravitational Settling (the Maxey Effect).* For completeness on closure, it is insightful to recall the way the FN closure term for the net turbulent driving force $\bar{f}$ accounts for the enhancement of gravitational settling of particles in homogeneous statistically stationary turbulence (the Maxey effect). This behavior is related to the underlying temporal inhomogeneity in the turbulence, to the eddying motion of the turbulence and the way particles respond to the spatial structure. More specifically it is to do with the way a body force like gravity imposes a bias on the motion of the particles enveloped by these structures in the direction of the body force. In the kinetic equation, it is accounted for by the body force $\bar{\kappa}$ in the direction of gravity and to the trajectory biasing of the particle motion imposed by gravity. We refer to the expression for $\bar{\kappa}$ given in Eq. (21) based on the FN closure method and in particular to the dependence of the coupling of the response function $G^p(\mathbf{x}, t|s)$ and the Eulerian spatial correlation $R(\mathbf{x}, t)$ on the trajectory biasing imposed by gravity.

9.5 *Interparticle Collisions.* Important contributions have been made in the application of the kinetic approach to particle pair dispersion: to the way it quantifies interparticle collision rates and the influence, this has on the particle continuum equations and also to the way particles cluster and coagulate in a flowing gas-particle suspension. Both processes involve the particle pair phase space (probability) density involving the position and velocity of both pair members at some instant of time. Collision rates are quantified by the value of the collision kernel Γ defined in terms of the particle pair pdf and the relative velocity $\mathbf{v}_1 - \mathbf{v}_2$ between particle pair members, Eqs. (105) and (107) and the dependence of those collision rates on the particle response to the large scales of the turbulence and the small dissipating scales of the turbulence responsible for the demixing and clustering of particles.

9.5.1 *Influence of the Particle-Fluid Velocity Correlation.* While there is an obvious similarity to collision rates of molecules in a gas, there are important differences regarding the legitimacy of the molecular chaos assumption when applied to particles colliding in a turbulent gas and the influence of particle-fluid drag forces on the collision rate. Due to the pioneering work of Simonin and Fede and their coworkers, these problems have been resolved by a consideration of the way the particles collision rate is influenced by the correlation of the two colliding particles with the local fluid and the way that depends upon their separation at the point of collision and the particle Stokes number St_L (as the ratio of the particle response time to that of the large and inertial range of turbulent scales). The effect is to reduce the collision rate approaching zero for $St_L \ll 1$ at zero separation. These features are incorporated into the formula for the collision kernel that depends upon the relative velocity between particle pairs at the point of collision and the particle fluid velocity covariance based on a local equilibrium approximation. This forms an essential part of the Boltzmann integral for the rate of loss/increase of particles

due to collisions within and outside an elemental volume of phase space for single particles. To illustrate the influence of the particle fluid velocity correlation, the particle kinetic stresses in a developing shear were evaluated using two methods: one based on the molecular chaos assumption and the other based on the particle fluid velocity correlation. Both models used Grad's third-order moment expansion for the particle velocity distribution Eq. (128). See figure indicating the values of the kinetic stresses for the molecular chaos model are noticeably greater than those based on the particle fluid flow velocity correlation.

9.6 Clustering of Monodisperse and Bidisperse Particle Suspensions. The solutions of the kinetic equation for particle pairs at the small dissipating scales of the turbulence have added much to our understanding of the mechanisms for clustering and demixing of suspended particles. In particular how the clustering depends upon the particle Stokes number St_K with a maximum at $St_K \sim 1$; the occurrence of RUM and singularities in the particle concentration field with the formation of caustics and finally the fractal nature of pair concentration at very small separations r where the RDF $g(r) \sim r^{-\chi}$, $\chi \propto St_K^2$. It was noted that the kinetic equation for particle pair separation for monodisperse particles is the same as that for particle transport in a turbulent boundary, exhibiting similar features: the buildup of concentration close to the wall and the dependence of the particle mean square velocity as a function of wall distance y^+ and τ^+ being compared with the clustering measured in terms of the RDF and the radial particle-structure functions $S_{22}^p(r)$ and their dependence on r and St_K equivalent to τ^+ .

The kinetic equation in the form used by Zaichik (with $\bar{\kappa} - \nabla \cdot \bar{\lambda} = 0$) has been used to obtain a closed set of coupled equations for the particle-structure functions S_2^p and particle pair RDF from which solutions, the RUM and MEVPM components of the total kinetic energy have been extracted as a function of St_K over a range of values of Re_λ in good agreement with the results of numerical simulations, Fig. 26 Further investigations using measurements of the *incompressibility* of the particle suspension along particle trajectories [79] have also revealed the RUM component as the source of singularities and intermittency within the highly filamental regions of the caustics and responsible for particle collisions. Here the activation of singularities precedes the crossing of trajectories in the RUM component.

The application of kinetic theory to the dispersion and clustering of bidisperse particle suspensions of particles is especially important because it can easily be extended to include the transport and collisions of polydisperse particles which makes the approach much more useful for the application to real suspensions; the growth and breakup of particle suspensions and the subsequent evolution of their size distribution can then be properly dealt with. Much of this is due to the pioneering work of Zaichik and Simonin [137] for generalizing the kinetic model for monodisperse particle pairs given in Eq. (169), with Eq. (171) for the phase space diffusion current involving the phase space diffusion coefficients given in Eq. (171). However, the bidisperse kinetic equation is significantly different from that of monodisperse particles in that the net turbulent driving force acting on any one component particle of the bidisperse mixture depends on a gradient diffusion contribution from both particle types (as reflected in their contribution to the stress tensors $\lambda^{(ij)}$, $\mu^{(ij)}$). Whilst following a similar approach for clustering of monodisperse particles, the approach followed by Zaichik and Simonin for bidisperse particles is more complex [137] because, unlike monodisperse particles, the rate of separation of bidisperse particles cannot be disentangled from the motion of the center of mass of the particle pair. So it was therefore necessary to deal explicitly with the particle pair pdf of the individual particle positions and velocities of the particle pair in the kinetic equation as given in Eq. (169). From this equation, the momentum equation for both members of the bidisperse mixture was obtained by suitable integration over

all particle velocities, Eq. (198). So unlike the case for monodisperse particles, the momentum equations for each component are coupled. We recall that the momentum equation for monodisperse particles contains advection-gradient diffusion terms that represent a balance between turbophoretic drift (dependent on spatial gradients of the particle velocity covariance) and gradient diffusion (dependent on spatial gradients of the particle concentration and a tensor of diffusion coefficients based on a combination of kinetic and interfacial stresses). In the case of bidisperse particles, the turbophoretic drift and gradient diffusion terms contain additional contributions that depend on the coupling between both component sets of particles and involving spatial gradients of the velocity covariance of both components and a diffusive flux with a set of diffusion coefficients that likewise depends on averages involving both components, see Eq. (199). So in comparison with monodisperse particles, the bidisperse momentum equations for each component involve two sets of diffusion coefficients, one identical in form to that for monodisperse particles and the second set of diffusion coefficient that depends on the coupling between both components. We noted that Zaichik [137] changes the spatial and velocity variables in these transport equations to consider directly the relative motion of particle pairs. The momentum equations are thus reduced to a balance between the gradient of the particle structure function (turbophoresis) and the gradient of the radial distributions function of the particle bidisperse particle pair, see Eq. (209) with a diffusion coefficient tensor ϵ_p , Eq. (210) that is a combination of the three sets of diffusion coefficients in the bidisperse momentum equations, Eq. (198).

9.7 Improvements and Future Prospects. It is useful to recall some of the deficiencies with both GLM and KM methods where improvements can be made and how both methods can compliment and support one another in practice. Its also highly appropriate to comment on future prospects, on how, for instance, this kinetic theory is open to further development and application to other types of particle suspensions exploiting the same methods and approach that are described in detail here for gas-particle flows.

