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Eulerian and Lagrangian approaches for predicting the behaviour of discrete particles in turbulent flows

G. Gouesbet*, A. Berlemont

Laboratoire d'Energétique des Systèmes et Procédés, UMR 6614-CORIA-CNRS, Université and INSA de ROUEN, Place Emile Blondel, BP 08, 76131 Mont Saint Aignan Cedex, France

Abstract

A review of the work carried out during the last two decades by a group in Rouen, on Eulerian and Lagrangian approaches for predicting the behaviour of discrete particles in turbulent flows, is presented. The opportunity of this review is taken to direct the reader to a much larger literature and to point out unsolved problems.

Keywords: Two phase flow; Turbulent dispersion; Particle tracking; Two-way coupling; Particle interactions; Vaporisation

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* Corresponding author.

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1. Introduction

The study of multiphase flows is a very vast domain of research of utmost practical interest because the number of potential applications is almost infinite. Forgetting about slug flows, annular flows, and the big realm of transitions and combinations between these regimes [1], we focus on the topic to be discussed in this paper, namely the case when discrete particles are transported by flows. Usually, this case may be subdivided into three subclasses: suspensions, bubbly flows and droplet flows. Although some specific features are attached to each of the subclasses, they will be considered here in a unified perspective. Furthermore, we assume that flows are turbulent. The basic issue to address is therefore to understand and predict the dispersion of particles induced by continuous turbulent motion.

During the last century, much effort has been devoted by researchers and engineers to the study of turbulent *diffusion*, starting with the celebrated pioneer observation by Reynolds that turbulent motion is much more efficient than molecular motion, by orders of magnitude. The word diffusion is used here when quantities to be dispersed do not react to inertial effects and cannot drift under buoyancy in isothermal flows. They may possess a scalar or vectorial, more generally tensorial, character. Examples include marked fluid particles, chemical species, heat, momentum, velocity curl, and velocity correlations. Conversely, for discrete particles which react to inertia and to other various effects produced by the fact that they are aliens with respect to the carrier fluid, we use the word *dispersion*. When the diameter d of the particles tends to zero, dispersion tends to diffusion. This, however, requires neglecting molecular diffusion as is usual in turbulent flows. One of the consequences of molecular diffusion for fluid particles is that their entity is not preserved in contrast with the case of discrete particles, leading to micro-mixing effects. Therefore, the concept of dispersion appears to be more general than that of diffusion.

Industrial applications of turbulent dispersion are miscellaneous and concern the design and control of various multiphase processes such as droplet combustion in furnaces, diesel engines, droplet cooling, cyclone separation, and pneumatic transport. Some processes are directly connected with energy conversion problems (chemical reactors like fluidised beds, spray and coal combustion). Bubbly flows are extensively studied in nuclear reactor engineering. Pollution transport and dispersal in geophysical flows is another issue of interest, including military purposes because chemical and biological attacks may rely on the use of aerosols and droplets [2].

Therefore, the chemical and mechanical engineer can hardly avoid coping with the turbulent dispersion mechanism of mass transfer. The researcher will be confronted with a difficult topic in which some fundamental problems are still unsolved. For example, we would like to know in closed form or to predict the relation between Eulerian and Lagrangian spectral densities, and also the relation between associated scales. Knowledge or prediction of Lagrangian correlation tensors would be particularly welcome. The absence of any rigorous solution to such problems will be troublesome.

In the simplest case, we have to deal with a one-way problem: given a turbulent flow, to predict the dispersion behaviour of transported discrete particles. However, particles are not passive contaminants. The mere presence of a particle locally modifies the turbulence since, inside the particle, there is no flow field, i.e. no eddies. This kind of local modification is expected to be negligible if the particle diameter is much smaller than the Kolmogoroff scale (note that this statement implies a sufficient condition). Up to now, we have always neglected such local turbulence modifications, even when the sufficient condition is not satisfied, apparently without any damage. This problem must, however, be considered an open one. However, when the particle mass loading ratio is increased, global turbulence modifications may be induced. For example, shear stresses may be reduced. Introducing particles to it decreases the expansion of a turbulent jet. Generally, the existence of a relative motion between particles and the carrier fluid leads to an extra dissipation of the turbulence energy. We are then faced with a two-way coupling problem: turbulence modifies particle behaviour which, in return, modifies the turbulence. The return may be viewed as the consequence of a micro-turbulence produced by extra gradients around the particle.

More difficult problems arise in the case of additional heat and mass transfers between particles and fluid (evaporation), possibly with simultaneous occurrence of chemical reactions and radiative transfer (combustion). Again, these issues may be addressed in a one-way or a two-way coupling formulation. Furthermore, if the particle number-density is sufficiently large, we may have to account for particle–particle interactions. This is a four-way coupling problem which, at the present time, should not be considered as completely solved, although significant progress has been made, in particular concerning the influence of collisions between particles.

To handle such a large variety of phenomena, two theoretical approaches are at our disposal, namely the Eulerian and the Lagrangian approaches, with many variants. In both cases, however, the underlying physics is essentially the same, but the Eulerian approach conceptually elaborates much on it, while the Lagrangian approach remains close to it. As a consequence, the most complex versions of the Eulerian approach take the status of models, while the Lagrangian approach essentially leads to simulations.

More specifically, the underlying physics is as follows. We must consider a large number of particulate trajectories that we may call trajectory realisations and, by averaging over these realisations, we deduce the quantities we want to know such as particle velocities and particle velocity fluctuations, or number–densities versus space and time.

However, in the Eulerian approach such as that discussed in this paper, trajectory constructions and subsequent averaging are not explicitly carried out at a computational level. Instead these operations are implicitly achieved at a conceptual level, leading to the introduction of a dispersion tensor. Therefore, the discrete character of the underlying process is washed out to provide us with a theory involving a continuum associated with the particles. The dispersion tensor is introduced in an equation of transport for mean number–densities (or probabilities of presence) to be solved. The conceptual part of the work being carried out by the brain (not by a computer), Eulerian codes are fast-running. The price paid for this computational efficiency is that assumptions must be introduced to succeed in the formulation of the dispersion tensor, i.e., the range of applications of the Eulerian approach is limited to cases when the concept of the dispersion tensor makes sense, resulting in a loss of generality. Other authors have, however, provided extensions outside of such limited cases, with an intensive modelling effort. In particular, they appear to be well adapted for the study of densely laden two-phase flows, as we shall comment later.

Conversely, in the Lagrangian approach, trajectory realisations are explicitly simulated by the computer which also carries out subsequent required averaging. Therefore, the range of applications is dramatically increased, including those cases when the concept of dispersion in the Fick sense is no more acceptable. The price paid is more time-consuming runs.

Previously, the price was thought to be high by many users (or potential users). Nowadays, due to the dramatic progress in the quality and speed of computers, the situation has changed. In particular, all computations we carried out with the Lagrangian approach can be reasonably performed on workstations.

Other comments on the relative advantages and disadvantages of both approaches are available from Refs. [3, 4]. The question of which of these approaches is preferable is not solved and, in fact, it is likely that this question does not make sense. The problem addressed is extremely complex, and it is certainly better to possess two lines of attack, rather than only one. Furthermore, to some extent, these approaches are complementary in many respects. For instance, any progress achieved in one approach may help make progress in the other. Examples of such inter-relations between the Eulerian and the Lagrangian approaches have recently proved to be of great interest for the study of particle collision [5].

The paper is organised as follows. Section 2 discusses turbulence predictions. This is required because, whatever the chosen approach (Eulerian or Lagrangian), prior knowledge of the turbulence field in which particles will move is required. Section 3 discusses the particle equation of motion which is necessary to build trajectories, with some specificity, depending on the considered approach. Section 4 is devoted to the Eulerian approach. Section 5 and Section 6 concern the Lagrangian approach, Section 5 for the fluid particle trajectories and Section 6 for the discrete particle trajectories. All these sections only concern the one-way coupling case. The two-way coupling problem is discussed in Section 7. Section 8 discusses the case when additional heat and mass transfers, not considered in the previous sections, occur, with the typical example of vaporisation of droplets, both for one-way and two-way couplings. Section 9 is devoted to the four-way coupling problem. Section 10 is the conclusion.

In addition, the bulk of the paper is written as a guideline, avoiding mathematical expressions. Technicalities are better reported in Appendices.

2. Knowledge of the turbulence field

Any turbulence modelling or simulation will inevitably produce inaccuracies which will partly spoil the results on particle behaviour. Therefore, in order to test particle predictions without such a spoiling effect, it is highly recommended to rely on experimental data for the turbulence field when they are available with enough accuracy. A typical case for which this situation is encountered is grid turbulence. However, a full code for practical applications, with a two-way coupling, typically proceeds via the following steps:

1. Turbulence predictions.
2. Particulate predictions (Eulerian approach) or simulations (Lagrangian approach).
3. Iterations involving the two previous steps when two-way coupling is significant (Lagrangian approach).

Any approach to the description of the turbulence field may then be used for the first step as far as it provides us with the required quantities with enough accuracy. Methods such as direct numerical simulation (DNS) or kinematic simulation (KS) provide unique opportunities to study specific effects like particle trapping in eddies [6–9] but are limited to small Reynolds number flows (DNS) or do not incorporate all of the physics involved in the Navier–Stokes equations (KS). Large eddy simulation (LES) allows

one to handle complex flows [10–12] but the best quality/price ratio is, up to now, obtained by using a complete stochastic modelling on which we shall focus in this paper.

Thus, in practice, we rely on a (k–ε) model supplemented with Rodi algebraic relations (ASM, algebraic stress model) for a more accurate prediction of Reynolds stresses. Details of this approach are available from [13–17], in the framework of our work, from which the prior literature may be accessed. In this section, we also restrict ourselves to one-way coupling so that the equations for these models are by now quite classical. Later, for two-way coupling, they will have to be supplemented by many extra-terms to account for the influence of the particles on the turbulence, leading to much more complex variants. Basic features are then recalled below.

For the (k–ε) model, we use an improved code originally based on the Teach-T from the Imperial College of Science and Technology [18]. Governing equations are the continuity equation, the momentum equation, transport equations for turbulence energy k and its dissipation ϵ, closure being obtained by using a last relation expressing eddy viscosity. Outputs are mean velocities U_i, turbulence energy k, dissipation ϵ and the production P of turbulence energy through the interaction between the mean and fluctuating fields.

In a second step, (k–ε) outputs are fed to second-order Rodi algebraic relations [19] to determine the Reynolds tensor components. These relations take the form of a linear system of equations (Cramer system) in which the Reynolds tensor components are the indeterminates. Although originally written with Cartesian tensors by Rodi, they have been later rewritten with general tensors under a form invariant with respect to co-ordinate system transformations, and specified for the case of axisymmetric flows [13, 17, 20]. We insist here on the fact that the use of general tensor calculus in this context is not only a smart sophistication but, conversely, we found that it provides the only practical and efficient way to obtain Rodi relations in arbitrary co-ordinate systems. Algorithms for the resolution of the obtained Cramer system are discussed in Ref. [21].

At this stage, the information gained on the structure of the turbulence field is not sufficient for the prediction and simulation of the behaviour of transported discrete particles. Extra knowledge requires in particular:

1. The functional shape of the Lagrangian velocity correlation coefficient R_{fL}.
2. The evaluation of scales, such as the Lagrangian macroscale τ_{L} involved in R_{fL}, or Eulerian spatial macroscales.

Note here that, for convenience, these quantities are discussed in a one-dimensional (1D)-framework. More generally, tensors should be used and, in particular, we would have to deal with a tensor $R_{\mathrm{fL},ij}$. We shall reintroduce such a tensorial character later.

Such knowledge is required for both the Eulerian and Lagrangian approaches, but it is of particular relevance to the Lagrangian approach. Conceptually, the definition and the use of R_{fL} is rather simple if the turbulence is assumed to be statistically stationary, an assumption which is therefore made throughout this paper. The development of Eulerian and Lagrangian approaches for statistically unsteady flows must be considered as an open subject of research, difficult enough to provide work to many researchers for many years.

Also, R_{fL} has a particularly clear meaning for homogeneous turbulence. However, restricting ourselves to such turbulence would be an unacceptable limitation. This difficulty is bypassed by using a trick which, although not perfect, will prove to be effective. This trick consists of using what we may call a tangent homogeneous field, i.e. a homogeneous field which, in one sense, is tangent to the actual nonhomogeneous field predicted by the previous stochastic modelling. In other words, if the turbulence is not homogeneous, the dispersive behaviour at any point is assumed to depend on the local properties of the turbulence at that point. Therefore, we may use a homogeneous field tangent at that point, having the properties of the nonhomogeneous field at that point. For instance, assume that the Lagrangian macroscale τ_{L} reads as $\tau_{\mathrm{L}}(k,\varepsilon)$. Then, at a point $\vec{x}_0$, τ_{L} may be evaluated by using $k(\vec{x}_0)$ and $\varepsilon(\vec{x}_0)$ and we may think of the dispersive behaviour as taking place in a homogeneous field, tangent at $\vec{x}_0$, having $k(\vec{x}) = k(\vec{x}_0)$ and $\varepsilon(\vec{x}) = \varepsilon(\vec{x}_0)$, hence $\tau_{\mathrm{L}} = \tau_{\mathrm{L}}(\vec{x}_0)$.

Since statistical steadiness may be viewed as homogeneity in time, instead of homogeneity in space, it is likely that the case of unsteady flows could similarly be investigated by using the concept of a homogeneous field, tangent with respect to the time evolution.

Another difficulty is that the determination of the functional shape of the Lagrangian velocity correlation coefficient R_{fL} is an unsolved problem. We therefore have to rely on an assumption, with possibilities discussed in Appendix A. A classical one assumes an exponential decrease with a characteristic time equal to the Lagrangian time macroscale. Such an assumption however contradicts Lin's results (see Ref. [22]) stating that, for homogeneous turbulence, there is no finite macroscale associated with the Lagrangian acceleration correlation coefficient. We thus demand in our approach that the coefficient R_{fL} exhibits at least one negative loop (Appendix B). To account for these remarks, our proposal is to use the exp–cos Frenkiel [23] correlation which involves a loop parameter m associated with the occurrence and the importance of negative loops. With $m = 0$, the classical exponential decrease form is recovered. The best value of m has not been determined theoretically up to now but, from our experience, we recommend the value $m = 1$. Note that we have shown that there is an upper bound for m to avoid negative values of particle dispersion coefficients, namely $m \sim 3.6$. An interesting feature is that the existence of negative loops implies that dispersion may be more efficient than diffusion, even for dense particles in homogeneous turbulence [24].

Finally, for the evaluation of scales, the reader should

refer to Ref. [16] and to references quoted in the sections on the Lagrangian approach.

3. Equation of motion of discrete particles

The discussion of the equation of motion of discrete particles encompasses a long story and also a complex one because it has been controversial. In this section, one of our aims is to provide a summary of this controversy.

A good starting point is the so-called BBO equation arising from the works of Basset (1888), Boussinesq (1903) and Oseen (1927), see Refs. [25–29].

For primary access to it, we would recommend Basset (1888) (Refs. [25, 26]) whose work can easily be revisited, leading to the conclusion that the equation is safe. BBO concerns the case of a spherical, solid particle moving vertically in a fluid at rest under gravity, with velocity zero at time 0. The restriction to a solid particle is important to write shear stresses on the surface of the particle but, to some extent, not essential in so far as, in practice, bubbles or droplets may have their surface contaminated and then behave as solid particles (see later comments). Also, as a consequence of the assumptions, the particle is non-rotating. Obviously, no particle/particle interaction is involved in the process since the particle is unique, and the motion is slow enough so that no micro-turbulence is produced. The assumptions imply that we are working in a linear approximation of the Navier–Stokes equation. It is then found that the force exerted upon the particle contains a drag term, the so-called Stokes drag previously described by Stokes [30], an added mass term extensively discussed by Boussinesq, a so-called history term (or Basset term), and possibly a buoyancy term.

Tchen [31] attacked the problem of generalising the BBO equation to the case when the fluid is no longer at rest. The demonstration is carried out in two steps. First, we consider the case of a particle moving with a velocity $(V_p - V_f)$ in a fluid at rest. This actually adds no physics but simply is a change of notation in which the particle velocity is assigned the term $(V_p - V_f)$. Next, the mechanical system (particle + fluid) is endowed with a time-dependent velocity $V_f(t)$, leading to the case of a particle with velocity V_p moving in a fluid with velocity V_f. Due to the fluid acceleration, Tchen states that it becomes necessary to introduce an extra pressure gradient term. Integrating the corresponding normal stresses on the surface of the sphere produces an extra force which did not appear in the original BBO equation, leading to the so-called Tchen equation (Appendix C). However, the Tchen procedure partly relies on intuition, giving rise to a long controversy.

Having criticised the Tchen equation, Corrsin and Lumley [32] have proposed a new equation which appears to be nonlinear with respect to velocities and involves a second-order fluid velocity derivative with respect to spatial co-ordinates. In the Eulerian approach, these terms are troublesome because they cannot be introduced in the standard theory of dispersion (Section 4), at least not in a simple way. Criteria are, however, given for neglecting these terms, allowing us to recover the Tchen equation, which is the one we use in the Eulerian approach.

Buevich [33] simultaneously criticises again the Tchen equation, explicitly stating that the Tchen procedure was intuitive, and the Corrsin and Lumley equation leading to results that he qualifies as being strange. For example, Buevich discusses a simple case, that of a steady particle motion in a fluid whose velocity is constant with respect to time and also with respect to the space co-ordinate along the trajectory of the particle moving in a constant direction. Furthermore, particle and fluid densities are assumed to be equal. The Corrsin and Lumley equation implies that the relative velocity between particle and fluid may take on arbitrary values. The underlying reason for such a physically incorrect result would lie in an incorrect transformation of the BBO equation from a co-ordinate system attached to the fluid to the laboratory co-ordinate system. Relying on a formulation from Oldroyd and Sedov, Buevich then demonstrates that the artificial introduction by Tchen of an extra pressure force disappears and obtains a new equation.

However, according to Maxey and Riley [34], the Buevich equation is also incorrect. Again, the statement is demonstrated by considering a simple case leading to results which cannot be accepted on physical grounds. Thereafter, they propose a new equation which is a generalisation of a previously established Riley equation [35].

Maxey and Riley's equation accounts for the influence of velocity profile curvatures. When this influence is neglected, the Riley equation is recovered (Appendix C). We also mention the Gatignol [36] equation which is similar to the Maxey and Riley equation.

In the Eulerian approach, we recall that the equation of motion does not appear explicitly but is implicitly introduced in the dispersion term of the particle transport equation by using a standard theory of dispersion (STDisp, Section 4). We use the Tchen equation although it is incorrect. In practice, introduced errors have been found to be small enough to be irrelevant. For instance, when both Eulerian and Lagrangian approaches are used, they lead to nearly identical results. The use of another linear equation is possible but requires a modification of some involved mathematical expressions without, however, altering the structure of the STDisp. For nonlinear equations, we believe that modifications for the STDisp are not feasible due to mathematical difficulties associated with nonlinearities but we have never seriously attempted to solve this issue.

In the Lagrangian approach, there is no difficulty in implementing any equation of motion because such a change of equation only requires modifying a few program statements. We may then easily handle more complicated equations than Riley's. This is actually required in many situations because Riley's equation is limited to the case when particulate Reynolds numbers are small enough. For

large particulate Reynolds numbers, a modified Riley equation is used (Appendix C). The modifications introduce empirical correcting factors C_D, C_A, C_H for the drag term, added mass term and the Basset term, respectively. The C_D factor is given by Clift et al. [37]. For C_A and C_H, we refer to Odar and Hamilton [38]. For fluid discrete particles (droplets, bubbles), internal recirculation associated with a modification of the boundary condition at the surface of the particle may arise, leading to an extra modification of the drag term. However, in practice, pollutants accumulating at the particle surface may restore the validity of the solid boundary condition. Then, fluid discrete particles behave as solid particles do [37].

Although originally designed for non turbulent conditions, the Tchen and modified Riley equations are used for turbulent flows, the first for the Eulerian approach, the second for the Lagrangian approach. We then assume that they are instantaneously valid. However, to establish them, it was necessary to detail limit conditions at an infinite distance from the sphere. These limit conditions conflict with the space- and time-dependent character of turbulent flows, i.e. they are, in principle, never satisfied. If we consider a Kolmogoroff eddy (length scale η_k) as being the smallest relevant domain of space, then we may expect that limit conditions at an infinite distance of the sphere make sense when the particle diameter d is much smaller than η_k. In these circumstances, equations of motion valid for non turbulent flows could remain valid for turbulent flows. Again, the condition $d < \eta_k$ is thought as being a sufficient condition. In practice, it did not appear to be necessary because we did not observe significant and systematic discrepancies between predictions/simulations and experiments when the condition was not satisfied. However, no clear limit can be stated for the particle diameter: particles do not respond to all the fluid fluctuations and thus the particle diameter must be smaller than the scale to which the solid particle will quickly respond to [39]. Let us mention that an extensive discussion on the relevant turbulent and particle scales has been proposed by Stokes [40]. The issue must nevertheless be considered open, and interest in specific studies is warranted.

In some cases, it might also be necessary to add lift forces to the equation of motion of particles. The reader is referred to Clift et al. [37] Rubinow and Keller [41], Julien et al. [42], Saffman [43] and Bretherton [44]. We point out that Saffman result is erroneous by a factor of 4π, as later corrected by Saffman himself in an erratum [45].

In order to estimate in specific cases whether or not lift forces may be neglected, we suggest reliance on the comparison between lift drift velocity (evaluated by writing a balance between lift drift forces and drag forces opposing them) and particle dispersion velocity. If the lift drift velocity is much smaller than the dispersion velocity, then lift forces may presumably be neglected. For instance, in Arnason's experiments [46], we estimated lift velocity and dispersion velocity to be 1 and 50 cm/s, respectively. In the converse case, we may tentatively add lift forces to the modified Riley equation. We point out that such a procedure is, however, not entirely safe. First, for big particulate Reynolds numbers, creeping flow assumption around the particle is no longer valid, i.e. the problem to be solved is no longer linear. Therefore, the principle of superposition of solutions is not valid and we must not expect that adding lift expressions to the modified Riley equation provides us with the correct answer. Next, assumptions underlying the work of Rubinow and Keller [41] and Saffman [43] are not satisfied. In particular, these works assume steadiness (which is never instantaneously satisfied in turbulent flows). They provide us with a lift force which is the rotational equivalent of the translational Stokes drag force when there is no rotation of the particle. As far as we know, the problem of lift forces exerted on rotating particles in unsteady flows is an unsolved issue. Very likely, the unsteady case would add new lift forces. For example, we expect the occurrence of a rotational history integral which would correspond to the Basset history integral of the translational problem.

Finally, in turbulent flows, we note that the particulate Reynolds number should be given a statistical meaning. Even if the average relative velocity between a particle and the fluid is zero (null value of the average particulate Reynolds number), the instantaneous value of the particulate Reynolds number can only be zero at discrete times. This issue is discussed in Ref. [47].

4. Eulerian approach

We assume monodispersed particles. The polydispersed case would be trivially considered by splitting the range of diameters in a number of subclasses, assuming that each subclass behaves independently of the others, as discussed in Ref. [48]. Also, in this section, we essentially concentrate on a simple version of the Eulerian approach, such as that used in the so-called codes DISCO-1 and DISCO-2, postponing a brief discussion of more complex versions to the end of the section.

The essential idea in the Eulerian approach is to handle particulate trajectories at a conceptual level, so that they eventually do not appear explicitly any more. Thus, in the Eulerian approach, a continuous scalar field represents particles. The scalar quantity may be an averaged local particle number–density, or a probability of presence defined over a large number of realisations of the laden turbulent flow. The scalar field is determined by writing and solving a particle transport equation. As usual, this transport equation involves a dispersion term representing the effect of turbulence on particles.

The core of the problem thus appears to be the determination of a dispersion coefficient (more generally of a dispersion tensor) for this dispersion term. For such a determination, we ideally should not rely on empirical correlations which are always more or less risky to use

and also add nothing to the understanding, although some earlier attempts used such an ad hoc approach. Instead, we shall rely on the construction of a standard theory of dispersion (in short STDisp) which, although involving limiting assumptions, provides us with a firm theoretical framework. This STDisp is extensively discussed in Refs. [47–51]. The word standard here refers to the fact that the amount of modelling is very small and, in well defined cases relying on a set of sufficient assumptions, there is even no modelling at all, thus justifying the use of the word 'theory' which is ipso-facto redundant to the use of the word 'standard'.

The STDisp relies on a standard theory of diffusion (STDiff) developed by Batchelor [52] and generalising previous works by Taylor [53, 54], Kampé de Fériet [55] and Frenkiel [23], among others. Batchelor assumes a non-isotropic, homogeneous, stationary turbulence. Molecular effects are neglected.

At initial time $t = 0$ in Batchelor's formulation, we consider a volume V of marked fluid and assume that the marking quantity is uniformly distributed within the volume. The analysis of the problem leads to the conclusion that subsequent modifications in the centre location of V and mean concentration diffusion do not depend on the shape of the volume V. Marked fluid particle diffusion with respect to the mean trajectory of the cloud centre is fully determined by the statistical behaviour of a single fluid particle. Assuming that the displacements in the various directions of space are characterised by Gaussian probability density functions, one then finds that the diffusion quantity evolves according to the Fick law expressed by using a diffusion tensor.

The representation of diffusion processes with the aid of the Fick law is indeed classical for long diffusion times, analogous with molecular diffusion [22]. From experimental data, one finds that the probability density functions of mean displacements are indeed Gaussian when the turbulence is homogeneous without any mean shear, for long diffusion times but also for short diffusion times. This also theoretically results from simple expressions relating mean displacements and velocity fluctuation variances, velocity fluctuations being normally distributed [22]. However, the assumption of mean displacement normality is not necessarily justified for intermediary diffusion times. Therefore, Batchelor points out that the Fick law owns a phenomenological character rather than a fundamental one.

The Fick law diffusion tensor is expressed in a simple way in terms of a displacement tensor which may be expressed in terms: (i) of a Lagrangian correlation tensor; or (ii) of a Lagrangian spectral tensor related to the Lagrangian correlation tensor by a Fourier transform. Therefore, knowing the Lagrangian correlation tensor, the time-dependent diffusion tensor may be obtained. Then the transport equation may be integrated. At this stage, the STDiff formulation is completed.

Batchelor formulation assumes spatial and temporal homogeneity of turbulence. Therefore, in steady turbulence, statistical characterisation of fluid particle motion at a point is also steady. However, for discrete particles, this is not always the case due, for instance, to inertia. Therefore, the statistical future of particle motion depends on initial conditions at time $t = 0$. If we intend to generalise the Batchelor formulation to the case of dispersion, we must assume that the statistical characterisation of discrete particle motion at a point is steady. In particular, it must be the same at time $t = 0$ than at any time after. This is the so-called stationary assumption [50].

If the stationary assumption is not satisfied, the definition of a tensor (or a coefficient) of dispersion does not make any sense. The spreading behaviour of a cloud of particles does not only reflect the Fickian dispersive influence of turbulence but also contains information on the initial conditions at the injection point (initial particle velocity and also initial fluctuations of particle velocity). Due to the existence of a particulate relaxation time, initial conditions require time to be forgotten. In extreme cases, measured dispersion coefficients would have nothing to do with turbulence characteristics but would rather characterise the injection process. Checking of the validity of the stationary assumption requires the comparison of two time scales: the particle relaxation time, telling us how fast initial conditions are forgotten; and the transit time in the turbulence field, telling us how much time is given to the particles for such a loss of memory. This assumption is not required in the Lagrangian approach.