9.7.1 KM Versus GLM, Defects and Improvements. We refer in particular to a detailed comparison between KM and GLM given in Reeks et al. [150] concerned with the realizability of the KM kinetic equation and its relationship to the GLM kinetic equations. Both kinetic equations invoke approximations in the description of the turbulence of the underlying flow transporting the particles which in the case of GLM are not rigorously justifiable [150]. The GLM is based on a model for the turbulence, whereas in KM the relevant proprieties of the underlying turbulence are inputs based on experimental measurement or from DNS/LES and using legitimate closures approximations for the net turbulence forces which take account of the spatiotemporal structure of the turbulence and the difference between particle and carrier flow Lagrangian timescales. However whilst accepting these limitations of GLM, one important and obvious advantage of the GLM over the KM approach is that it includes an extra phase space variable for the flow velocity sampled along a particle trajectory. So a solution to the corresponding kinetic equation in principle contains more information about the dispersion process than the solution of the KM equation. However, as was stated in Sec. 9.2.1 the GLM equations do not properly take account of the fact that fluid element motion is different from the fluid element motion sampled along a particle trajectory. In the GLM, the term which accounts for this difference is only strictly accounted for through the mean shear of the flow with the influence of the fluctuating shear swept under the carpet of the white noise generating function or its effect modeled by making the timescale in the Langevin model a prescribed function of the particle response time τ_p . In contrast, in KM, the difference between a particle and fluid element motion and the dependence on particle inertia is formally accounted for and an intrinsic part of the closure approximation.

In particular, it is captured through the dependence of λ , μ , and κ on the correlation tensors of the fluid velocity field evaluated along the inertial particle trajectories. So for GLM, the reality is closure is required for the net value of the fluctuating shear measured along particle trajectories. The same closure schemes, FN/LHDI can be used to close this term as were used for the net turbulent driving force in KM $\bar{f}$. In principle, these terms should enable the prediction of crossing trajectories and the way Lagrangian timescales depend upon the gravitational settling.

9.7.2 Incorporation of Boundary Conditions in Complex Flows. Only simple examples have been referred to in this review to illustrate how the kinetic theory handles the natural boundary conditions of scattering and absorption at solid boundaries. See Figs. 10 and 11. What boundary conditions that have been applied to the solutions of the particle momentum equations have assumed perfect reflection or been purely artificial. In reality, the natural boundary conditions have to do with the particles' response to the surface molecular forces which for impacting particles at a solid surface express a relationship between the distribution of particle velocities before and after impact with possible deposition/absorption and subsequent resuspension of the deposited particles sometime later. So whilst the velocity distribution at the wall is an important feature of the boundary conditions, it is not known a priori but is an intrinsic part of the calculation. To incorporate these natural boundary conditions it has had been necessary to solve the kinetic equations directly for the particle phase space density $W(\mathbf{x}, \mathbf{v}, t)$. This is possible close to the wall or at small particle separation, but is not possible in complex flow and geometries. So some kind of matching is necessary of the near-wall solution for $W(\mathbf{x}, \mathbf{v}, t)$ with the solution of the mass momentum kinetic stress equation of the bulk flow. It suggests the use of wall functions similar to that used in RANS turbulence modeling, see, e.g., Knopp et al. [151].

9.7.3 The Inclusion of Convective Mass Fluxes for the Turbulent Aerodynamic Force $\bar{f}$. It is to be noted that in all the examples where the kinetic equations have been solved both for single particle and particle pair, mono and bidisperse suspensions where the turbulence is inhomogeneous, the convective mass flux derived from the turbulent stresses of λ and μ and the body force κ have been neglected. Only the influence of the convective flux associated with the kinetic stresses $\overline{\mathbf{v}\mathbf{v}'}$ and likewise those stresses $\overline{\mathbf{w}\mathbf{w}'}$ associated with the relative velocity $\mathbf{w}$ between particle pairs have been considered in the corresponding moment equations of Zaichik and Simonin [31,81,137,141]. These extra convective fluxes will play an important part in the buildup of the near-wall concentration in turbulent boundary layers and in particle pair concentration at small separation where the concentration is necessarily a balance between convective and diffusive fluxes. Stafford and Swailes [132] have recently calculated these extra convective fluxes and their contribution to the near-wall concentration qualitatively assessed, see Sec. 7.6. So those calculations of Zaichik and Simonin must be repeated with the inclusion of these extra convective terms. In the case of the GLM approach, these convective fluxes can readily be accounted for by adding them artificially as body forces to the particle equation of motion. It is important to appreciate that the interfacial momentum transfer term between particle and carrier flow is the same as that given by the closed form of the net drag and the closed form of the aerodynamic driving force $-\beta\mathbf{v} + \bar{f}$ which of necessity includes these extra convective fluxes and body forces as well as the diffusive components of $\bar{f}$. The contribution of these extra convective fluxes in Euler-Euler models for reactive flows and in particular their contribution to the interphase momentum transfer needs to be investigated.

9.7.4 Other Flows and Particle Flow/Density Ratios. Reference is made here to the considerable body of work of Simonin, Fede and Masi and their coworkers in extending the GLM approach to model dense reactive flows, common to many industrial flows [152] involving fluidized beds [153–155] and chemical

combustion plants [156] where two-way coupling between particle and carrier flow is dominant and interparticle collisions are crucial features [155]. The work of Swailes et al. [17] has already been mentioned on the added mass effect in flows concerned with the transport of droplets in liquids pipelines in the petroleum industry. But it is also relevant in other flows where the particle/carrier flow density ratio ~ 1 in addition to the role of history forces in accelerating flows captured by the BBO equation [157]. Finally, we refer to the work of Marchioli et al. [158] who have made considerable progress in recent years in the development and application of LES for particle transport in the turbulent flows using Euler-Euler closure models for the subgrid scale modeling of the type reviewed here [159]. Here again, it would be important to consider the influence of the convective fluxes on the particle pair transport at the small dissipating scales of the turbulence for both bidisperse and monodisperse particles. There remains the application of this kinetic theory for the dispersion of nonspherical particles of different shapes and sizes. Whilst accurate methods for calculating the drag and lift in turbulent flows have been developed successfully and applied in DNS/LES, see, e.g., Wachem et al. [160], a kinetic theory for such particles has as yet to be developed and implemented in any formal way. The formulation and the application of suitable closure approximation based on FN methods still apply and open to future development.

9.7.5 A Personal Note. It was deeply satisfying to have followed in the footsteps of Albert Einstein (see Sec. 4.1.1) using exactly the same arguments he used to evaluate the diffusion coefficient of Brownian particles and which lead to the well-known Stokes-Einstein relation [64]. In the case considered here of small particles suspended at equilibrium in a homogeneous statistically stationary turbulent flow, an expression for the particle diffusion coefficient was obtained Eq. (68) based as with Einstein's formula for the Brownian diffusion coefficient on the balance of the particle pressure gradient due to the turbulence with the weight of the suspended particles Eq. (66).

9.7.6 Dedication. This review is dedicated to the memory of Dave Stock for his contribution to our understanding of gas-particle flows through the ingenuity of his experiments and for the modeling and simulation he has inspired. It is also dedicated to the memory of Leonid Zaichik for the immense contribution he has made to the development and application of the kinetic theory presented here.

Acknowledgment

Financial support for the research reported in this review has been gratefully received from EPSRC-GB. 'Droplet clouds in a "box" of turbulence' EPSRC Grant # EP/E029973/1.

Nomenclature

Upper Case Roman Symbols

$B_{LP}(r, \tau)$	= Lagrangian velocity correlation of particle pair separated initially by a distance r	3811
$C(\psi)$	= collision term to be added to the transport equation for property ψ , e.g., ψ = mass, momentum, kinetic energy, and third-order moments, etc	3812 3813 3814
C_p	= specific heat of the particle/droplet	3815
$D_f(\infty)$	= long term fluid element (passive scalar) diffusion coefficients	3816
$D_{ij}(t)$	= particle diffusion coefficients = covariances of particle position and velocity $\langle x_i^*(t)v_j^*(t) \rangle$	3817
$D_p(\infty)$	= long term particle diffusion coefficients	
D_v	= molecular diffusion coefficient of vapor	
$F(r)$	= longitudinal spatial correlation between carrier flow velocities separated by a distance r	3818 3819