When the transit time is much longer than the particle relaxation time, the stationary assumption is satisfied and the STDiff may be generalised to a STDisp. Mathematical expressions of the STDiff remain valid for the STDisp with the proviso that quantities concerning fluid particles must be replaced by quantities concerning discrete particles. In particular, the dispersion tensor is now expressed in terms of the Lagrangian velocity correlation tensor of discrete particles or, through the Fourier transform, in terms of the corresponding Lagrangian spectral tensor.

We again assume that we know the fluid Lagrangian spectral tensor (see Section 2). From the Tchen equation of motion, one shows that the discrete particle Lagrangian spectral tensor is equal to the fluid Lagrangian spectral tensor multiplied by η^2. The so-called Tchen amplitude ratio η only depends on fluid (not turbulence) and particle properties. It may be physically understood as resulting from a particle filtering effect, turbulence frequencies being imperfectly transmitted to particle motion. At this stage, dispersion coefficients may be computed and introduced in a particle transport equation. The STDisp is completed.

The computation of dispersion coefficients requires time-consuming numerical integrations. However, when the Basset term is neglected, integration may be analytically performed leading to simple algebraic relations [50]. Circumstances under which the Basset term may be neglected, and/or procedures to check whether this is possible, are discussed in Ref. [56]. Ref [47] expresses the

Eulerian formulation in terms of a fundamental ratio of two time scales: the particle relaxation time and the Lagrangian macroscale of turbulence. Ref. [47] also examines under which conditions the Stokes drag term involved in the Tchen equation remains valid for turbulent flows.

Although the STDisp is, in principle, designed for homogeneous turbulence, nonhomogeneous turbulence may be in practice considered, at least approximately, by:

1. adding a convection term to the transport equation
2. introducing spatial derivatives of the dispersion tensor
3. computing quantities in a local way. For example, evaluation of the Lagrangian time macroscale τ_L is carried out with an expression involving the dissipation ε of turbulence energy. ε Is obtained from the turbulence model as a space-dependent variable. Therefore, the macroscale τ_L also becomes a space-dependent variable in contrast with its uniform character in the case of STDisp in homogeneous flows. In other words, the dispersion at one point is locally controlled by a fictitious turbulent field which is tangent to the actual field, i.e. what we previously called a tangent homogeneous field.

We now come to the discussion of a limitation of the STDisp which is produced by Tchen equation assumptions. The use of this equation requires assuming that a discrete particle must permanently remain in the same fluid particle. One states that no overshooting is allowed [22]. Even in the most favourable case when fluid and particle densities are equal, this assumption cannot be perfectly justified because of the loss of individuality of any fluid particle which is stretched, deformed and eventually destroyed by molecular diffusion.

But furthermore, in most cases of practical interest, there is a drift between discrete particles and fluid particles due, for instance, to the influence of volume forces like gravity. Therefore, overshooting is the rule. The trajectories of one discrete particle and one fluid particle coinciding at time t diverge when time goes on to the future or is reversed to the past. This is the so-called crossing-trajectory effect (CTE) [57–59]. Owing to this effect, particles cross eddies, leading to an enhanced loss of memory. One then concludes that dispersion efficiency is reduced in agreement with experiments. In the Eulerian approach, CTE is taken into account by introducing a multiplicative semi-empirical correcting factor to the dispersion coefficient of the STDisp. This factor contains a new constant C_β [15]. Bear in mind, however, that the C_β-value given in Ref. [15] is erroneous. The published value should be divided by 2 (all other results are unchanged).

Here we would like to provide a striking image of the fact that a loss of memory is associated with a reduction of the dispersion efficiency. In the first case, assume N gentlemen grouped together inside a circle in a desert and, at $t = 0$, they all start walking in random directions. By definition, a gentleman only drinks water. Therefore, once a direction of walking is chosen, it is preserved. After one hour, the gentlemen will be dispersed much. Here, a high memory leads to high dispersion efficiency. In the second case, we still have N men, but they are not gentlemen. Thus, once a direction of walking is chosen, it is not preserved. In extreme cases, some of the men will fall down but, in any case, even if they preserve their speed (a scalar), they will not preserve their velocity (a vector). Here, a loss of memory leads to low dispersion efficiency. To some extent, this is the essence of the CTE where the enhanced effect of collisions with eddies is replaced by the deleterious effect of alcohol.

The above discussed Eulerian approach has been implemented in codes generically called DISCO (for DISpersion COmputing). Results and validations are provided in Refs. [13–15, 60, 61] which are specifically devoted to the Eulerian approach. Other results are discussed in Ref. [3] and incidentally provided in references concerning the Lagrangian approach for the sake of comparisons (see quoted references in the following sections).

More general Eulerian approaches may be designed, then relying on modelling. Some assumptions of the STDisp may be removed with a more intense conceptual effort. This enables us to go beyond the range of applications of the STDisp which, even extended to nonhomogeneous flows and corrected for CTE, remains limited due to underlying assumptions. For instance, the STDisp transport equation involves mean particulate number–densities but does not account for number–density fluctuations which, by analogy with the Reynolds stresses, must certainly play a role in a refined description. Such generalisations for the STDisp also lead to specific difficulties in a closure problem generated by the presence of particles, in particular in the description of interfacial transfers between the two phases. A consequence is the introduction of new modelling constants, a somehow unpleasant feature. Obviously, checking such more complex Eulerian approaches by intensive experiments becomes essential. For details, the reader is referred to Refs. [62–64]. In any case, the STDisp should be recovered from these generalised approaches as a limit case, providing a test of validity and consistency. We should also mention that significant progress, somehow analogous to the Eulerian approach, has been accomplished by relying on an analogy with the kinetic theory of gases, but many developments are still necessary [65, 66].

Generalised Eulerian approaches, generically called Eulerian models, then become akin to so-called two-fluid models [1] and, conversely, a two-fluid model may be viewed as a Eulerian model. Such two-fluid models appear well suited to the study of dense multiphase flows, for instance for the understanding and prediction of fluidised beds.

However, we believe that these models lead to considerable difficulties in accounting for complex phenomena such as vaporisation and combustion, particle/wall interactions, coalescence and break-up, big particulate Reynolds number cases, two-way coupling and particle/particle interactions (four-way coupling). Although interest in the development

of Eulerian models for such more complex phenomena is warranted, we here have a strong motivation for the development of another approach, namely the Lagrangian approach that we are now going to study.

5. Lagrangian approach for fluid particle trajectories

5.1. Generalities

We provide in this subsection some general information aiming to introduce classification of the different Lagrangian approaches which have been developed and used during about the last two decades. Whatever the Lagrangian method used, the main problem in turbulent flows, is determining the fluid instantaneous velocity field at the discrete particle location, all along the trajectory of the tracked discrete particle. Obviously, this problem is crucial because, owing to various effects such as inertia and gravity, discrete particle trajectories and fluid particle trajectories do not coincide. However, fluid particle trajectories may be viewed as reference trajectories and, in any case, we have to predict them. The equation for such a prediction is, in principle, very simple due to the fact that a fluid particle (or a discrete particle exhibiting special properties such as being nonbuoyant and/or having a vanishing diameter) instantaneously follows the surrounding velocity field. Therefore, we have:

$$x_i(t + \delta t) = x_i(t) + U_i \delta t$$

in which $x_i(t)$ is the location of the fluid particle at time t, U_i is the instantaneous fluid velocity and δt an increment of time, small enough so that U_i is essentially constant during δt. The instantaneous velocity U_i is equal to the mean velocity which is known (for instance from turbulence model predictions) plus a fluctuation u_i, which is unknown. However, we know the variances of each component of u_i (again from the turbulence model predictions) and we may assume, for simplicity, that u_i satisfies a Gaussian probability density function. This is not enough to toss a value of the fluctuation u_i since it is compulsory to also satisfy the Lagrangian velocity correlation coefficient R_{fL} discussed previously (Section 2 and Appendices A and B). Indeed, we have commented on the strong relationship existing between R_{fL} (more or less memory) and the dispersion (diffusion) efficiency (Section 4). We may then introduce a classification of the Lagrangian approaches depending on how this issue is handled. This classification starts from the simplest approach to the more sophisticated one, introducing an order which, not surprisingly, coincides with the chronological order.

1. *degree 0*. There, forces acting on discrete particles are expressed only in terms of mean values. In other words, the velocity fluctuations u_i are taken as equal to 0 meaning that the relevance of R_{fL} is not even considered. Obviously, the subsequent problem to determine the relationship between fluid particle trajectories and discrete particle trajectories does not make sense in such an approach. It may be viewed as a ballistic approach in which the influence of the turbulent field on the discrete particles is not taken into account. This crude approach may be successful in some cases, for instance for large and dense particles travelling in a turbulent flow like bullets. However, this approach is, to some extent, outside of the scope of this paper since the stochastic ingredient required to generate dispersion phenomena is lacking. This is why we symbolically assign a degree 0 to it.
2. *degree 1*. There, fluid velocity fluctuations are generated by a stochastic process in which velocity is maintained constant during constant time intervals equal to the Lagrangian time macroscale τ_L. This is the so-called eddy lifetime approach which has been, and still is, very popular [67–71]. The correlation coefficient R_{fL} is not explicitly considered in this approach but, clearly, some memory effect is introduced in the stochastic process. In fact, it may be analytically demonstrated that the chosen stochastic process generates a correlation coefficient R_{fL}, which linearly decreases from 1 at a delay equal to 0 down to 0 at a delay equal to $2\tau_L$. This is the shape (A_1) of Appendix A. Although this shape is crude, the eddy lifetime approach may provide reasonable results. As we shall soon see, this must be partially due to compensating effects in the evaluation of scales.
3. *degree 2*. This approach is similar to the previous one but the times in which velocity fluctuations are kept constant are no more constant. Instead, these times are randomly chosen and satisfy a Poisson distribution based on the time macroscale τ_L. This approach may then be called a modified eddy lifetime approach, or a random eddy lifetime approach. Again the correlation coefficient R_{fL} is not explicitly considered but it may be analytically demonstrated that the present process generates a decreasing exponential shape of R_{fL}. This is shape (A_2) of Appendix A, i.e. Frenkiel shape with $m = 0$. This approach is conceptually more attractive than the previous one since an exponential decrease of R_{fL} is more realistic than a linear decrease. For details, see Refs. [72–74].
4. *degree 3*. Degree 0 is not relevant to dispersion simulations, as previously mentioned. At degrees 1 and 2, a stochastic process is a priori chosen, generating a posteriori a Lagrangian correlation coefficient which cannot be controlled. In degree 3, we account for the fact that R_{fL} is actually a predominant quantity, at least conceptually, and takes it as an input. More importantly, the procedure is designed in such a way that any R_{fL}-shape may be a priori chosen and introduced in the code. The stochastic process, in its details (but not in its whole scheme) is then slaved to the chosen correlation. We may then call this approach the correlation slaved approach. In particular, it allows one to easily test the influence of the shape of the

correlation coefficient on the particle diffusion (dispersion) phenomenon. However, in practice, as previously mentioned, we favour the exp–cos Frenkiel shape with $m = 1$. With $m = 0$, degree 2 is then automatically recovered as a special case and we may check that predictions from degree 3 with $m = 0$ agree with predictions from degree 2.

5.2. The slaving process

The slaving process satisfies the following properties:

1. The probability density function of the velocity fluctuations is assumed to be normal. This assumption may, in principle, be relaxed, allowing possibly to test the influence of pdfs on diffusion (or dispersion). For predictions in turbulent flows, the relaxation of this assumption would require knowledge of the actual pdf. The accuracy with which this pdf should be known depends on the sensitivity of particle behaviour to it. Up to now, this issue has not been studied but interest in such a study is warranted.
2. The stochastic process must reproduce one point correlation of velocity fluctuations, known from the turbulence model (or from experiments).
3. Finally, this stochastic process must also correctly reproduce the fluid particle Lagrangian correlation function of velocities along the trajectory, according to the chosen shape of R_{fL}.

The chosen Lagrangian correlation function is rewritten under the form of a matrix A (the correlation matrix) which is symmetric and definite positive. Matrix components are velocity correlations at times $i\delta t$ and $j\delta t$, in which δt is the time step for trajectory simulations. From matrix A, we may deduce uniquely another matrix B by invoking a so-called Cholesky factorisation. The aim is to generate a vector **U** whose components are velocity fluctuations along the trajectory, at time steps regularly separated by the increment δt, and complying with the chosen Lagrangian correlation. A vector **Y** with uncorrelated, centred, unit variance components is first randomly generated. One then shows that $\mathbf{U} = \mathbf{BY}$ (see Appendix D for details).

This process involves many operations so that the reader may wonder whether it would not be too time-consuming. Actually, due to the fact that the correlation history is well reproduced, time steps in the slaving process may be much larger than in eddy lifetime approaches, so that runs are essentially not more time-consuming.

Originally designed for 1D-dispersion, the procedure has later been generalised to 2D- and 3D-cases. Details may be found in Refs. [3, 75–81]. In these references, we also provide validations relying on comparisons between the Lagrangian approach (computer program PALAS: PArticle LAgrangian Simulation) and the Eulerian approach, theoretical results, experimental data. The quoted references also contain results and validations concerning the case of discrete particles that we are now going to discuss.

Also, Appendix E provides an extra discussion, with emphasis on scales and the influence of inaccuracies when evaluating these scales.

6. Lagrangian approach for discrete particle trajectories

The simulation of the trajectory of a discrete particle relies on integrating the equation of motion of the particle. Very often, the following simplifications may be introduced:

1. Basset term is neglected. The interest in this simplification when it is allowed is that the Basset term is an history integral which is time-consuming to evaluate. Conditions allowing one to neglect the Basset term are discussed in Ref. [56].
2. When turbulence intensities are small enough, temporal derivatives of velocity fluctuations may be neglected with respect to mean velocity derivatives.

Now, the simulation of a discrete particle trajectory is a far more complicated task than for fluid particles. The main problem is that, to integrate the equation of motion from time t to time $(t + \delta t)$, we must know the fluid velocity fluctuation at the location of the discrete particle. However, velocity fluctuations along the discrete particle trajectory are correlated, but they are not correlated via the fluid particle Lagrangian correlation function that is assumed to be known. They are correlated via a discrete particle Lagrangian correlation function that is unknown. Therefore, the simulation technique described in the previous section cannot be used along the discrete particle trajectory.