3820	$G(r)$ = lateral spatial correlation between carrier flow	j^+ = particle deposition velocity normalized on the	3866
3821	velocities separated by a distance r	friction velocity in fully developed turbulent	3867
	$\mathbf{F}_A$ = aerodynamic force	pipe flow	3868
	$\mathbf{F}_D$ = aerodynamic drag force	k_g = thermal conductivity of the gas flow	3869
	$\mathbf{F}_L$ = aerodynamic lift force	k_p = particle kinetic energy	3870
3822	Nu = Nusselt number of the particle	k_p = particle kinetic energy contribution from the	
	$\langle P \rangle$ = pdf for particle velocity, position and fluid	MEPVF	3871
3823	velocity viewed by the particle	l_e = length scale of the turbulence	3872
	$P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ = phase space density at $(\mathbf{v}, \mathbf{u}, \mathbf{x})$ at time t	$n_i, i = 1, 2$ = number concentration of particles, $i = 1, 2$	
	$P^0(\mathbf{v}, \mathbf{x})$ = equilibrium Maxwell distribution of particle	n_p = particle number density	3873
3824	velocities	p = particle pressure tensor due to the suspended	3874
3825	Pr = Prandtl number of the gas/vapor mixture	particles' turbulent motion	3875
	$R_E(0, y)$ = carrier flow spatial velocity correlation (in a	p = rate constant for the removal of particles from	3876
3826	frame moving with the settling velocity with a	an adhering surface	3877
3827	separation y measured in the direction of		
3828	gravity	$\bar{r} = r/\eta_K r_c$ = defines the location of the center of one of a	
	$\mathbf{R}_{ki}$ = Eulerian two-point, two-time correlation ten-	pair of a colliding particles with respect to the	3878
3829	sor of the turbulent force field $\mathbf{f}$	center of the other particle at their point of	3879
3830	Re_p = particle Reynolds number	contact. For two colliding spherical particles r_c	3880
	Re_p = particle Reynolds number based on the net rel-	is the radius of the collision sphere that defines	3881
3831	ative velocity between particle and local car-	the point of contact for the two colliding	3882
3832	rier flow	particles	3883
	Re_λ = Reynolds number based on Taylor microscale	$\mathbf{u}(\mathbf{x}, t)$ = gas flow velocity flow field local to the	3884
3833	$\mathbf{S}$ = strain rate tensor	particle	
3834	S_c = vapor Schmidt number	u' = fluid rms velocity or turbulence intensity	
3835	S_r = heat source due to the external field (radiation)	$\mathbf{u}''$ = the average carrier flow velocity relative to $\langle \mathbf{u} \rangle$	
	$\mathbf{S}_2(\mathbf{r})$ = Eulerian fluid point pair second-order structure	encountered by a particle	3885
3836	function tensor at a separation $\mathbf{r}$	$\mathbf{v}$ = particle velocity	3886
	$\mathbf{S}_2^p$ = Eulerian second-order structure function	$\tilde{\mathbf{v}}_p(\mathbf{x}, t, \mathcal{H}_f)$ = MEPVF contribution to the instantaneous par-	
	$\mathbf{S}_3^p$ = the particle pair density weighted triple rela-	ticle velocity	3887
3837	tive velocity (i.e., the third-order	$\mathbf{v}_g$ = gravitational settling velocity	
	particle-structure function) at a separation $\mathbf{r}$	w_r = the relative velocity between particle pairs	3888
	$\mathbf{S}_2^p(\mathbf{r})$ = second-order particle-structure function at	measured along their line of centers	3889
3838	particle pair separation r , i.e., the pair density	$ \overline{w_r} $ = the net velocity toward any individual particle	
3839	weighted relative velocity covariance	of neighboring particles at the collision radius	3890
	$S_{2,II}^p$ = second-order particle-structure functions at	along their line of centers	3891
3840	particle pair separation r for velocities II = a-	x = particle position	3892
3841	long line of centers	$\mathbf{x}_p(t s)$ = particle position evaluated at time s along all	
	$S_{2,nn}^p$ = second-order particle-structure functions at	particle trajectories passing through $\mathbf{x}$ and $\mathbf{v}$ at	3893
3842	particle pair separation r for velocities	time t	3894
3843	nn = normal to line of centers	z = parameter characterizing the interrelation	3895
3844	Sh = droplet Sherwood number	between the effects of gravity and turbulence	3896
3845	St = particle Stokes number	on the collision kernel	3897
3846	St_K = Stokes number based on the ratio of the parti-	$\bar{z}$ = the net collision rate of an individual particle	
3847	cle response time to the timescales of Kolmo-	with surrounding particles	3898
3848	gorov dissipating scales of the turbulence		
3849	T = absolute temperature	Upper Case Greek Symbols	3899
3850	T_e = the microscale time scale ε_f/u'^2	St_L = particle Stokes number $1/\beta T_L$	3900
3851	T_E = the Eulerian integral time scale of the carrier	Γ = particle collision kernel (the net collision rate	3901
3852	flow turbulence at a point moving with the	of an individual particle with surrounding	3902
3853	mean carrier flow velocity	particles normalized by the local average	3903
3854	T_L = integral timescale of the carrier flow turbu-	number concentration of particles within a	3904
3855	lence along a fluid element trajectory	control volume)	3905
3856	$\mathbf{W}$ = particle phase space density	$\Delta \mathbf{v}_j(t)$ = changes in velocity for a particle starting	
	$\langle W \rangle$ = pdf for particle velocity and position	somewhere in particle phase space at some ini-	3906
	$W^{(0)}(\mathbf{v}, \mathbf{x}, t)$ = the particle phase space density in the absence	tial time $s = 0$ and arriving at the point $\mathbf{x}, \mathbf{v}$ at	3907
3857	of turbulence $\mathbf{f}(s) = 0$	time $s = t$	3908
		ΔH = the difference in enthalpy between the droplet	
3858	Lower Case Roman Symbols	and vapor mass flux	3909
3859	d_p = particle diameter	$\Delta H \dot{m}$ = energy exchange during the evaporation/	
3860	e_c = coefficient of restitution for particle collisions	condensation	3910
	$\mathbf{f}(\mathbf{x}, t)$ = fluctuating (zero mean) aerodynamic driving	$\Delta \mathbf{x}_j(t)$ = changes in position for a particle starting	
3861	force	somewhere in particle phase space at some ini-	3911
3862	$g(r)$ = radial distribution of particle pairs a distance r	tial time $s = 0$ and arriving at the point $\mathbf{x}, \mathbf{v}$ at	3912
3863	apart	time $s = t$	3913
	$g(r_c) = n(r_c)/\bar{n}$ = radial distribution function	Σ_{12} = collision rate of type 1 particles with type 2	
	$g_{12}(r)$ = radial distribution of particle 2 with	particles	3914
3864	respect 7to particle 1 separated by a radial dis-	$\Theta(\mathbf{v} \mathbf{u})$ = wall scattering probability density	
3865	tance r	Θ = matrix of ensemble covariances of φ	
		$\mathbf{X}$ = particle phase space vector	3915