In the slaving process approach, this problem is handled by simultaneously launching a fluid particle and a discrete particle, which coincide at the initial time of the trajectory construction. The fluid particle trajectory will serve to drive the discrete particle trajectory. This fluid particle trajectory is simulated by using the technique presented in Section 5. At each time step, one then knows the velocity fluctuation of the fluid at the fluid particle location. In order to determine the required fluid velocity fluctuation at the particle location, we use Eulerian transfer of velocity fluctuations from the fluid particle location to the discrete particle location, i.e. fluid velocity fluctuations at the discrete particle location are determined by a random process satisfying a Eulerian spatial correlation between trajectories. At this stage, knowledge of spatial Eulerian scales is therefore required (Section 2). The mathematical formulation of the Eulerian transfer again relies on the introduction of a correlation matrix and of a Cholesky factorisation as in the previous section.

However, the driving fluid particle can only play its role when the distance between trajectories is smaller than an Eulerian spatial macroscale. Otherwise, trajectories become uncorrelated. Therefore, the distance between trajectories is

compared with the Eulerian macroscale at each time step. When it becomes too large, a new driving fluid particle is launched from the discrete particle location while tracking of the old one is given up (see Appendix F for details).

The above procedure allows the simulation of discrete particle trajectories constrained to satisfy essential Lagrangian and Eulerian correlations appearing in any turbulence field. When the discrete particle drifts with respect to the turbulence field, it travels through eddies leading to an enhanced loss of memory, so that (as we have seen) the dispersion efficiency is decreased (crossing trajectory effects).

Our present procedure for discrete particle trajectories naturally simulates the CTE without introducing any new constant. More generally, Lagrangian simulations discussed in Sections 5 and 6 do not introduce new constants. It is the basic reason why they have the status of a simulation, not of a model. Any involved constant is associated with the turbulence field, not with the particle behaviour.

We must however remark that the Eulerian transfer process is not conceptually perfect. Effectively, let $\overline{AB}$ be the correlation between two velocity fluctuations along the fluid particle trajectory, and $\overline{BC}$ the correlation between two velocity fluctuations, B being taken on the fluid particle trajectory and C on the discrete particle trajectory, then $\overline{AC} \pm \overline{AB}\ \overline{BC}$. The consequence of this mathematical fact may be illustrated as follows. We assume that we simultaneously track two fluid particles, one driving and the other driven. The fluid particle Lagrangian correlation function along the driving trajectory is correctly simulated because it is an input to the Cholesky factorisation. However, after Eulerian transfer, it will not be perfectly recovered along the driven fluid particle trajectory. More sophisticated procedures in the same kind of spirit might be imagined to overcome this problem. However, in practice, the effort has not been found to be necessary.

Numerous comparisons between simulations and experiments are provided in Refs. [3, 75–81]. Refs. [80, 81] discuss a case of 3D-particle dispersion with CTE in which ferrofluid droplets are submitted to a nonhomogeneous magnetic field. From the results presented in these papers, we conclude that the Lagrangian approach is satisfactory.

7. Two-way coupling

When the mass-loading ratio of particles increases, it becomes necessary to take into account the influence of particles on the turbulence. The problem has been extensively studied in the past and is still a main research topic in the two-phase flow community. Due to the complexity of the involved mechanisms, both experimental studies and numerical attempts have been developed. Among them, let us mention experiments in particle laden jets [82–84], direct numerical simulations that are mostly devoted to the influence of particles on the fluid turbulence energy and its dissipation [7, 10], large eddy simulations to account for preferential concentration [9] and theoretical studies [85, 86].

Gore and Crowe [87] defined a criterion which is based on the ratio of the particle diameter d_p and the integral length scale of the flow L_E. They found that turbulence is attenuated for small values of d_p/L_E (<0.1) and increased for large values (>0.1). Nevertheless, the relevant parameters which are involved in the two-way coupling are not restricted to the ratio d_p/L_E. If the particle diameter is larger than the Kolmogorov scale, the particle will affect the energy distribution of the surrounding flow. The particle Reynolds number ($Re_p = d_p|V_p\text{-}U_f|/\nu$) is linked to the structure of the flow around the particle. For large Re_p particles are generating turbulent wakes which will modify the turbulence of the carrier fluid. An important parameter is the particle relaxation time ($\tau_p = (\rho_p + \rho_f/2)d_p^2/18\mu$), which leads to the Stokes number $S_t = \tau_p/\tau_f$ when it is compared to the fluid integral time scale τ_f. As quoted by Sato [88] for Stokes number of the order of unity, a mean slip velocity between the two phases is observed and thus it leads to momentum transfer from the particle to the fluid. This transfer increases with an increase in the loading ratio. Direct numerical simulations [7, 10] have shown the complexity of the problem, which should not be considered as completely solved at the present time, although significant progress has been achieved.

The most commonly used turbulence model remains the so-called (k–ε) model. To introduce the two-way coupling in the simulations, the equations of the turbulence model are then modified by adding source terms in the balance equations for momentum, turbulence energy and dissipation. For momentum and turbulence energy, it is not necessary to introduce any new constant. Corresponding source terms can be accurately computed from the record of particle energy and momentum at the entrance and at the exit of finite difference cells [89]. Conversely, a new constant is required to model the particle source term in the dissipation equation. Therefore, the simulation becomes a model. The obtained governing equations for the prediction of the turbulence field then generalise the (k–ε) ones. They will later be given in a more general context (Appendix H).

The structure of the code PALAS is then also modified to account for the two-way coupling. In a first step of the run, the nonladen turbulence field is predicted by using the original governing equations of the (k–ε) model (supplemented by ASM ones), and a sufficient amount of particle trajectories is simulated.

From these simulations, source terms are evaluated and introduced in the modified turbulence model. A new set of trajectories is later simulated in the new turbulence field, and so on. The number of iterations between the turbulence and the particulate modules to obtain convergence of the process is typically 3. However, in dense or strongly coupled two-phase flows, possibly with phase change or chemical reaction, the convergence can be quite difficult to reach [90].

Validations by comparisons with experimental data have been found satisfactory [79, 91], more particularly in particle laden jets.

8. Heat and mass transfers

The Lagrangian approach is very suitable to handle complex phenomena. Here, we discuss the case when additional heat and mass transfers occur between the discrete particles and the surrounding fluid, with the typical example of droplet vaporisation. We have then also to track heat and mass transfers along the discrete particle trajectories. We start with a description of vaporisation models.

8.1. Droplet vaporisation models

One of the main assumptions in vaporisation models is the so-called 'corrected spherical symmetry' assumption, which means that spherical symmetry is assumed for heat and mass transfers between the droplets and the surrounding fluid, and that convection effects are taken into account by introducing correlation laws [92, 93].

A more complete list of assumptions is as follows:

1. spherical symmetry
2. quasi-steady gas film around the droplet
3. uniform physical properties of the surrounding fluid
4. uniform pressure around the droplet
5. liquid/vapour thermal equilibrium on the droplet surface.

To take advantage of the assumption of thermal equilibrium on the surface of the droplets, the droplet temperature (particularly on this surface) must be determined. This may rely on the so-called 'infinite conductivity model' in which the temperature inside the droplet is assumed to be uniform, or on the 'conduction limit model' in which the conduction temperature equation is solved inside the droplet, or more completely, on the 'circulation model' where internal circulation can also be involved [94–97]. See details in Appendix G.

These models include more or less sophisticated simulations of the vaporising droplet behaviour but do not provide any information on the influence of turbulence on the particle behaviour. Such an influence may be predicted by implementing these models in an one-way Lagrangian approach where, besides tracking the dynamical behaviour of the droplets, we also track simultaneously their vaporising behaviour. For instance, simulations have been carried out for methyl alcohol droplets in grid turbulence [98]. Particular attention has been paid to the respective influence of fluctuating temperatures, fluctuating vapour mass fractions and fluctuating velocities on mean diameters and diameter distributions. An important result is that the turbulence produces a broadening of the probability density function of diameters, which cannot be neglected, particularly when significant temperature fluctuations occur in the flow under study. This broadening has a strong influence on the spatial distribution of droplets, since the dispersion efficiency depends on the diameter of particles. Hence, in the case of spray combustion, the structure of the flame will depend much on the diameter pdf broadening induced by turbulent fluctuations.

8.2. Two-way coupling

In many situations, the mass loading particle/fluid ratio is too large to allow one to be satisfied with the one-way approach discussed in the previous subsection. We then have to use a two-way coupling scheme, describing the modification of the turbulence field by the particles, similarly to that discussed in Section 7. In particular, the structure of the code again implements iterations between turbulence predictions and particulate predictions. Besides momentum and energy exchanges between the continuous and the discrete phases (involved in Section 7), we now also have to implement other exchanges produced by the vaporisation [99]. The vapour, which is given by droplets to the fluid, is a source of mass and, furthermore, vaporisation induces modifications in momentum and energy exchanges. The most difficult work in implementing such a two-way coupling consists of adequately rewriting the governing equations for turbulence predictions. Details are provided in Appendix H.

9. Four-way coupling

9.1. Generalities

Let us start from a two-way coupling case, in its full generality, i.e. including phase exchanges between the particles and the carrier fluid. Now, assume that the number–density of particles is so big that particles will interact, either in an indirect way through hydrodynamic forces on a particle induced by the presence of the other particles, or directly, such as by collisions or coalescence. We are then faced with a full four-way coupling problem in full generality, to be discussed, in this paper, in the framework of Lagrangian approaches.

The terminology 'four-way' comes from the fact that, if a particle A influences a particle B, then, reciprocally, particle B must influence particle A, by action and reaction. The terminology 'hydrodynamical' arises from the literature but does not mean that the carrier fluid is necessarily in a liquid state.

A classification of particle laden flows in terms of the importance of inter-particle collisions is based on the ratio of the particle relaxation time τ_p and the characteristic time of collisions τ_c [100]. In the framework of the kinetic theory, for a statistically homogeneous distribution of dynamically identical particles, τ_c depends on the particle volume fraction α, the particle diameter and the particle kinetic energy k_p ($\tau_c = [24/\sqrt{\pi}\alpha/d_p\sqrt{2k_p/3}]^{-1}$). The dilute regime is

defined for $\tau_p/\tau_c \ll 1$ and the dense regime is for $\tau_p/\tau_c \gg 1$. For dense two-phase flow the averaged time between two collisions is smaller than the particle relaxation time, so that the particles do not have time to recover their own behaviour between two collisions. In dilute two-phase flow, the fluid influence is the dominant effect, since the time between two collisions is large enough for the particle motion to be mainly controlled by the fluid.

The four-way coupling problem in its full generality is still unsolved, but, in recent years, was the object of much effort. This problem can be viewed as representing the present frontier of two-phase flows with discrete particles. Different approaches have been recently and are currently being studied [5], leading to very encouraging results and, in some cases, to definite ones, namely (i) the use of a direct numerical simulation of both the fluid flow and of the embedded particles, giving insights on underlying physical phenomena [101, 102]; (ii) an Eulerian approach in which collisions between particles are described by using a kinetic theory approach [102]; (iii) a Lagrangian simulation based on a single particle tracking [103, 104]; and (iv) a Lagrangian simulation based on several particle trajectories [105, 106].

Let us focus on Lagrangian approaches and assume that we only consider particle collisions. Also assume that probabilities for collision events can be evaluated. Then it is possible to simulate single particle trajectories. Along each trajectory realisation, a random process may be used to decide when a collision occurs and, tossing the characteristics of the particle partner in the collision, to describe this collision. Here, we may view a discrete particle as surrounded by a cloud of probability acting on this particle. By analogy with the double solution interpretation in quantum mechanics where a microparticle is accompanied by a probability wave, we shall call this approach the double solution approach. This is approach (iii) above.

Approach (iv) is the most natural one to account not only for collisions but also for hydrodynamic interactions between particles. Here, N particles are simultaneously launched and hydrodynamic forces may be evaluated at each time step, allowing one to provide a Lagrangian simulation of the simultaneous trajectories for a cloud of particles. This is the approach to which the rest of this paper is devoted.

Obviously, there is a drastic limitation in it, namely the fact that N cannot be too big. We however forecast that realisations over N-particle trajectories may help to define probabilities of events so that this approach could allow the development of refined double solution approaches (although this last statement is still more or less intuitive). We shall return to this issue on several occasions.

Also, at the present time, the usual two-way coupling is not yet considered so that the four-way coupling problem is considered in a restricted framework that we may call a degenerated four-way coupling problem.

9.2. Hydrodynamic interactions

In the N-trajectory Lagrangian approach, N particles are simultaneously tracked and we evaluate hydrodynamic interactions and/or collisions between particle pairs, at each time-step along particle trajectories, so that the motion of a single particle is correlated with the motion of the other surrounding particles. Of course, a given particle is more influenced by those particles which are close to it, rather than by particles which are far away from it. This is why the N-trajectory approach may be realistic in practice, although, in an actual flow, the number N is actually infinite from the point of view of computer capabilities.

Hydrodynamic interactions are deduced from the sedimentation theory relying on the use of a mobility matrix. For small enough particle Reynolds numbers, the mobility matrix allows one to express the instantaneous velocities of interacting particles versus their distance, diameters, velocity differences, and also fluid properties. The inverse matrix, known as the resistance matrix, may then be used to define a set of differential equations for particle displacements (see Appendix I for details). When compared with one-way equations of motion (such as Riley [35] or Maxey and Riley [34] ones), the main difference then arises in the drag term which now involves the hydrodynamic coupling between particles. We then obtain a set of equations whose cardinality is equal to the number of interacting particles to be solved (Appendix J).