3916	$\Psi_{\mathcal{L}p}(\tau)$ = Lagrangian autocorrelation coefficient of fluid	χ = power law exponent in $g(\bar{r}) = C_g \bar{r}^\chi$ given as a	3962
3917	velocity fluctuations measured along the tra-	function of St_K	3963
	jectory of a particle $p = 1, 2$ at time τ	$\chi^{(1,2)}$ = particle-particle kinetic energy transfer from	3964
		particle 1 $\rightarrow$ 2 due to collisions	3964
3918	Lower Case Greek Symbols	Superscripts	3965
	α = inverse response time in GLM model	" = refers to random variable relative to mean	
3919	α_p = volume fraction of particle phase	flow, e.g., $\mathbf{v}'' = \mathbf{v} - \langle \mathbf{u} \rangle$	3966
	α_{vs} = mass fraction of saturated vapor	0 = refers to initial values	3967
	α_v = mass fraction of vapor	$^\dagger = \mathbf{A}^\dagger$ is the transpose of $\mathbf{A}$	
3920	β = inverse particle response time	' = refers to random variable relative to particle	
	δk_p = particle kinetic energy contribution from the	density weighted average, e.g., $\mathbf{v}' = \mathbf{v} - \bar{\mathbf{v}}$	3968
3921	RUM		
	$\delta \mathbf{v}_p^m(t)$ = RUM contribution to the instantaneous particle	Mathematical Symbols	3969
3922	velocity	$\frac{D_p}{Dt}$ = particle substantial derivative	
3923	ε_f = the turbulent energy dissipation rate	$\mathcal{G}$ = response tensor for small changes in particle	
	ε_p = bidisperse pair diffusivity tensor for pair	position subject to small changes in the aero-	3970
3924	separation	dynamic driving force	3971
	$\varepsilon_{p,ll}(r)$ = longitudinal component of the particle pair dif-	$\mathcal{H}_f$ = RUM contribution to the instantaneous particle	
3925	fusivity tensor ε_p along the line of centers of	velocity	3972
3926	the particle pair	$\bar{n}(\mathbf{x}_1, t)$ = the average number concentration of particles	
	$\varepsilon^{(1,1)}, \varepsilon^{(1,2)}$ = dissipative parts of collision terms in kinetic	at $\mathbf{x}_1$ at time t	3973
3927	stress transport equation due to nonelastic	$\underline{\varrho}$ = vector (x, v)	
3928	collisions	$\langle \rangle$ = the ensemble average	
3929	ε_{ij} = component of diffusion tensor relating pres-	$\overline{(\dots)}$ = particle density weighted average	
3930	sure tensor $\mathbf{p}$ to gradient diffusion in particle		
3931	equation of state		
	ε_{12} = tensor of diffusion coefficients determining the	Abbreviations	3974
3932	extra contribution to the momentum equation	BBO = Basset Boussinesq Oseen equation	3975
3933	of particles of type 1 arising from spatial gra-	C-E = Chapman-Enskog approximation	3976
3934	dients of the particle pair concentration $\langle n_{12} \rangle$	CFD = computational fluid dynamics	3977
3935	in $\mathbf{x}_2$ of particles of type 2	CKT = classical kinetic theory	3978
	ε_{ij}^S = diffusion coefficients in a simple shear flow	DNS = direct numerical simulation	3979
3936	relating diffusive current to particle concentra-	DPS = direct particle simulation	3980
3937	tion gradient	FN = Furutsu-Novikov closure method	3981
3938	η = net friction coefficient	FP = Fokker-Planck equation	3982
3939	η_K = Kolmogorov length scale associated with the	FSS = Fevrier, Simonin, and Squires JFM (2005)	3983
3940	viscous dissipating length scale of the	G&M = Gustavsson and Mehlig, Phys. Rev. E (2011)	3984
3941	turbulence	GLM = generalized Langevin model	3985
	κ = a body force per unit particle mass which	KM = kinetic method	3986
3942	depends upon inhomogeneity in the turbulence	LES = large eddy simulation	3987
3943	and biasing of the particle trajectories	LHA = local homogeneous approximation	3988
3944	ν_f = the kinematic viscosity of the carrier gas flow	LHDI = Lagrangian history direct interaction method	3989
	ν_{pf}' = fluid-particle turbulent viscosity in Boussinesq	MEF = mesoscopic Eulerian formalism	3990
3945	approximation for fluid-particle covariance in	MEPVF = mesoscopic Eulerian particle velocity field	3991
3946	SDM model for kinetic stresses	PDF = probability density function	3992
3947	ξ = the particle-fluid velocity correlation coeffi-	RDF = radial distribution function	3993
3948	cient based on local equilibrium between parti-	RUM = random uncorrelated motion	3994
3949	cle and carrier flow	S&S = Stafford and Swailes, Phys. Rev. E (2020)	3995
	λ = stress tensor for variations in real x -space (per	SDM = Simonin, Deutsch, and Minier	3996
3950	particle mass)	VK = Van Kampen operator representation methods	3997
	$\lambda^{(j,i)}$ = bidisperse dispersion tensor for particle spatial	for closure of kinetic equations	3998
3951	displacements for particles of type $i, j = 1, 2$	Z&A = Zaichik and Alipchenkov, New J. Phys. 11	
	μ = diffusion tensor for particle velocity	(2009)	3999
	$\mu^{(j,i)}$ = bidisperse dispersion tensor for particle velocity		
3952	displacements for particles of type $i, j = 1, 2$		
	$\langle \rho \rangle$ = the ensemble average of ρ (the mean mass	References	
3953	density)	[1] Maxey, M. R., and Riley, J. J., 1983, "Equation of Motion for a Small Rigid	
3954	ρ = the mass density of the particles for one real-	Sphere in a Nonuniform Flow," <i>Phys. Fluids</i> , 26 (4), p. 883.	4000
3955	ization of the flow field	[2] Crowe, C. T., Schwarzkopf, J. D., Sommerfeld, M., and Tsujii, T., 2012, <i>Mul-</i>	
3956	ρ_g = gas density	<i>tiphase Flow With Droplets and Particles</i> , CRC Press, Boca Raton, FL.	4001
3957	ρ_p = particle material density	[3] Elghobashi, S. E., and Abou-Arab, T. W., 1983, "A Two Equation Turbulence	
	σ = external flow stresses	Model for Two Phase Flows," <i>Phys. Fluids</i> , 26 (4), pp. 931-983.	4002
3958	τ_c = interparticle collision time	[4] Crowe, C. T., Troutt, T. R., and Chung, J. N., 1995, "Particle Interactions	
3959	τ_e = eddy decay time	With Vortices," <i>Fluid Mech. Appl.</i> , 30 , pp. 829-861.	4003
3960	τ_p = particle response time = $1/\beta$	[5] Squires, K. D., and Eaton, J. K., 1991, "Preferential Concentration of Particles	
	τ_c^k = standard kinetic theory interparticle collision	by Turbulence," <i>Phys. Fluids</i> , 3 (5), pp. 1169-1178.	4004
3961	time based on molecular chaos assumption	[6] Sundaram, S., and Collins, L. R., 1997, "Collision Statistics in an Isotropic	
	τ^+ = particle response time τ_p in wall units	Particle-Laden Turbulent Suspension: Part I—Direct Numerical Simulations,"	4005
		<i>J. Fluid Mech.</i> , 335 , pp. 75-109.	4006
		[7] Wilkinson, M., Mehlig, B., Östlund, S., and Duncan, K. P., 2007, "Unmixing	
		in Random Flows," <i>Phys. Fluids</i> , 19 (11), p. 113303.	4007

- [8] Fevrier, P., Simonin, O., and Squires, K. D., 2005, "Partitioning of Particle Velocities in Gas-Solid Turbulent Flows Into a Continuous Field and a Spatially Uncorrelated Random Distribution; Theoretical Formalism and Numerical Study," *J. Fluid Mech.*, **533**, pp. 1–46.
- [9] Herranz, L. E., Ball, J., Auvinen, A., Bottomley, D., Dehbi, A., Housiadas, C., Piluso, P., Layly, V., Parozzi, F., and Reeks, M., 2010, "Progress in Understanding Key Aerosol Issues," *Prog. Nucl. Energy*, **52**(1), pp. 120–127.
- [10] Kissane, M., Zhang, F., and Reeks, M., 2012, "Dust in HTRs: Its Nature and Improving Prediction of Its Resuspension," *Nucl. Eng. Des.*, **251**, pp. 301–305.
- [11] Gray, I., Sievwright, B., and Reeks, M., 2010, "Modelling of Release of Particulate Material From Transport Containers," *J. Packag., Transp., Storage Secur. Radioactive Mater.*, **21**(1), pp. 13–18.
- [12] Devenish, B. J., Bartello, P., Brenguier, J.-L., Collins, L. R., Grabowski, W. W., Ijzermans, R. H. A., Malinowski, S. P., Reeks, M. W., Vassilicos, J. C., Wang, L.-P., and Warhaft, Z., 2012, "Droplet Growth in Warm Turbulent Clouds," *Q. J. R. Meteorol. Soc.*, **138**(667), pp. 1401–1429.
- [13] Simonin, O., 1996, "Statistical and Continuum Modelling of Turbulent Reactive Particulate Flows Part II: Application of a Two-Phase Second-Moment Transport Model," *Combustion and Turbulence in Two-Phase Flows, 1995–1996 Lecture Series Programme*, Von Karman Institute for Fluid Dynamics, Belgium.
- [14] Haworth, D. C., and Pope, S. B., 1986, "A Generalized Langevin Model for Turbulent Flow," *Phys. Fluids*, **29**(2), pp. 387–405.
- [15] Pope, S. G., 1991, "Application of the Velocity-Dissipation Probability Density Function Model to Homogeneous Turbulent Flows," *Phys. Fluids A*, **3**(8), pp. 1947–1957.
- [16] MacInnes, J. M., and Bracco, F. V., 1992, "Stochastic Particle Dispersion Modeling and the Tracer Particle Limit," *Phys. Fluids A*, **4**(12), pp. 2809–2824.
- [17] Skartlien, R., Drazen, D., Swailes, D., and Jensen, A., 2009, "Suspensions in Turbulent Liquid Pipe Flow: Kinetic Modelling and Added Mass Effects," *Int. J. Multiphase Flow*, **35**(11), pp. 1017–1035.
- [18] Buyevich, Y., 1971, "Statistical Hydromechanics of Disperse Systems—Part 1: Physical Background and General Equations," *J. Fluid Mech.*, **49**(03), pp. 489–507.
- [19] Buyevich, Y., 1972, "Statistical Hydromechanics of Disperse Systems—Part 2: Solution of the Kinetic Equation for Suspended Particles," *J. Fluid Mech.*, **52**(2), pp. 345–355.
- [20] Buyevich, Y., 1972, "Statistical Hydromechanics of Disperse Systems—Part 3: Pseudo-Turbulent Structure of Homogeneous Suspensions," *J. Fluid Mech.*, **56**(2), pp. 313–336.
- [21] Reeks, M. W., 1977, "Eulerian Direct Interaction Applied to the Statistical Motion of Particles in a Turbulent Fluid," *J. Fluid Mech.*, **83**(3), pp. 569–590.
- [22] Reeks, M. W., 1983, "The Transport of Discrete Particles in Inhomogeneous Turbulence," *J. Aerosol Sci.*, **14**(6), pp. 729–739.
- [23] Reeks, M. W., 1991, "On a Kinetic Equation for the Transport of Particles in Turbulent Flows," *Phys. Fluids*, **3**(3), pp. 446–456.
- [24] Reeks, M. W., 1992, "On the Continuum Equations for Dispersed Particles in Non Uniform Flows," *Phys. Fluids*, **4**(6), pp. 1290–1303.
- [25] Swailes, D. C., and Darbyshire, K. F. F., 1997, "A Generalized Fokker-Planck Equation for Particle Transport in Random Media," *Phys. A: Stat. Mech. Appl.*, **242**(1–2), pp. 38–48.
- [26] Bragg, A., Swailes, D. C., and Skartlien, R., 2012, "Drift-Free Kinetic Equations for Turbulent Dispersion," *Phys. Rev. E*, **86**(5), p. 056306.
- [27] Swailes, D. C., Darbyshire, K. F. F., and Reeks, M. W., 1995, "Analysis of Particle Dispersion Using a PDF Equation; Results for Simple Shear and Rotating Flows," *ASME FED-Vol. 228*, pp. 257–263.
- [28] Swailes, D. C., Sergeev, Y. A., and Parker, A., 1998, "Chapman-Enskog Closure Approximation in the Kinetic Theory of Dilute Gas-Particulate Suspensions," *Phys. A Stat. Mech. Appl.*, **254**(3–4), pp. 517–547.
- [29] Derevich, I., and Zaichik, L., 1988, "Precipitation of Particles From a Turbulent Flow," *Izv. Akad.Nauk SSR, Mekh. Zhid. i Gaza*, pp. 96–104.
- [30] Zaichik, L., 1991, "Simulation of Particle Diffusion, Segregation, and Intermittency in Turbulent Flows," *Eighth International Symposium on Turbulent Shear Flows*, Technical University of Munich, Munich, Germany, p. 16.
- [31] Alipchenkov, V. M., and Zaichik, L. I., 2005, "Dispersion and Clustering of Bidisperse Particles in Isotropic Turbulence," *Fluid Dyn.*, **40**(1), pp. 83–94.
- [32] Zaichik, L. I., and Alipchenkov, V. M., 2007, "Refinement of the Probability Density Function Model for Preferential Concentration of Aerosol Particles in Isotropic Turbulence," *Phys. Fluids*, **19**(11), p. 113308.
- [33] Pozorski, J., and Minier, J.-P., 1999, "Probability Density Function Modelling of Dispersed Two-Phase Turbulent Flows," *Phys. Rev. E*, **59**(1), pp. 855–863.
- [34] Zhou, L. X., 1993, *Theory and Numerical Modeling of Turbulent Gas-Particle Flows and Combustion*, CRC Press, Boca Raton, FL.
- [35] Li, Y., and Zhou, Z. X., 1996, "A $k-\epsilon$ Model for Simulating Gas-Particle Flows," *6th Erlangen-Merseberg Workshop on Two-Phase Flow Predictions*, M. Sommerfeld, ed., Merseberg, Apr. 13–16, pp. 99–112.
- [36] Pandya, R. V. R., and Mashek, F., 2001, "Probability Density Functions Modeling of Evaporating Droplets Dispersed in Isotropic Turbulence," *AIAA J.*, **29**(1), pp. 561–568.
- [37] Simonin, O., Deutsch, E., and Minier, J. P., 1993, "Eulerian Prediction of the Fluid/Particle Correlated Motion in Turbulent Two-Phase Flows," *Appl. Sci. Res.*, **51**(1–2), pp. 275–283.