9.3. Applications

The above formalism may be used to describe the behaviour of N sedimenting particles in a fluid at rest and, actually, was originally designed for such applications. See Refs. [107–111] for examples. It can also be implemented in a Lagrangian approach in which N particles are simultaneously followed in a turbulence field. It is then found that the influence of hydrodynamic interactions becomes small when the turbulence intensity increases, say beyond 1%, smaller in particular than the influence of collisions. An inverse behaviour is observed for collision effects, depending on the investigated velocity direction with respect to particle alignment (increase of fluctuating velocities in particle centre direction, decrease in perpendicular direction). No influence on particle behaviour for 50 randomly distributed particles has been observed in isotropic turbulence. For non-isotropic flows, an effect of return to isotropy of the fluctuating motion of the particles is observed. The significance of this effect is strongly dependent on particle turbulent dispersion and particle relaxation time. The influence of collisions is decreased by increasing turbulence intensity (the more the particles are rapidly dispersed, the more the influence of collision is reduced), and increased by increasing particle relaxation time. The simultaneous tracking of N particles, however, allows one to evaluate collision probabilities which could, in the next step, be included in a double

solution approach. This leads us to the frontier of our present knowledge, to the point where our ideas would become too speculative for such a paper.

10. Conclusion

In this paper, Eulerian and Lagrangian approaches to predict and/or simulate the dispersion behaviour of discrete particles in turbulent flows have been presented and discussed. From numerous validations carried out by comparing theoretical results and experimental data, we conclude that both approaches are suitable for the purpose.

The main focus, however, concerned the Lagrangian approach which is well suited to the simulation of complex phenomena, avoiding a significant increase of model constants. Examples of such complex phenomena may be found in two-way coupling situations when the turbulence acts on the transported particles which, in return, react on the turbulence and modify its properties when the mass-loading ratio is large enough. The two-way coupling problem has also been considered when additional heat and mass transfers take place between the particles and the carrier fluid, such as in the case of vaporising droplets. In the presence of evaporation (one-way or two-way), it is found that a monodispersed cloud of droplets becomes a polydispersed cloud with skewed diameter probability density function. Since dispersion phenomena depend on the diameter, we also obtain a space-dependent diameter probability density function in which the smallest droplets typically tend to disperse faster towards the edges of the flow. A next step would be to consider the case of combustion, leading to enhanced complexity produced by the occurrence of chemical reactions and of radiative transfer.

Besides this line of research leading from isothermal dispersion to combustion problems, current efforts are devoted to the so-called four-way problem in which particle–particle interactions take place, under the form of hydrodynamical interactions and/or collisions. In the Lagrangian approach, instead of successively launching particles in the flow, the basic idea relies on a simultaneous launching allowing, conceptually, an easy handling of particle–particle interactions. In this form, the problem is very challenging. More Eulerian correlations must be taken into account, leading to a random process of greater complexity. Also, simultaneous launching of particles leads to a dramatic increase of storage requirements such as the number N of particles to be simultaneously tracked cannot be very large. Although limited in its range of applications, this approach can, however, provide relevant information. It may help to design a double solution approach in which only one particle would be tracked, being nevertheless surrounded by a cloud of probability such as defining the probability of collision. Such an approach might also be used for coalescence or break-up.

Some of our assertions concerning the four-way problem may be a bit speculative. However, currently intense efforts are being devoted to this issue and forthcoming results will certainly help to clarify it. In any case, starting from a well-established knowledge, we felt it necessary to project ourselves to the future.

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Appendix A. Functional shape of the Lagrangian velocity correlation coefficient R_{fL}

The simplest available shape is the linear decrease according to:

$$R_{\mathrm{fL}}(\tau) = 1 - \frac{\tau}{2\tau_{\mathrm{L}}} \tag{A1}$$

decreasing from 1 at $\tau = 0$ down to 0 at $\tau = 2\tau_{\mathrm{L}}$. Next, we have the classical exponential decrease:

$$R_{\mathrm{fL}}(\tau) = \exp(-\tau/\tau_{\mathrm{L}}) \tag{A2}$$

and the Frenkiel [23] family:

$$R_{\mathrm{fL}}(\tau) = \exp\left[\frac{-\tau}{(m^2+1)\tau_{\mathrm{L}}}\right]\cos\left[\frac{-m\tau}{(m^2+1)\tau_{\mathrm{L}}}\right] \tag{A3}$$

in which m is the loop parameter, giving back the exponential decrease for $m = 0$.

Finally, we mention Sawford's [112] expression reading as:

$$R_{\mathrm{fL}}(\tau) = \frac{1}{1-\sqrt{Re*}}\left[\exp\left(-\sqrt{Re*}\tau/T_{\mathrm{L}}\right) - \sqrt{Re*}\exp(\tau/T_{\mathrm{L}})\right] \tag{A4}$$

in which:

$$T_{\mathrm{L}} = \tau_{\mathrm{L}}\left(1 + \frac{1}{\sqrt{Re*}}\right)^{-1} \tag{A5}$$

$$Re* = \frac{16a_0^2}{C_0^4}\,\frac{Re_\lambda}{15} \tag{A6}$$

$$Re_\lambda = \frac{\lambda\sqrt{\bar{u}^2}}{\nu} \tag{A7}$$

$$a_0 = 0.13Re_\lambda^{0.64} \tag{A8}$$

Here, the Reynolds number Re_λ is based on a Taylor turbulent scale, a velocity fluctuation scale $\sqrt{\bar{u}_2}$ and on the kinematic viscosity ν. C_{O} is taken as the Kolmogoroff

constant or as a solution of the relation:

$$\frac{\tau_L}{\tau_k} = \frac{2}{C_O}\frac{Re_\lambda}{\sqrt{15}} + \frac{C_O}{2a_0} \tag{A9}$$

in which τ_k is the Kolmogoroff time scale. Let us mention that this correlation is fairly insensitive to the exact value of C_O.

Eqs. (A1)–(A3) do not satisfy the requirement:

$$\frac{dR_{fL}(\tau)}{d\tau}|_{\tau=0} = 0 \tag{A10}$$

but Eq. (A3) exhibits negative loops (for $m \neq 0$) as we require to satisfy as closely as possible relation Eq. (A14) in Appendix B. The fact that Eq. (A3) does not satisfy Eq. (A10) is not very troublesome. Indeed, Fourier transforming, it appears that the fluid Lagrangian spectrum is badly estimated for high frequencies which have little influence on particulate dispersion, which is controlled by rather big eddies.

Sawford's expression satisfies Eq. (A10) so that it may be possibly preferred. It has, however, not been extensively used in the historical development of the topic discussed in this paper. However, in practice, uncertainties in the shape of R_{fL} may be compensated by uncertainties in the evaluation of scales [104], so that the interest in an investigation of Sawford's expression is not warranted.

Appendix B. On the shape of $R_{fL}(t)$

Let us consider a one-dimensional turbulent motion in a homogeneous stationary turbulence [22]. Let *v(t)* and *a(t)* be the fluid fluctuating Lagrangian velocity and the fluid fluctuating Lagrangian acceleration, respectively. Then, we have:

$$v(t) = v(0) = \int_0^t a(t')\,dt' \tag{A11}$$

Defining the acceleration correlation coefficient as:

$$A_L(\tau) = \frac{\overline{a(t)a(t+\tau)}}{\overline{a^2}} \tag{A12}$$

we find:

$$\frac{dR_{fL}(t)}{dt} = cste\int_0^t A_L(\tau)\,d\tau \tag{A13}$$

But the limit of $\frac{dR_{fL}(t)}{dt}$ for $t \to \infty$ is zero, leading to:

$$\int_0^\infty A_L(\tau)\,d\tau = 0 \tag{A14}$$

i.e. there is no acceleration integral time scale. This implies that $A_L(\tau)$ possesses at least one negative loop. But we also have from Eq. (A13):

$$A_L(t) = cste\frac{d^2R_{fL}(t)}{dt^2} \tag{A15}$$

and, therefore, the second derivative of R_{fL} must also exhibit at least one negative loop. This condition is not satisfied by the correlations Eq. (A1) and Eq. (A2) of Appendix A. It may, however, be better satisfied if R_{fL} itself possesses one negative loop, hence our demand leading to the use of Frenkiel's expression.

Note, however, that negative loops may be absent from R_{fL} and hence Eq. (A15) will be satisfied. Indeed, using Eq. (A14) and Eq. (A15), we find:

$$\int_0^\infty A_L(\tau)\,d\tau = cste\int_0^\infty \frac{d^2R_{fL}(\tau)}{d\tau^2}d\tau = cste\frac{dR_{fL}(\tau)}{d\tau}|_0 \tag{A16}$$

Thus, when the first derivative of the correlation function is 0 at $t = 0$ and for $t \to \infty$ (as it should), the non-existence of an acceleration integral time scale is automatically satisfied. Such is the case for the Sawford correlation, but not for the linearly and exponentially decreasing shapes. Frenkiel's family provides a (partial) remedy to this situation because, in this case, $R'_{fL}(\tau)$ at $\tau = 0$ is proportional to $1/(m^2 + 1)$.

Appendix C. Equations of motion

This appendix provides equations of motion which are relevant to the topic of this paper. For the Eulerian approach, we use the Tchen equation [29] reading as:

$$\frac{d\mathbf{V}}{dt} + a\mathbf{V} + c\int_{-\infty}^t \frac{d\mathbf{V}}{dt}(t-\tau)^{-1/2}\,d\tau = a\mathbf{U} + b\frac{d\mathbf{U}}{dt} + c\int_{-\infty}^t \frac{d\mathbf{V}}{dt}(t-\tau)^{-1/2}\,d\tau - \frac{2(s-1)}{2s+1}\mathbf{g} \tag{A17}$$

in which:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + V_j\frac{\partial}{\partial x_j} \tag{A18}$$

$$a = \frac{18\nu}{(s+1/2)d^2} \tag{A19}$$

$$b = \frac{3}{2(s+1/2)} \tag{A20}$$

$$c = \frac{9(\nu/\pi)^{1/2}}{(s+1/2)d} \tag{A21}$$

and:

$$s = \frac{\rho_p}{\rho_f} \tag{A22}$$

The temporal derivative is evaluated along the discrete particle trajectory. Also, d is the diameter of the particle while ρ_p and ρ_f are the density of the particle material and of the surrounding fluid, respectively, **V** and **U** are the velocity vector of the particle and of the fluid respectively, and **g** is the gravity vector. The extra force resulting from the

extra pressure gradient term reads as:

$$F_{\text{press}} = \frac{\pi d^3}{6}\rho_{\text{f}}\frac{\text{d}\mathbf{U}}{\text{d}t} \tag{A23}$$

and is incorporated in the term $b\text{d}\mathbf{U}/\text{d}t$ of Eq. (A17). This term is the one which has mainly been discussed in the controversy concerning the Tchen equation.

For the Lagrangian approach, we use a modified Riley equation [35] reading as:

$$\begin{aligned}\rho_{\text{p}}\frac{\pi d^3}{6}\frac{\text{d}\mathbf{V}}{\text{d}t} = &-\frac{\pi d^2}{8}\rho_{\text{f}}C_{\text{D}}(\mathbf{V}-\mathbf{U})|\mathbf{V}-\mathbf{U}| \\ &- \rho_{\text{f}}\frac{\pi d^3}{6}C_{\text{A}}\frac{\text{d}(\mathbf{V}-\mathbf{U})}{\text{d}t} + \frac{\pi d^3}{6}\left(\rho_{\text{p}}-\rho_{\text{f}}\right)\mathbf{g} \\ &+ \rho_{\text{f}}\frac{\pi d^3}{6}\frac{\text{D}\mathbf{U}}{\text{D}t} - \frac{\pi d^2}{4}C_{\text{H}}\frac{\sqrt{\rho_{\text{f}}\mu}}{\pi} \\ &\times\int_{-\infty}^{t}\frac{\text{d}(\mathbf{V}-\mathbf{U})}{\text{d}t}(t-\tau)^{-1/2}\,\text{d}\tau\end{aligned} \tag{A24}$$

in which:

$$C_{\text{D}} = \frac{24}{Re_{\text{p}}}\left(1 + 0.15Re_{\text{p}}^{0.687}\right)\ Re_{\text{p}} \le 200 \tag{A25}$$

$$C_{\text{A}} = 1.05 - 0.0066/\left(A_{\text{C}}^2 + 0.12\right) \tag{A26}$$

$$C_{\text{H}} = 2.86 - 3.12/\left(A_{\text{C}}^2 + 1\right)^3 \tag{A27}$$

$$A_{\text{C}} = \frac{|\mathbf{V}-\mathbf{U}|^2}{\text{d}|\dfrac{\text{d}(\mathbf{V}-\mathbf{U})}{\text{d}t}|}\ A_{\text{C}} \le 60 \tag{A28}$$

with the particulate Reynolds number reading as:

$$Re_{\text{p}} = \frac{|\mathbf{V}-\mathbf{U}|d}{\nu} \tag{A29}$$

and

$$\frac{\text{D}}{\text{D}t} = \frac{\partial}{\partial t} + U_j\frac{\partial}{\partial x_j} \tag{A30}$$

that means the extra pressure gradient term is now evaluted along the fluid motion.

If $Re_{\text{p}} < 1$, then the Riley equation is recovered. Modifications introduced to account for large particulate Reynolds numbers are available from equations in Clift et al. [37] and Odar and Hamilton [38].

Appendix D. The slaving process for fluid particles

For the sake of simplicity, the procedure is explained in a 1D-formulation.

Let $u(n\delta t)$ be the fluid fluctuating velocity at time $(n\delta t)$. Our aim is then to determine a vector of correlated random variables:

$$U = (u(0),\ u(\delta t),\ u(2\delta t)\ldots,\ u(i\delta t),\ldots) \tag{A31}$$

the correlation between the components of U having to agree with R_{fL}.