- [38] Novikov, E. A., 1965, "Functionals and the Random-Force Method in Turbulence Theory," *Sov. Phys. JETP*, **20**, pp. 1290–1294.
- [39] Furutsu, K., 1963, "On the Theory of Radio Wave Propagation Over Inhomogeneous Earth," *J. Res. Natl. Bur. Stand., Sect. D*, **67D**(1), pp. 39–62.
- [40] Hyland, K. E., Reeks, M. W., and McKee, S., 1999, "Derivations of a PDF Kinetic Equation for the Transport of Particles in Turbulent Flow," *J. Phys. Math. Gen.*, **32**(34), pp. 6169–6190.
- [41] Zaichik, L. I., 1999, "A Statistical Model of Particle Transport and Heat Transfer in Turbulent Shear Flows," *Phys. Fluids*, **11**(6), pp. 1521–1543.
- [42] Derevich, I. V., and Zaichik, L. I., 1990, "An Equation of Probability Density of Velocity and Temperature of Particles in a Turbulent Flow Modeled by a Random Gaussian Field," *Appl. Math. Mech.*, **54**(5), pp. 631–637.
- [43] Zaichik, L. I., 1997, "Modelling the Motion of Particles in Non-Uniform Turbulent Flow Using the Equation for Its Probability Density Function," *Appl. Math. Mech.*, **61**(1), pp. 127–133.
- [44] Derevich, I. V., 2000, "Statistical Modelling of Mass Transfer in Turbulent Two-Phase Dispersed Flows I. Model Development," *Int. J. Heat Mass Transfer*, **43**(19), pp. 3709–3723.
- [45] Zaichik, L. I., Oesterlé, B., and Alipchenkov, V. M., 2004, "On the Probability Density Function Model for the Transport of Particles in Anisotropic Turbulent Flow," *Phys. Fluids*, **16**(6), pp. 1956–1964.
- [46] Kraichnan, R. H., 1965, "Lagrangian History Direct Interaction for Turbulence," *Phys. Fluids*, **8**(4), p. 575.
- [47] Reeks, M. W., and McKee, S., 1991, "The Importance of Random Galilean Transformation Invariance in Modeling Dispersed Particle Flows," *ASME Paper No. G20329*.
- [48] Frisch, U., 1995, "Turbulence: The Legacy of A. N. Kolmogorov," CUP, Cambridge, UK, p. 87.
- [49] Kraichnan, R. H., 1970, "Diffusion by a Random Velocity Field," *Phys. Fluids*, **13**(1), pp. 22–31.
- [50] Bragg, A., Swailes, D. C., and Skartlien, R., 2012, "Particle Transport in a Turbulent Boundary Layer: Non-Local Closures for Particle Dispersion Tensors Accounting for Particle-Wall Interactions," *Phys. Fluids*, **24**(10), p. 103304.
- [51] Corrsin, S., 1974, "Limitations of Gradient Transport Models in Random Walks and in Turbulence," *Adv. Geophys.*, **18A**, pp. 25–60.
- [52] Swailes, D. C., and Darbyshire, K. F. F., 1997, "A Generalised Fokker-Planck Equation for Particle Transport in Random Media," *Phys. A*, **242**(1–2), pp. 38–48.
- [53] Monin, A. S., and Yaglom, A. M., 1973, *Statistical Fluid Mechanics*, Vol. 1, MIT, Cambridge, MA.
- [54] Reeks, M. W., 2005, "On Probability Density Function Equations for Particle Dispersion in a Uniform Shear Flow," *J. Fluid Mech.*, **522**, pp. 263–302.
- [55] Hyland, K. E., Reeks, M. W., and McKee, S., 1999, "Exact Analytic Solutions to Turbulent Particle Flow Equations," *Phys. Fluids*, **11**, pp. 1240–1261.
- [56] Stock, D. E., 1996, "Particle Dispersion in Flowing Gases-1994 Freeman Scholar Lecture," *ASME J. Fluids Eng.*, **118**(1), pp. 4–17.
- [57] Reeks, M. W., 1977, "On the Dispersion of Small Particles Suspended in an Isotropic Turbulent Flow," *J. Fluid Mech.*, **83**(3), pp. 529–546.
- [58] Squires, K. D., and Eaton, J. K., 1991, "Measurements of Particle Dispersion Obtained From Direct Numerical Simulations of Isotropic Turbulence," *J. Fluid Mech.*, **226**, pp. 1–35.
- [59] Wells, M. R., and Stock, D. E., 1983, "The Effects of Crossing Trajectories on the Dispersion of Particles in a Turbulent Flow," *J. Fluid Mech.*, **136**(1), pp. 31–62.
- [60] Csanady, G. T., 1963, "Turbulent Diffusion of Heavy Particles in the Atmosphere," *J. Atmos. Sci.*, **20**(3), pp. 201–208.
- [61] Tavoularis, S., and Corrsin, S., 1985, "Effects of Shear on the Turbulent Diffusivity Tensor," *Int. J. Heat Mass Transfer*, **28**(1), pp. 265–276.
- [62] Serafini, J. S., 1954, "Impingement of Water Droplets on Wedges and Double-Wedge Airfoils at Supersonic Speeds," N.A.S.A. NACA, Report No. 1159.
- [63] Zaichik, L. I., Alipchenkov, V. M., and Sinaiski, E. G., 2008, *Particles in Turbulent Flows*, Wiley-VCH, Hoboken, NJ.
- [64] Einstein, A., 1905, "On the Theory of Brownian Motion," *Ann. Phys. IV*, **322**(8), pp. 549–560.
- [65] Daly, B. J., and Harlow, F. H., 1970, "Transport Equations in Turbulence," *Phys. Fluids*, **13**(11), p. 2634.
- [66] Simonin, O., 1996, "Statistical and Continuum Modelling of Turbulent Reactive Particulate Flows: Part I—Theoretical Derivation of Dispersed Phase Eulerian Modelling From Probability Density Function Kinetic Equation," *Combustion and Turbulence in Two-Phase Flows, 1995–1996 Lecture Series Programme*, Von Karman Institute for Fluid Dynamics, Belgium.
- [67] Fevrier, P., and Simonin, O., 1998, "Constitutive Relations for Fluid-Particles Velocity Correlations in Gas-Solid Turbulent Flows," *Third International Conference on Multiphase Flows, ICMF'98*, Lyon, France, June 8–12, pp. 208–225.
- [68] Rogers, C. B., and Eaton, J. K., 1990, "The Behavior of Solid Particles in a Vertical Turbulent Boundary Layer in Air," *Int. J. Multiphase Flow*, **16**(5), pp. 819–834.
- [69] Hishida, K., and Maeda, M., 1990, "Turbulent Characteristics of Gas-Solid Two-Phase Confined Jet: Effect of Particle Density," *Proceedings of Fifth Workshop on Two Phase Flow Predictions*, Erlangen, Mar. 19–22, pp. 3–14.
- [70] Darbyshire, K. F. F., and Swailes, D. C., 1996, "A PDF Model for Particle Dispersion With Stochastic Particle-Surface Interactions, Fed-236, Gas-Solid Flows," *ASME Paper No. 51–56*.
- [71] Reeks, M. W., and Swailes, D. C., 1997, "The Near Wall Behaviour of Particles in a Simple Turbulent Flow With Gravitational Settling and Partially Absorbing Wall," *J. Fluid Mech. Res.*, **22**(2), pp. 31–39.

- [72] Swailes, D. C., and Reeks, M. W., 1994, "Particle Deposition From a Turbulent Flow: A Steady-State Model for High Inertia Particles," *Phys. Fluids*, **6**(10), pp. 3392–3403.
- [73] Devenish, B. J., Swailes, D. C., Sergeev, Y. A., and Kurdyumov, V. N., 1999, "A PDF Model for Dispersed Particles With Inelastic Particle-Wall Collisions," *Phys. Fluids*, **11**(7), pp. 1858–1868.
- [74] Li, A., and Ahmadi, G., 1992, "Dispersion and Deposition of Spherical Particles From Point Sources in Turbulent Channel Flow," *Aerosol Sci. Technol.*, **16**(4), pp. 209–226.
- [75] Soldati, A., and Marchioli, C., 2009, "Physics and Modelling of Turbulent Particle Deposition and Entrainment: Review of a Systematic Study," *Int. J. Multiphase Flow*, **35**(9), pp. 827–839.
- [76] Reeks, M. W., 1993, "On the Constitutive Relations for Dispersed Particles in Nonuniform Flows—I: Dispersion in a Simple Shear Flow," *Phys. Fluids*, **5**(3), pp. 750–761.
- [77] van Dijk, P., and Swailes, D. C., 2012, "Hermite-DG Methods for PDF Equations Modelling Particle Transport and Deposition in Turbulent Boundary Layers," *J. Comp. Phys.*, **231**(14), pp. 4094–4920.
- [78] Sikovsky, D. P., 2013, "Singularity of Inertial Particle Concentration in the Viscous Sublayer of Wall-Bounded Turbulent Flows," International Conference on Turbulence Heat and Mass Transfer 2012, Palermo, Italy, pp. 51–56.
- [79] Meneguz, E., and Reeks, M. W., 2011, "Statistical Properties of Particle Segregation in Homogeneous Isotropic Turbulence," *J. Fluid Mech.*, **686**, pp. 338–351.
- [80] IJzermans, R. H. A., Meneguz, E., and Reeks, M. W., 2010, "Segregation of Particles in Incompressible Random Flows: Singularities, Intermittency and Random Uncorrelated Motion," *J. Fluid Mech.*, **653**, pp. 99–136.
- [81] Zaichik, L. I., Drobyshevsky, N. I., Filippov, A. S., Mukin, R. V., and Strizhov, V. F., 2010, "A Diffusion-Inertia Model for Predicting Dispersion and Deposition of Low-Inertia Particles in Turbulent Flows," *Int. J. Heat Mass Transfer*, **53**(1–3), pp. 154–162.
- [82] Arrhenius, S., 1889, "On the Reaction Rate of the Inversion of Non-Refined Sugar Upon Souring," *Z. Phys. Chem.*, **4**, p. 226.
- [83] Logan, S. R., 1982, "The Origin and Status of the Arrhenius Equation," *J. Chem. Educ.*, **59**(4), pp. 279–282.
- [84] Reeks, M. W., Reed, J., and Hall, D., 1988, "On the Resuspension of Small Particles by a Turbulent Flow," *J. Phys D App. Phys.*, **21**(4), pp. 574–589.
- [85] Reeks, M. W., and Hall, D., 2001, "Kinetic Models for Particle Resuspension in Turbulent Flows: Theory and Measurement," *J. Aerosol Sci.*, **32**(1), pp. 1–39.
- [86] Zhang, F., Reeks, M., and Kissane, M., 2013, "Particle Resuspension in Turbulent Boundary Layers and the Influence of non-Gaussian Removal Forces," *J. Aerosol Sci.*, **58**, pp. 103–128.
- [87] Zhang, F., Reeks, M. W., Kissane, M., and Perkins, R. J., 2013, "Resuspension of Small Particles From Multilayer Deposits in Turbulent Boundary Layers," *J. Aerosol Sci.*, **66**, pp. 31–61.
- [88] Williams, M. M. R., 1992, "An Exact Solution of the Reeks-Hall Resuspension Equation for Particulate Flow," *J. Aerosol Sci.*, **23**(1), pp. 1–10.
- [89] Zhou, Y., Wexler, A. S., and Wang, L. P., 1998, "On the Collision Rate of Small Particles in Isotropic Turbulence: II—Finite Inertia Case," *Phys. Fluids*, **10**(5), pp. 1206–1216.
- [90] Laviéville, J., Deutsch, E., and Simonin, O., 1995, "Large Eddy Simulation of Interaction Between Colliding Particles and a Homogeneous Isotropic Turbulence Field," *ASME*, New York.
- [91] Laviéville, J., Simonin, O., Berlemont, A., and Chang, Z., 1997, "Validation of Inter-Particle Collision Models Based on Large-Eddy Simulation in Gas-Solid Turbulent Homogeneous Shear," *ASME*, New York.
- [92] Zaichik, L. I., and Alipchenkov, V. M., 2003, "Pair Dispersion and Preferential Concentration of Particles in Isotropic Turbulence," *Phys. Fluids*, **15**(6), pp. 1776–1787.
- [93] Laviéville, J., 1997, "Numerical Simulations and Modelling of Interactions of Turbulence Dragging and Inter-Particle Collisions Applied to Gas-Solid Two Phase Flows," These de Doctorat de l'Université de Rouen.
- [94] Zaichik, L. I., Alipchenkov, V. M., and Sinaiski, E. G., 2008, "Chapter 4," *Particles in Turbulent Flows*, Wiley-VCH, Hoboken, NJ.
- [95] Saffman, P. G., and Turner, J. S., 1956, "On the Collision of Drops in Turbulent Clouds," *J. Fluid Mech.*, **1**(01), pp. 16–30.
- [96] Abrahamson, J., 1975, "Collision Rates of Small Particles in a Vigorously Turbulent Fluid," *J. Chem. Eng. Sci.*, **30**(11), pp. 1371–1379.
- [97] Simonin, O., Zaichik, L. I., Alipchenkov, V. M., and Février, P., 2006, "Connection Between Two Statistical Approaches for Modeling of Particle Velocity and Concentrations Distributions in Turbulent Flow: The Mesoscopic Eulerian Formalism and the Two-Point Probability Density Function Method," *Phys. Fluids*, **18**(12), p. 125107.
- [98] He, J., and Simonin, O., 1995, "Modelisation Numerique Des Ecoulement Turbulent Gas-Solide en Conduite Verticale," Rapport EDF, Report No. HE-44/94/021A.
- [99] Simonin, O., 1991, "Eulerian Formulation for Particle Dispersion in Turbulent Two-Phase Flows," Proceedings of Fifth Workshop on Two-Phase Flow Predictions, Erlangen 1990, M. Sommerfeld and D. Wenneberg (Editors), Bilateral Seminars of the International Bureau/Forschungszentrum Julich GmbH, 4, pp. 156–166.
- [100] Oesterlé, B., and Pettjean, A., 1993, "Simulation of Particle-to-Particle Interactions in Gas-Solid Flows," *Int. J. Multiphase Flow*, **19**, pp. 199–211.
- [101] Sommerfeld, M., 1995, "The Importance of Inter-Particle Collisions in Horizontal Gas-Solid Channel Flows," ASME Paper No. 24.
- [102] Grad, H., 1949, "On the Kinetic Theory of Rarefied Gases," *Commun. Pure Appl. Math.*, **2**(4), pp. 331–407.
- [103] Jenkins, J. T., and Richman, M. W., 1985, "Grad's 13-Moment System for a Dense Gas of Inelastic Spheres," *Arch. Ration. Mech. Anal.*, **87**(4), pp. 355–377.
- [104] Zaichik, L. I., and Alipchenkov, V. M., 1997, "Simulation of Transport of Colliding Particles Suspended in Turbulent Shear Flows," Proceedings of Second International Symposium on Turbulence, Heat and Mass Transfer, pp. 823–832.
- [105] Moreau, M., Fede, P., Simonin, O., and Villedieu, P., 2003, "Monte Carlo Simulation of Colliding Particles Suspended in Gas-Solid Homogeneous Turbulent Shear Flows," ASME Paper No. FEDSM2003-45736.
- [106] Moreau, M., Fede, P., Simonin, O., and Villedieu, P., 2004, "Stochastic Lagrangian Modeling and Monte Carlo Simulation of Collisions in Gas-Solid Homogeneous Shear Turbulent Flows," Fifth International Conference on Multiphase Flow, ICMF2004 Yokohama, Japan, May 30–June 4, Paper No. 426.
- [107] Fessler, J. R., Kulick, J. D., and Eaton, J. K., 1994, "Preferential Concentration of Heavy Particles in a Turbulent Channel Flow," *Phys. Fluids*, **6**(11), pp. 3742–3749.
- [108] Crowe, C. T., Chung, J. N., and Trout, T. R., 1993, "Chapter 18," *Particulate Two-Phase Flow*, M. C. Roco, ed., Vol. 626, Heinemann, Oxford, pp. 1–1.
- [109] Falkovich, G., Fouxon, A. S., and Stepanov, M. G., 2002, "Acceleration of Rain Initiation by Cloud Turbulence," *Nature*, **419**(6903), pp. 151–154.
- [110] Chen, L., Goto, S., and Vassilicos, J. C., 2006, "Turbulent Clustering of Stagnation Points and Inertial Particles," *J. Fluid Mech.*, **553**(1), pp. 143–154.
- [111] Balkovsky, E., Falkovich, G., and Fouxon, A., 2001, "Intermittent Distribution of Inertial Particles in Turbulent Flows," *Phys. Rev. Lett.*, **86**(13), pp. 2790–2793.
- [112] Chun, J., Koch, D., Rani, S., Ahluwalia, S., and Collins, L., 2005, "Clustering of Aerosol Particles in Isotropic Turbulence," *J. Fluid Mech.*, **536**, pp. 219–251.
- [113] Zaichik, L. I., and Alipchenkov, V. M., 2009, "Statistical Models for Predicting Pair Dispersion and Particle Clustering in Isotropic Turbulence and Their Applications," *New J. Phys.*, **11**(10), p. 103018.
- [114] Masi, E., 2010, "Theoretical and Numerical Study of the Modeling of Unsteady Non-Isothermal Particle Laden Turbulent Flows by an Eulerian-Eulerian Approach," Ph.D. thesis, Institut National Polytechnique de Toulouse.
- [115] Masi, E., Simonin, O., and Bedat, B., 2011, "The Mesoscopic Eulerian Approach for Evaporating Droplets Interacting With Turbulent Flows," *Flow Turbul. Combust.*, **86**(3–4), pp. 563–583.
- [116] Masi, E., Simonin, O., Riber, E., Sierra, P., and Gicquel, L., 2014, "Development of an Algebraic-Closure-Based Moment Method for Unsteady Eulerian Simulations of Particle-Laden Turbulent Flows in Very Dilute Regime," *Int. J. Multiphase Flow*, **58**, pp. 257–278.
- [117] Masi, E., and Simonin, O., 2014, "Algebraic-Closure-Based Moment Method for Unsteady Eulerian Simulations of Non-Isothermal Particle-Laden Turbulent Flows at Moderate Stokes Numbers in Dilute Regime," *Flow, Turbul. Combust.*, **92**(1–2), pp. 121–145.
- [118] Bragg, A. D., and Collins, L. R., 2014, "New Insights From Comparing Statistical Theories for Inertial Particles in Turbulence: I—Spatial Distribution of Particles," *New J. Phys.*, **16**(5), p. 055013.
- [119] Wang, L. P., Wexler, A. S., and Zhou, Y., 2000, "Statistical Mechanical Description and Modelling of Turbulent Collision of Inertial Particles," *J. Fluid Mech.*, **415**, pp. 117–153.
- [120] Salazar, J. P. L. C., DE Jong, J., Cao, L., Woodward, S. H., Meng, H. U. I., and Collins, L. R., 2008, "Dissipation Rate Estimation From PIV in Zero-Mean Isotropic Turbulence," *J. Fluid Mech.*, **600**, pp. 245–56.
- [121] Falkovich, G., and Pumir, A., 2007, "Sling Effect in Collisions of Water Droplets in Turbulent Clouds," *J. Atmos. Sci.*, **64**(12), pp. 4497–4505.
- [122] Derevyanko, S., Falkovich, G., and Turitsyn, S., 2008, "Sling Effect in Collisions of Water Droplets in Clouds," *New J. Phys.*, **10**(7), p. 075019.
- [123] Falkovich, G., and Pumir, A., 2004, "Intermittent Distribution of Heavy Particles in a Turbulent Flow," *Phys. Fluids*, **16**(7), pp. L47–L50.
- [124] Maxey, M. R., 1987, "The Gravitational Settling of Aerosol Particles in Homogeneous Turbulence and Random Flow Fields," *J. Fluid Mech.*, **174**, pp. 441–465.
- [125] Reeks, M. W., 2012, "Particle Drift in Turbulent Flows: The Influence of Local Structure and Inhomogeneity," arXiv: 1205.2731v3.
- [126] Wang, L. P., Wexler, A. S., and Zhou, Y., 2001, "Modelling Turbulent Collision of Bidisperse Inertial Particles," *J. Fluid Mech.*, **433**, pp. 77–104.
- [127] Bragg, A. D., and Collins, L. R., 2014, "New Insights From Comparing Statistical Theories for Inertial Particles in Turbulence: II—Relative Velocities," *New J. Phys.*, **16**(5), p. 055014.
- [128] Gustavsson, K., and Mehlig, B., 2011, "Distribution of Relative Velocities in Turbulent Aerosols," *Phys. Rev. E*, **84**(4), p. 045304.
- [129] Salazar, J. P. L. C., and Collins, L. R., 2012, "Inertial Particle Acceleration Statistics in Turbulence: Effects of Filtering, Biased Sampling and Flow Topology," *Phys. Fluids*, **24**(8), p. 083302.
- [130] Bec, J., Biferale, L., Cencini, M., Lanotte, A. S., and Toschi, F., 2011, "Spatial and Velocity Statistics of Inertial Particles in Turbulent Flows," *Phys. Conf. Ser.*, **333**, p. 012003.
- [131] Reeks, M. W., 1983, "The Transport of Discrete Particles in Inhomogeneous Turbulence," *J. Aerosol Sci.*, **14**(6), pp. 729–739.