We then define a correlation matrix A, with elements a_{ij}, reading as:

$$A = \begin{bmatrix} \overline{u(0)^2} & . & . \\ \overline{u(0)u(\delta t)} & \overline{u(\delta t)^2} & . \\ \overline{u(0)u(2\delta t)} & \overline{u(\delta t)u(2\delta t)} & \overline{u(2\delta t)^2} \end{bmatrix} \tag{A32}$$

This matrix is positive definite and symmetric. It is, in fact, convenient to use a reduced matrix R, with elements r_{ij}, according to:

$$r_{ij} = \overline{u^*(i\delta t)u^*(j\delta t)} = \frac{\overline{u(i\delta t)u(j\delta t)}}{\sqrt{\overline{u^2(i\delta t)}}\sqrt{\overline{u^2(j\delta t)}}} \tag{A33}$$

so that, instead of U (Eq. A31), we now have to determine a vector U^* reading as:

$$U^* = (u^*(0),\ u^*(\delta t),\ u^*(2\delta t),\ldots,\ u^*(i\delta t),\ldots) \tag{A34}$$

Starting from a vector Y (y_{i}) of noncorrelated random numbers with a Gaussian distribution (such that $\overline{y_i} = 0$ and $\overline{y_i y_j} = \delta_{ij}$), and assuming a matricial linear relation between R and Y, we then search for a matrix B^* satisfying:

$$U^* = B^*Y \tag{A35}$$

Since A (and then R) is positive definite and symmetric, we may invoke the so-called Cholesky factorization telling us that:

$$R = B^*B^{*\text{T}} \tag{A36}$$

in which $B^{*\text{T}}$ is the transpose of B^*. Knowing the correlation matrix R, Eq. (A36) allows one to determine B^* and then, by Eq. (A35), we obtain U^*.

Of course, as time goes on, the size of the correlation matrix could grow without any limit. This is actually avoided by limiting the size of the correlation matrix, for example by assuming that correlations are 0 when the time delay τ exceeds 5 times the Lagrangian time macroscale τ_{L}.

Finally, if R_{fL} is chosen to have a Frenkiel [23] shape, let us mention that the elements r_{ij} of R read as:

$$r_{ij} = \exp\left[\frac{-|j-i|\delta t}{(m^2+1)\tau_{\text{L}}}\right]\cos\left[\frac{m|j-i|\delta t}{(m^2+1)\tau_{\text{L}}}\right] \tag{A37}$$

Appendix E. On scales

For fluid particle trajectories, the Lagrangian time macroscale τ_{L} must be evaluated. We may consider the ideal case of homogeneous and isotropic turbulence to exemplify problems associated with this evaluation (for more real

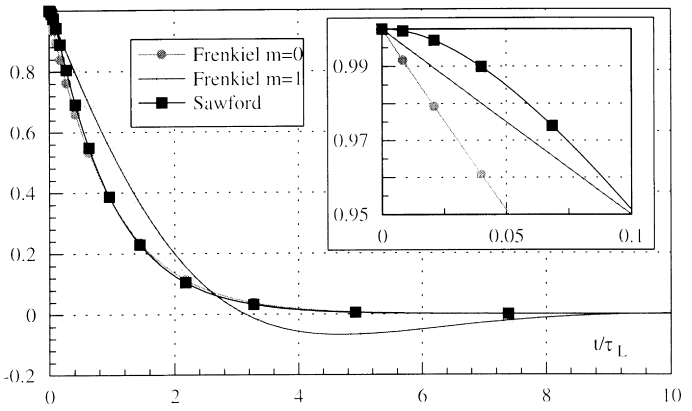

Fig. A1. Different shapes for the Lagrangian velocity correlation coefficient R_{fL}.

cases, see the literature, in particular Ref. [16] in which τ_L is extended to a tensorial time τ_{Lij}).

Then, following Tennekes and Lumley [113], the eddy viscosity ν_t may be estimated by:

$$\nu_t \approx \overline{u_{fL}^2}\tau_L \tag{A38}$$

in which u_{fL} is the fluid Lagrangian velocity fluctuation. Relying on the $(k-\varepsilon)$ closure equation, we also have:

$$\nu_T = C_\mu \frac{k^2}{\varepsilon} \tag{A39}$$

in which $c_\mu = 0.09$. We then have:

$$\tau_L \approx 0.14\frac{k}{\varepsilon} \approx 0.2\frac{\overline{u_{fL}^2}}{\varepsilon} \tag{A40}$$

Unfortunately, the above constant 0.2 actually depends on the authors. From experiments and simulations, it should be somewhere between 0.2 and 0.6, as extensively discussed in Ref. [114].

Therefore, it is important to discuss the influence of an uncertainty in the value of τ_L on the diffusion phenomenon.

We start with Fig. A1 explicitly showing different shapes for R_{fL}, namely according to the Frenkiel expression (for $m = 0$, and for $m = 1$) and to the Sawford expression. Here, we have considered a homogeneous, isotropic, and steady turbulence, with a rms fluctuating velocity corresponding to $\overline{u_f^2}$ equal to $0.017\ m^2/s^2$ and a Lagrangian time macroscale equal to $\tau_L = 91$ ms. Under such circumstances, the Frenkiel expression with $m = 0$ and the Sawford expression lead to similar results (excepted if we zoom in on small time delays).

Now, anticipating a bit on the Lagrangian approach for discrete particles, Fig. A2 presents mean square displacements $\overline{y^2}$ of discrete particles, versus time, again for different R_{fL}-shapes. The turbulence is a grid turbulence with characteristics of the flow studied by Snyder and Lumley [115], previously discussed in Ref. [104]. The discrete particles are pollen particles and the results of the experiments by Snyder and Lumley are also reported in the figure. We see that the Frenkiel correlation with $m = 1$ agrees very well with the experimental results, while the Sawford expression leads to smaller values, and the exponential decrease correlation still with smaller values. The relative difference between extreme values is about 20%. Here, such comparisons between different R_{fL}-shapes make sense because the scales have been evaluated from the experiments and directly introduced in the predictions. These scales are the time macroscale τ_L (involved in R_{fL}) and Eulerian scales used to account for crossing trajectory effects (Section 6).

A less favourable situation is when scales have to be evaluated by modelling expressions, such as Eq. (A40) for τ_L. The $\pm 10\%$ of relative difference between extreme values in Fig. A2 can then be generated by a $\pm 10\%$ change in the value of τ_L. See also Ref. [116] for further details on this issue. This discussion exemplifies the importance of a precise enough knowledge of the turbulence field, including the prediction of scales. Direct numerical simulations [10] or large eddy simulations [11] may help to improve such scale predictions, by possibly providing more accurate expressions of scale evaluations.

Appendix F. The slaving process for discrete particles

We simultaneously track a fluid particle (with trajectory built as in Appendix D) and a discrete particle (with trajectory built from the equation of motion), starting from the same point at some initial time t_0. The fluid velocity fluctuation at location P of the particle is determined by transferring the fluid velocity fluctuation at location F of the fluid particle to P, by using Eulerian correlations (Fig. A3). The fluid particle is surrounded by a spherical domain of radius L_D, in which L_D is a correlation length scale. When the discrete particle leaves the correlation domain surrounding the fluid particle, both trajectories become uncorrelated and the discrete particle trajectory can no longer be driven by the pilot fluid particle trajectory. Then a new pilot fluid particle trajectory is used, starting at the location of the discrete

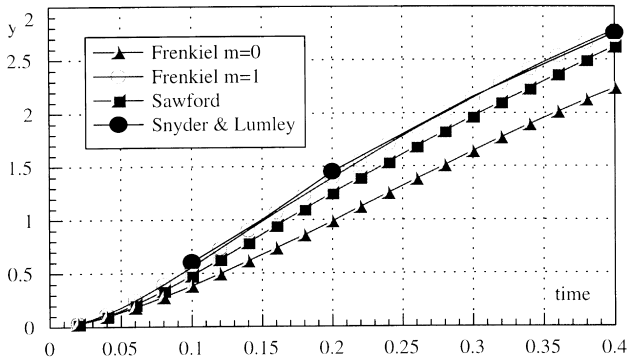

Fig. A2. Influence of R_{fL}-shapes on dispersion, and comparisons with experiments.

particle (Fig. A3). This procedure simulates the effect of crossing trajectories. In a simpler version, we may also change the fluid particle at each time step, but this scheme requires much smaller time steps for the construction of fluid particle trajectories and thus longer computing time.

The transfer from the fluid particle location F to the discrete particle location P also uses a correlation matrix and a Cholesky factorisation. The correlation matrix is now a spatial correlation matrix involving Eulerian correlations, reading as (in the case of a 2D-formulation):

$$\begin{bmatrix} \overline{u_1^2(F)} & . & . & . \\ \overline{u_1(F)u_2(F)} & \overline{u_2^2(F)} & . & . \\ \overline{u_1(F)u_1(P)} & \overline{u_2(F)u_1(P)} & \overline{u_1^2(P)} & . \\ \overline{u_1(F)u_2(P)} & \overline{u_2(F)u_2(P)} & \overline{u_2(P)u_1(P)} & \overline{u_2^2(P)} \end{bmatrix} \tag{A41}$$

If we use again a Frenkiel shape for Eulerian correlations, we then have:

$$\overline{u_i(F)u_i(P)} = \sqrt{\overline{u_i^2(F)}}\sqrt{\overline{u_i^2(P)}} \times \exp\left[\frac{-r}{(n^2+1)L_{Ei}}\right]\cos\left[\frac{nr}{(n^2+1)L_{Ei}}\right]$$

$$\overline{u_i(F)u_j(P)} = \overline{u_i(F)u_j(F)} \times \exp\left[\frac{-r}{(n^2+1)L_{Eij}}\right]\cos\left[\frac{nr}{(n^2+1)L_{Eij}}\right] \tag{A42}$$

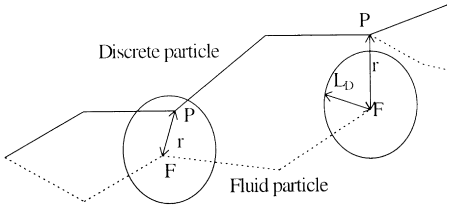

Fig. A3. The pilot fluid particle trajectories and the driven discrete particle trajectory.

When scales have to be evaluated they are expressed as follows:

$$L_{Ei} = C_i\tau_{Li}\sqrt{\overline{u_i^2(F)}} \text{ and } L_{Eij} = C_{ij}\tau_{Lij}\sqrt{|\overline{u_iu_j(F)}|} \tag{A43}$$

where the constants C_i and C_{ij} are fixed to 1 when no information can be used from experimental data.

Appendix G. Vaporisation models

With the assumptions of corrected spherical symmetry, the non-dimensional vapour mass flow rate Λ reads as [88]:

$$\Lambda = \frac{2}{Le_1}\ln(1+B_M) = \frac{\mathring{m}C_{vap}}{\pi D\lambda} \tag{A44}$$

in which Le_1 is the Lewis number and B_M the Spalding mass transfer number, reading as:

$$Le_1 = \frac{\lambda}{C_{vap}\rho D_1} \tag{A45}$$

$$B_M = \frac{Y_1^s - Y_1^\infty}{1 - Y_1^s} \tag{A46}$$

Also, $\mathring{m}$ is the vapour mass flow rate, C_{vap} is the specific heat of the vapour, D is the droplet diameter, λ is the thermal conductivity of the fluid, ρ is the fluid density, D_1 is the diffusion coefficient of the vapour, and Y_1^s and Y_1^∞ are vapour mass fractions on the droplet surface and far from the droplet, respectively.

It is then found that the equation of evolution of the droplet diameter reads as:

$$\frac{dD}{dt} = \frac{-2\Lambda\lambda}{\rho_l DC_{vap}} \tag{A47}$$

where ρ_l is the liquid droplet density.

In the infinite conductivity model, it is possible to explicitly provide a rather simple equation of evolution of the temperature T^s of the surface of the droplet. This

equation reads as:

$$\frac{dT^s}{dt} = \frac{6}{D^2}\frac{\lambda}{\rho_l C_l} \times \left[(T^\infty - T^s) Nu - \frac{L}{C_{vap}} \Lambda \right] \quad \text{(A48)}$$

where C_l is the specific heat of the liquid, T^∞ is the fluid temperature, L is the latent heat of vaporisation, and Nu is the Nusselt number defined by:

$$Nu = \frac{\Lambda}{\exp(\Lambda/2) - 1} = \frac{q_g}{\frac{\lambda(T^\infty - T^s)}{D}} \quad \text{(A49)}$$

where q_g is the heat flow rate on the droplet surface.

In order to account for the influence of convection on droplet vaporisation, correlation laws are used both for heat and mass transfer modifications under the film theory assumption. Following Faeth [117], the Nusselt number Nu is then expressed as:

$$Nu = Nu^* \ln(1 + B_T) \text{ and } Nu^* = 2 + \frac{0.55 Re_p^{1/2} Pr^{1/3}}{\left(1 + \frac{1.232}{Re_p Pr^{4/3}}\right)^{1/2}} \quad \text{(A50)}$$

where B_T is the Spalding heat transfer number, Re_p is the particle Reynolds number and Pr is the Prandtl number. A similar relation is written for the Sherwood number, but with the Prandtl number replaced by the Schmidt number. Several other correlations are available for the Nusselt and Sherwood numbers which have been compared in Ref. [118].

An important issue in droplet vaporization rate is the knowledge of the physical properties in the gaseous film around the droplet. Following Hubbard et al. [119], the averaging '1/3 rule' should be used, namely physical properties of the fluid in the gaseous film around the particle have to be approximated at a reference state '2/3 of the droplet surface + 1/3 of the fluid far from the droplet'. That leads to change of the drag coefficient C_D of the equation of motion of the particle because the kinematic viscosity ν involved in the particle Reynolds number must now be evaluated in the aforementioned reference state. From our experience, the behaviour of droplets is very sensitive to the physical properties around the droplet, i.e. to the definition of the reference state.

Appendix H. Turbulence governing equations for two-way coupling

Equations are written for a stationary, incompressible flow under conservative forms, in order to include source terms (mass, momentum, energy). We have to deal with mean flow equations (continuity, momentum, temperature, vapour mass fraction) and with turbulent quantity equations (turbulence energy, dissipation, scalar fluctuation transport) [95, 114].

The continuity equation reads as:

$$\frac{\partial}{\partial x_i}(\rho \overline{U_i}) = \bar{S}_m \quad \text{(A51)}$$

in which $\bar{S}_m$is the mass source term produced by the vaporisation process.

The momentum equation reads as:

$$\frac{\partial}{\partial x_j}(\rho \overline{U_i}\ \overline{U_j}) = \frac{\partial}{\partial x_i}\left[\bar{P} + \frac{2}{3}\rho k\right] - \frac{\partial}{\partial x_i}\left[\frac{2}{3}(\mu + \mu_T)\frac{\partial \overline{U_j}}{\partial x_j}\right] + \frac{\partial}{\partial x_j}(\mu + \mu_T)\left(\frac{\partial \overline{U_i}}{\partial x_j} + \frac{\partial \overline{U_j}}{\partial x_i}\right) + \overline{S_{u_i}} \quad \text{(A52)}$$

in which $\bar{P}$ is the mean pressure and μ_T the turbulent viscosity. $\overline{S_{u_i}}$ is the momentum source term, which is the sum of two contributions according to:

$$\overline{S_{u_i}} = \overline{S_{pu_i}} + \overline{S_{u_i}} \quad \text{(A53)}$$

The first contribution results from the interaction between the two phases, without any phase change, and depends on the interaction forces between the fluid and the particles. It reads as:

$$\overline{S_{pu_i}} = n\left\langle -m_p\left(\frac{dV_i}{dt} - g_i\right)\right\rangle \quad \text{(A54)}$$

in which n is the mean number of particles per unit volume, m_p is the particle mass, V_i is the particle velocity, g_i is gravity and $< >$ indicates mean values over all the particle trajectory realisations.

The second contribution $\overline{S_{mu_i}}$ is the gas momentum flux ejected by the particle during its vaporisation. Assuming that the vapour is discharged into the fluid with a mean velocity nearly equal to the droplet velocity, we get:

$$\overline{S_{mu_i}} = n\langle S_m V_i \rangle \quad \text{(A55)}$$

depending on the mass source S_m.

The mean temperature equation reads as:

$$\overline{U_j}\frac{\partial}{\partial x_j}\left(\rho \overline{U_j}\bar{T}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu}{Pr} + \frac{\mu_T}{Pr_T}\right)\left(\frac{\partial \bar{T}}{\partial x_j}\right) + \bar{S}_H/C_p \quad \text{(A56)}$$

where $\bar{T}$ is the mean temperature, $\bar{S}_H$ is the enthalpy source term, C_p is the fluid specific heat capacity, Pr and Pr_T are the molecular and turbulent Prandtl numbers, respectively. The enthalpy source term is the sum of two contributions:

$$\bar{S}_H = \bar{S}_{pH} + \bar{S}_{mH} \quad \text{(A57)}$$

The first contribution represents the heat captured by the droplet for its heating and for vaporising a mass $\dot{m}$ of liquid per unit time, while the second contribution represents the heat which is released by the droplet into the fluid as the result of mass transfer accompanying the change from the liquid state (at temperature T^s) to the gaseous state (at

temperature T_{ref}). These contributions read as:

$$\bar{S}_{mH} = n\left\langle \mathring{m} C_{vap}(T_s - T_{ref})\right\rangle \tag{A58}$$

$$\bar{S}_{pH} = n\left\langle -4\pi r_s^2 q_g\right\rangle \tag{A59}$$

The equation of transport of the mean vapour mass fraction reads as:

$$\frac{\partial}{\partial x_j}\left(\rho\overline{U_j}\bar{Y}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu}{Sc} + \frac{\mu_T}{Sc_T}\right)\left(\frac{\partial \bar{Y}}{\partial x_j}\right) + \bar{S}_m \tag{A60}$$

where Sc and Sc_T are the molecular Schmidt number and the turbulent Schmidt number, respectively.

For the two-way turbulence energy equation, we first apply the Reynolds decomposition to the momentum equation, yielding:

$$\frac{\partial}{\partial t}\rho u_i' + \frac{\partial}{\partial x_j}\rho(\overline{U_j}u_i^{'} + \overline{U_i}u_j^{'} + u_i'u_j' - \overline{u_i'u_j'}) = -\frac{\partial p'}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\frac{2}{3}\mu\frac{\partial u_k'}{\partial x_k}\right) + \frac{\partial}{\partial x_j}2\mu s_{ij}^{'} + S_{u_i}^{'} \tag{A61}$$

in which:

$$s_{ij}^{'} = \frac{1}{2}\left(\frac{\partial u_i^{'}}{\partial x_j} + \frac{\partial u_j^{'}}{\partial x_i}\right) \tag{A62}$$

is the fluctuating part of the strain tensor.

Multiplying Eq. (A61) by $u_i{}'$, summing on subscript i, and averaging, we obtain:

$$\begin{aligned}\frac{\partial}{\partial x_j}\left[\rho\overline{U_j}k + \frac{1}{2}\rho\overline{u_j'u_i'u_i'} - 2\mu\overline{u_i's_{ij}'} + \overline{p'u_j'}\right] &= -\rho\overline{u_i'u_j'S_{ij}} - 2\mu\overline{s_{ij}'s_{ij}'} && \text{(I)}\\ &\quad + \overline{S_{u_i'}u_i'} && \text{(II)}\\ -\rho k\frac{\partial\overline{U_k}}{\partial x_k} - \left(\frac{2}{3}\overline{u_i^{'}\frac{\partial}{\partial x_i}\frac{\partial u_k^{'}}{\partial x_k}}\right) - \frac{1}{2}\rho\overline{u_i'u_i'\frac{\partial u_k'}{\partial x_k}} + \overline{p'\frac{\partial u_k'}{\partial x_k}} &&\\ -\rho\overline{U_i}\overline{u_i'\frac{\partial u_k'}{\partial x_k}} && \text{(III)}\end{aligned} \tag{A63}$$

Part I corresponds to the usual turbulence energy equation of the (k–ε) model (Section 2). Part II is a two-way term produced by the fluctuations of the momentum source term. From Eq. (A53), we see that this term contains a contribution, which does not involve any phase change (corresponding to the two-way coupling in Section 7) and a contribution depending on the phase change. Part III is only generated by phase changes and we are now going to elaborate more on it.

Using Eq. (A51) and neglecting fluctuations of the fluid density we get:

$$\frac{\partial\overline{U_k}}{\partial x_k} = \frac{\bar{S}_m}{\rho} \tag{A64}$$

$$\frac{\partial u_k'}{\partial x_k} = \frac{S_m'}{\rho} \tag{A65}$$

so that part III may be rewritten as:

$$(\text{III}) = -k\bar{S}_m - \frac{1}{2}\overline{u_i'u_i'S_m'} - \overline{U_i'u_i'S_m'} - \frac{2}{3}\frac{\mu}{e}\rho u_i'\overline{\frac{\partial S_m'}{\partial x_i}} + \frac{1}{\rho}\overline{p'S_m'} \tag{A66}$$

The term (1) depends on the mean mass source term, while the other terms depend on correlations involving fluctuations of this mean mass source term. In the framework of a Lagrangian approach, terms (2) and (3) can be directly evaluated without any assumptions and therefore do not require any modelling [114]. Modelling is in principle required for terms (4) and (5). No solution has been established to model term (4); in practice, however, it appears reasonable to neglect the correlation between velocity fluctuations and spatial derivatives of mass source term fluctuations. Also, it appears reasonable to neglect the correlation between pressure fluctuations and mass source term fluctuations [term (5)], in analogy with the correlation $\overline{\rho' u_i'}$ which is exactly 0 in homogeneous and isotropic turbulence [22].

Eq. (A64) may then be rewritten as:

$$\frac{\partial}{\partial x_j}\rho\overline{U_j}k = \frac{\partial}{\partial x_j}\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial x_j} + \boldsymbol{S}_k \tag{A67}$$

$$\boldsymbol{S}_k = G - C_D\rho\varepsilon + S_k \tag{A68}$$

$$G = \mu_T\left[\frac{\partial\overline{U_i}}{\partial x_j} + \frac{\partial\overline{U_j}}{\partial x_i}\right]\frac{\partial\overline{U_i}}{\partial x_j} \tag{A69}$$

is the one-way usual turbulence energy production term. S_k is the two-way extra source term involving two contributions:

$$S_k = S_{pk} + S_{mk} \tag{A70}$$

The first contribution S_{pk} depends on the particle mass loading (without any phase change) while the second contribution S_{mk} is due to the vaporisation process. They read as:

$$S_{pk} = \overline{S_{pu_i}'u_i'} \tag{A71}$$

$$\begin{aligned}S_{mk} &= \overline{S_{mu_i}'u_i'} - k\bar{S}_m - \frac{1}{2}\overline{u_i'u_i'S_m'} - \bar{U}_i\overline{u_i'S_m'}\\ &= \overline{S_{mu_i}'u_i'} + \frac{1}{2}\bar{U}_i\bar{U}_i\bar{S}_m - \frac{1}{2}\overline{U_iU_iS_m}\end{aligned} \tag{A72}$$

Next, the extra dissipation due to the particles is assumed to be proportional to the extra energy production. Thus, we

Continuity equation: $\frac{\partial}{\partial x_j}\rho\overline{U_j} = \overline{S_m}$

Transport equation: $\frac{\partial}{\partial x_j}\rho\overline{U_j}\Phi = \frac{\partial}{\partial x_j}\frac{\mu_t}{\sigma_\Phi}\frac{\partial\bar{\Phi}}{\partial x_j} + \bar{S}_\Phi$

Φ	$\bar{S}_\Phi$ (turbulence model)	$\bar{S}_\Phi = \bar{S}_{p\Phi} + \bar{S}_{m\Phi}$ (extra source terms)
U_i	$\frac{\partial}{\partial x_i}(P + \frac{2}{3}k) - \frac{\partial}{\partial x_i}\frac{2}{3}\mu_t\frac{\partial\overline{U_j}}{\partial x_j} + \overline{S_{U_i}}$	$S_{pU_i} = \langle S_p n - m_p[\frac{dV_i}{dt} - g_i]\rangle$
		$S_{mU_i} = n\langle S_m V_i\rangle$
k	$G - C_D\rho\varepsilon + S_k$	$S_{pk} = \overline{S'_{pU_i}u'_i}$
		$S_{mk} = \overline{S_{mU'_i}u'_i} + \frac{1}{2}\bar{U}_i\bar{U}_i\bar{S}_m - \frac{1}{2}\overline{U_iU_iS_m}$
ε	$C_1\frac{\varepsilon}{k}G - C_2\rho\frac{\varepsilon^2}{k} + S_\varepsilon$	$S_\varepsilon = C_{\varepsilon3}\frac{\varepsilon}{k}S_k$
c_pT	S_H	$S_{pH} = -n\langle L\dot{m} + Q_L\rangle$
		$S_{mH} = n\langle\dot{m}C_{vap}(T_S - T_0)\rangle$
y	S_m	$S_m = n\langle\dot{m}\rangle$
$\overline{\theta'^2}$	$C_{\theta1}\mu_t\frac{\partial\bar{\theta}}{\partial x_j}\frac{\partial\bar{\theta}}{\partial x_j} - C_{\theta2}\rho\frac{\varepsilon}{k}\overline{\theta'^2} + S_{\theta'}$	$S_{\theta'} = \overline{S'_\theta\theta'} + \bar{\theta}\bar{\theta}\bar{S}_m + \overline{\theta\theta S_m}$

obtain a source term $S_{p\varepsilon}$ for the dissipation ε reading as:

$$S_{p\varepsilon} = C_{\varepsilon3}\frac{\varepsilon}{k}S_{pk} \tag{A73}$$

in which ε/k is the inverse of a characteristic time required for dimensional reasons, and $C_{\varepsilon3}$ is a new constant. In the presence of vaporisation, we similarly obtain a new extra-source $S_{m\epsilon}$ which is modelled as in Eq. (A73) with S_{pk} replaced by S_{mk}. The equation for the rate of dissipation then reads as:

$$\frac{\partial}{\partial x_j}\left(\rho\bar{U}_j\varepsilon\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_T}{\sigma_\varepsilon}\right)\left(\frac{\partial\varepsilon}{\partial x_j}\right) + \boldsymbol{S}_\varepsilon \tag{A74}$$

in which:

$$\boldsymbol{S}_\varepsilon = C_1\frac{\varepsilon}{k}G - C_2\rho\frac{\varepsilon^2}{k} + S_\varepsilon \tag{A75}$$

with the extra source term:

$$S_\varepsilon = C_{\varepsilon3}\frac{\varepsilon}{k}\left(S_{pk} + S_{mk}\right) \tag{A76}$$

Let us finally consider the transport equation for a scalar fluctuation, designated θ. The modelling approach is similar to that for the previously discussed quantities so that we shall be more concise. It is found that:

$$\frac{\partial}{\partial x_j}\left(\rho\bar{U}_j\overline{\theta'^2}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_T}{\sigma_\theta}\right)\left(\frac{\partial\overline{\theta'^2}}{\partial x_j}\right) + \boldsymbol{S}_{\theta'} \tag{A77}$$

in which σ_θ is a constant close to 1 as is usual in such modelling.

Furthermore, we have:

$$\boldsymbol{S}_{\theta'} = C_{\theta1}\mu_T\frac{\partial\bar{\theta}}{\partial x_j}\frac{\partial\bar{\theta}}{\partial x_j} - C_{\theta2}\rho\frac{\varepsilon}{k}\overline{\theta'^2} + S_{\theta'} \tag{A78}$$

in which the extra source term reads as:

$$\begin{aligned} S_{\theta'} &= \overline{S'_\theta\theta'} - \overline{\theta'^2S_m} - \overline{\theta'^2S_m} - 2\overline{\theta\theta'S_m} \\ &= \overline{S_{\theta'}\theta'} + \bar{\theta}\bar{\theta}\bar{S}_m - \overline{\theta\theta S_m} \end{aligned} \tag{A79}$$

This appendix provides an overview of the way to obtain governing equations for the two-way coupling case, in thepresence of phase exchanges. Checking these equations would require much work for the reader, i.e. our presentation is rather complete but too concise for a precise understanding of all the details. A more complete explanation would take too much time, spoiling the balance between the different parts involved in this paper. Further details may, however, be found in Refs. [95, 114].

However, we believe that it is convenient to the reader to provide below a table giving a summary of the structure of the two-way governing equations.