- [132] Stafford, C., 2020, "Improved Modeling of Disperse Multi-Phase Transport Based on Numerical Simulation and PDF Analysis," Ph.D. thesis, Newcastle University for Publication in Phys Rev. E.
- [133] Stafford, C., and Swailes, D. C., 2021, "Mass Flux of Dispersed Particles in Turbulence: Representations and the Influence of Correlation Structure in Gravitational Settling," *Phys. Rev. E*, **103**(3), p. 063101.
- [134] Maxey, M. R., and Corrsin, S. M., 1986, "Gravitational Settling of Aerosol Particles in Randomly Oriented Cellular Flow Fields," *J. Atmos. Sci.*, **43**(11), pp. 1112–1134.
- [135] Wang, L. P., and Maxey, M. R., 1993, "Settling Velocity and Concentration Distribution of Heavy Particles in Homogeneous Isotropic Turbulence," *J. Fluid Mech.*, **256**, pp. 27–68.
- [136] Dávila, J., and Hunt, J. C. R., 2001, "Settling of Particles Near Vortices and in Turbulence," *J. Fluid Mech.*, **440**, pp. 117–145.
- [137] Zaichik, L. I., Simonin, O., and Alipchenkov, V. M., 2006, "Collision Rates of Bidisperse Inertial Particles in Isotropic Turbulence," *Phys. Fluids*, **18**(3), p. 035110.
- [138] Fede, P., and Simonin, O., 2003, "Modeling of Kinetic Energy Transfer by Collision in a Non-Settling Binary Mixture of Particles Suspended in a Turbulent Homogeneous Isotropic Flow," *ASME* Paper No. FEDSM2003-45735.
- [139] Fede, P., and Simonin, O., 2005, "Application of a Perturbed Two-Maxwellian Approach for the Modeling of Kinetic Stress Transfer by Collision in Non-Equilibrium Binary Mixture of Inelastic Particles," *ASME* Paper No. FEDSM2005-77127.
- [140] Derevich, I. V., 1996, "Particle Collisions in Turbulent Flows," *Fluid Dyn.*, **31**(2), pp. 249–260.
- [141] Zaichik, L. I., Fede, P., Simonin, O. P., and Alipchenkov, V. M., 2009, "Statistical Models for Predicting the Effect of Bidisperse Particle Collisions on Particle Velocities and Stresses in Homogeneous Anisotropic Turbulent Flows," *Int. J. Multiphase Flow*, **35**(9), pp. 868–878.
- [142] Gourdel, C. I., Simonin, O., and Brunier, E., 1998, "Modeling and Simulation of Gas-Solid Particle Turbulent Flows With a Binary Mixture of Particles," Third International Conference on Multiphase Flow, ICMF'98, Lyon, France, June 8–12, pp. 1–10.
- [143] Alipchenkov, V. M., and Zaichik, L. I., 2001, "Particle Collision Rate in a Turbulent Flow Field," *Fluid Dyn.*, **36**(4), pp. 608–618.
- [144] Dodin, Z., and Elperin, T., 2002, "On the Collision Rate of Particles in Turbulent Flow With Gravity," *Phys. Fluids*, **14**(8), pp. 2921–2924.
- [145] Zaichik, L. I., Alipchenkov, V. M., and Sinaiski, E. G., 2008, "Chapter 1," *Particles in Turbulent Flows*, Wiley-VCH, Hoboken, NJ.
- [146] Zaichik, L. I., Alipchenkov, V. M., and Sinaiski, E. G., 2008, "Chapter 6," *Particles in Turbulent Flows*, Wiley-VCH, Hoboken, NJ.
- [147] Sawford, B. L., and Yeung, P. K., 2001, "Lagrangian Statistics in Uniform Shear Flows: Direct Numerical Simulation and Lagrangian Stochastic Models," *Phys. Fluids*, **13**(9), pp. 2627–2634.
- [148] Zhou, Y., Wexler, S., and Wang, L. P., 2001, "Modeling Turbulent Collision Rate of Bidisperse Inertial Particles," *J. Fluid Mech.*, **433**, pp. 77–104.
- [149] Pope, S. G., 1985, "PDF Methods for Turbulent Reactive Flows," *Prog. Energy Combust. Sci.*, **11**(2), pp. 119–192.
- [150] Reeks, M. W., Swailes, D. C., and Bragg, A. D., 2018, "Is the Kinetic Equation for Turbulent Gas-Particle Flows Ill Posed?," *Phys. Rev. E*, **97**(2), p. 23104.
- [151] Knopp, T., Alrutz, T., and Schwaborn, D., 2006, "A Grid and Flow Adaptive Wall-Function Method for RANS Turbulence Modelling," *J. Comput. Phys.*, **220**(1), pp. 19–40.
- [152] Hamidouche, Z., Masi, E., Fede, P., Ansart, R., Neau, H., Hemati, M., and Simonin, O., 2018, "Numerical Simulation of Multiphase Reactive Flows," *Adv. Chem. Eng.*, **52**, pp. 51–124.
- [153] Benoit, H., Ansart, R., Neau, H., Trinanes, P. G., Flamant, G., and Simonin, O., 2018, "Three-Dimensional Numerical Simulation of Upflow Bubbling Fluidized Bed in Opaque Tube Under High Flux Solar Heating," *AIChE J.*, **64**(11), pp. 3857–3867.
- [154] Ozel, A., Fede, P., and Simonin, O., 2013, "Development of Filtered Euler–Euler Two-Phase Model for Circulating Fluidised Bed: High Resolution Simulation, Formulation and a Priori Analyses," *Int. J. Multiphase Flow*, **55**, pp. 43–63.
- [155] Fede, P., Simonin, O., and Ingram, A., 2016, "3d Numerical Simulation of Lab-Scale Pressurized Dense Fluidized Bed Focusing on the Effect on Particle-Particle Restitution Coefficients and Particle-Wall Boundary Conditions," *Chem. Eng. Sci.*, **142**, pp. 215–235.
- [156] Hamidouche, Z., Masi, E., Fede, P., Simonin, O., Mayer, K., and Penthor, S., 2019, "Unsteady Three-Dimensional Theoretical Model and Numerical Simulation of a 120-kw Chemical Looping Combustion Pilot Plant," *Chem. Eng. Sci.*, **193**, pp. 102–119.
- [157] Reeks, M. W., and McKee, S., 1984, "The Dispersive Effects of Basset History Forces on Particle Motion in a Turbulent Flow," *Phys. Fluids*, **27**(7), p. 1573.
- [158] Marchioli, C., 2017, "Large-Eddy Simulation of Turbulent Dispersed Flows: A Review of Modelling Approaches," *Acta Mech.*, **228**(3), pp. 741–771.
- [159] Fox, R. O., 2012, "Large-Eddy-Simulation Tools for Multiphase Flows," *Ann. Rev. Fluid Mech.*, **44**(1), pp. 47–76.
- [160] van Wachem, B., Zastawny, M., Zhao, F., and Mallouppas, G., 2015, "Modelling of Gas-Solid Turbulent Channel Flow With Non-Spherical Particles With Large Stokes Numbers," *Int. J. Multiphase Flow*, **68**, pp. 80–92.
- [161] Gustavsson, K., Mehlig, B., Meneguz, E., and Reeks, M. W., 2012, "Inertial-Particle Dynamics in Turbulent Flows: Caustics, Concentration Fluctuations and Random Uncorrelated Motion," *New J. Phys.*, **14**(11), pp. 115017–115034.