Deleting all extra terms associated with heat and mass transfer exchanges, we then recover the simpler two-way coupling case discussed in Section 7. Deleting all extra terms, we recover the classical one-way governing equations of Section 2.

Appendix I. Description of hydrodynamic interactions

We assume that particles are solid and spherical, that the particle Reynolds number is small compared with 1 and, also, we neglect the effect of particle rotations.

Following Jeffrey and Onishi [120,121], particle hydrodynamic forces then read as:

$$\begin{bmatrix} \vec{F}(1) \\ \vec{F}(2) \end{bmatrix} = \mu \begin{bmatrix} A^{(1)(1)} & A^{(1)(2)} \\ A^{(2)(1)} & A^{(2)(2)} \end{bmatrix} \begin{bmatrix} \vec{V}_{\mathrm{p}}(1) - \vec{U}(\vec{x}(1)) \\ \vec{V}_{\mathrm{p}}(2) - \vec{U}(\vec{x}(2)) \end{bmatrix} \quad \text{(A80)}$$

in which $\vec{F}(\alpha)$ is the force exerted by particle α on the surrounding fluid, which can also be expressed as:

$$\vec{F}(\alpha) = -\int_{S_\alpha} \sigma.\vec{n}\ \mathrm{d}s \quad \text{(A81)}$$

where S_α designates the surface of the sphere, σ is the stress tensor, and $\vec{n}$ the unit vector perpendicular to the surface, pointing outward. Also, μ is the fluid viscosity, $A^{(\alpha)(\beta)}$ are the elements of the resistance matrix, $\vec{V}p(\alpha)$ is the translation velocity of particle α and $\vec{U}(\vec{x}(\alpha))$ is the fluid velocity at location $\vec{x}(\alpha)$. Furthermore, each element $A^{(\alpha)(\beta)}$ of the resistance matrix is actually a second-order tensor referring to particles α and β.

The resistance matrix is symmetric:

$$A_{ij}^{(\alpha)(\beta)} = A_{ji}^{(\alpha)(\beta)} \quad \text{(A82)}$$

and the exchange between two spheres with radii a_1 and a_2 must not change the hydrodynamical forces:

$$A^{(1)(2)}(\vec{r},\ a_1,\ a_2) = A^{(2)(1)}(-\vec{r},\ a_2,\ a_1) \quad \text{(A83)}$$

We may then write:

$$A_{ij}^{(\alpha)(\beta)}(\vec{r}) = X^{A^{(\alpha)(\beta)}}(\vec{r}) e_i e_j + Y^{A^{(\alpha)(\beta)}}(\vec{r})(\delta_{ij} - e_i.e_j) \quad \text{(A84)}$$

where $\vec{e} = \vec{r}/r$ is the unit vector between the sphere centres (oriented from α to β) and $X^{A^{(\alpha)(\beta)}}$ and $Y^{A^{(\alpha)(\beta)}}$ are scalar functions depending on the sphere radii and on the distance between their centres, called resistance functions.

We then make A dimensionless (but without changing the notation A, for convenience), according to:

$$A^{(\alpha)(\beta)} = \frac{A^{(\alpha)(\beta)}}{3\pi(a_\alpha + a_\beta)} \quad \text{(A85)}$$

$$s = \frac{2r}{a_\alpha + a_\beta} \quad \text{(A86)}$$

$$\lambda = \frac{a_\alpha}{a_\beta} \quad \text{(A87)}$$

The interaction force relation Eq. (A80) then can be rewritten as:

$$\begin{bmatrix} \vec{F}(1) \\ \vec{F}(2) \end{bmatrix} = 3\pi(a_1 + a_2)\mu \begin{bmatrix} A^{(1)(1)} & A^{(1)(2)} \\ A^{(2)(1)} & A^{(2)(2)} \end{bmatrix} \times \begin{bmatrix} \vec{V}_{\mathrm{p}}(1) - \vec{U}(\vec{x}(1)) \\ \vec{V}_{\mathrm{p}}(2) - \vec{U}(\vec{x}(2)) \end{bmatrix} \quad \text{(A88)}$$

At this stage, we are left with the evaluation of the functions $X^{A^{(\alpha)(\beta)}}$ and $Y^{A^{(\alpha)(\beta)}}$. These resistance functions have been determined by Jeffrey and Onishi [121], leading to functions which are different for X and Y, and depend on whether the particles are close or greatly separated. They are expressed as polynomial expansions in terms of powers of s (Eq. A86) and λ (Eq. A87).

For instance, in the case of separated spheres, we have:

$$X^{A^{(1)(1)}}(s,\ \lambda) = \sum_{k=0}^{\infty} f_{2k}(\lambda)(1+\lambda)^{-2k} s^{-2k} \quad \text{(A89)}$$

$$X^{A^{(1)(2)}}(s,\ \lambda) = \frac{-2}{1+\lambda} \sum_{k=0}^{\infty} f_{2k+1}(\lambda)(1+\lambda)^{-2k-1} s^{-2k-1} \quad \text{(A90)}$$

in which:

$$f_0 = 1 \quad \text{(A91)}$$

$$f_1 = 3\lambda \quad \text{(A92)}$$

…

$$f_6 = 16\lambda + 108\lambda^2 + 281\lambda^3 + 648\lambda^4 + 144\lambda^5 \quad \text{(A93)}$$

…

Explicit expressions for the resistance functions may be rather easily obtained by means of symbolic computations, for instance by using the formal calculus software Maple.

To provide the reader with explicit expressions, let us consider the case of two identical (same nature, same radius) particles, with $a_\alpha = a_\beta$, i.e. $\lambda = 1$. In the separated sphere approximation, we then obtain:

$$X^{A^{(1)(1)}} = 1 + \frac{9}{4}s^{-2} + \frac{93}{16}s^{-4} + \frac{1197}{64}s^{-6} + \ldots \quad \text{(A94)}$$

$$X^{A^{(1)(2)}} = -\frac{3}{2}s - \frac{19}{8}s^{-3} - \frac{387}{32}s^{-5} + \ldots \quad \text{(A95)}$$

$$Y^{A^{(1)(1)}} = 1 + \frac{9}{16}s^{-2} + \frac{465}{256}s^{-4} + \frac{14745}{4096}s^{-6} + \ldots \quad \text{(A96)}$$

$$Y^{A^{(1)(1)}} = -\frac{3}{4}s - \frac{59}{64}s^{-3} - \frac{2259}{1024}s^{-5} + \ldots \tag{A97}$$

and, in the case of the close sphere approximation, we have:

$$X^{A^{(1)(1)}} = \frac{1}{4}\frac{1}{1-4s^{-2}} - \frac{9}{40}\ln\left(\frac{1}{1-4s^{-2}}\right) - \frac{3}{112}\ln\left(\frac{1}{1-4s^{-2}}\right)\ln\left(\frac{1}{1-4s^{-2}}\right) + \frac{3}{4} + \frac{17}{10}s^{-2} + \frac{127}{560}s^{-4} - \frac{4057}{2240}s^{-6} + \ldots \tag{A98}$$

$$X^{A^{(1)(2)}} = \frac{1}{2}\frac{1}{s(1-4s^{-2})} - \frac{9}{40}\ln\left(\frac{s+2}{s-2}\right) - \frac{3}{112}\ln\left(\frac{1}{1-4s^{-2}}\right)\ln\left(\frac{s+2}{s-2}\right) + \frac{1}{140}s^{-1} + \frac{151}{280}s^{-3} + \frac{8077}{5600}s^{-5} + \ldots \tag{A99}$$

$$Y^{A^{(1)(1)}} = -\frac{1}{6}\ln(s-2) + 0.9951846 + \ldots \tag{A100}$$

$$Y^{A^{(1)(2)}} = \frac{1}{6}\ln(s-2) - 0.271199 + \ldots \tag{A101}$$

By studying these expressions, we found that $s = 2.5$ provides a good criterion as the frontier between the two limiting regimes of separated and close sphere approximations.

For three spheres (and more than three spheres), the situation appears to be much more complex than in the case of two particles, due to difficulties encountered in the analytical construction of the resistance matrix. However, under reasonable assumptions and following Durlofsky et al. [122], it remains possible to define a mobility matrix, which leads to a resistance matrix by inversion.

Following Durlofsky et al. [122], we then have a mobility matrix which reads as:

$$M = \begin{bmatrix} m^{(\alpha)(\alpha)} & m^{(\alpha)(\beta)} & m^{(\alpha)(\gamma)} & . \\ m^{(\beta)(\alpha)} & m^{(\beta)(\beta)} & m^{(\beta)(\gamma)} & . \\ m^{(\gamma)(\alpha)} & m^{(\gamma)(\beta)} & m^{(\gamma)(\gamma)} & . \\ . & . & . & . \end{bmatrix} \tag{A102}$$

in which the elements are second-order tensors given by:

$$m_{ij}^{(\alpha)(\beta)}(\vec{r}) = x_{\alpha\beta}^{m}(\vec{r})e_i.e_j + y_{\alpha\beta}^{m}(\vec{r})(\delta_{ij} - e_i.e_j) \tag{A103}$$

In a so-called fourth-order approximation, Durlofsky et al. established that:

$$x_{\alpha\alpha}^{m} = x_{\beta\beta}^{m} = 1 \tag{A104}$$

$$x_{\alpha\beta}^{m} = x_{\beta\alpha}^{m} = \frac{3}{2}s^{-1} - s^{-3} \tag{A105}$$

$$y_{\alpha\alpha}^{m} = y_{\beta\beta}^{m} = 1 \tag{A106}$$

$$y_{\alpha\beta}^{m} = y_{\beta\alpha}^{m} = \frac{3}{4}s^{-1} + \frac{1}{2}s^{-3} \tag{A107}$$

$$m_{11}^{(\alpha)(\alpha)} = m_{22}^{(\alpha)(\alpha)} = 1 \tag{A108}$$

$$m_{12}^{(\alpha)(\alpha)} = m_{21}^{(\alpha)(\alpha)} = 0 \tag{A109}$$

(while higher-order approximations would involve unknown terms).

In this approximation, the mobility matrix is well defined. It is also positive definite and symmetric, so that we can obtain its inverse, the resistance matrix, by using a Cholesky factorisation.

Appendix J. Equation of motion with hydrodynamic interactions

As an example, let us consider the case of sedimenting particles in a fluid at rest, in the Stokes regime. Then no fluid velocity is involved in the equation of motion of particles. For an isolated single particle, the equation of motion reads as:

$$\rho_p \frac{d\mathbf{V}_p}{dt} = \frac{3}{4}\frac{1}{d}\rho_f C_D \mathbf{V}_p|\mathbf{V}_p| + (\rho_p - \rho_f)\vec{\mathbf{g}} \tag{A110}$$

With hydrodynamic interactions it is generalised to:

$$\rho_p \frac{d\mathbf{V}_p}{dt} = \frac{3}{4}\frac{1}{d}\rho_f C_D \mathbf{V}_p\mathbf{F}_I + (\rho_p - \rho_f)\vec{\mathbf{g}} \tag{A111}$$

in which F_I possesses the same dimension as a velocity and incorporates the action on the tracked particle of another particle in its vicinity.

In the case of two spheres, we then obtain a system of two coupled equations reading as:

$$\frac{d}{dt}\begin{bmatrix}\vec{V}_p(\alpha)\\ \vec{V}_p(\beta)\end{bmatrix} = \frac{3}{4d}\frac{\rho_f}{\rho_p}\begin{bmatrix}A^{(1)(1)} & A^{(1)(2)}\\ A^{(2)(1)} & A^{(2)(2)}\end{bmatrix} \times \begin{bmatrix}C_D(\alpha)\vec{\mathbf{V}}_p(\alpha) & |\vec{\mathbf{V}}_p(\alpha)|\\ C_D(\beta)\vec{\mathbf{V}}_p(\beta) & |\vec{\mathbf{V}}_p(\beta)|\end{bmatrix} + (1 - \frac{\rho_f}{\rho_p})\vec{\mathbf{g}} \tag{A112}$$

When the distance between the two spheres is greater than a length scale L_i (taken as equal to 50 times the larger particle diameter), then interactions are negligible and the matrix A reduces to unity. The system (A112) may be integrated by using a fourth-order Runge–Kutta scheme.

More generally, for n interacting particles, we have to

integrate:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\vec{\mathbf{V}}_{\mathrm{p}}(k_1)\\ \ldots.\\ \vec{\mathbf{V}}_{\mathrm{p}}(k_i)\\ \ldots.\\ \vec{\mathbf{V}}_{\mathrm{p}}(k_n)\end{bmatrix}=\left(1-\frac{\rho_{\mathrm{f}}}{\rho_{\mathrm{p}}}\right)\vec{\mathbf{g}}$$

$$-\frac{3\rho_{\mathrm{f}}}{4\rho_{\mathrm{p}}d}\begin{bmatrix}R^{(1)(1)} & . & R^{(1)(j)} & . & R^{(1)(n)}\\ \ldots. & . & \ldots. & . & \ldots.\\ R^{(i)(1)} & . & R^{(i)(j)} & . & R^{(i)(n)}\\ \ldots. & . & \ldots. & . & \ldots.\\ R^{(n)(1)} & . & R^{(n)(j)} & . & R^{(n)(n)}\end{bmatrix} \tag{A113}$$

$$\times\begin{bmatrix}C_{\mathrm{D}}(k_1)\vec{U}_{\mathrm{rel}}(k_1)|\vec{U}_{\mathrm{rel}}(k_1)|\\ C_{\mathrm{D}}(k_j)\vec{U}_{\mathrm{rel}}(k_j)|\vec{U}_{\mathrm{rel}}(k_j)|\\ C_{\mathrm{D}}(k_n)\vec{U}_{\mathrm{rel}}(k_n)|\vec{U}_{\mathrm{rel}}(k_n)|\end{bmatrix}$$

References

[1] Wallis GB. One dimensional two-phase flow. New York: McGraw-Hill, 1969.

[2] Gouesbet G. Particules discrètes et défense. Conférence plénière d'introduction à la journée 'Aérosols et Défense' tenue dans le cadre des 4èmes journées d'étude sur les aérosols, GAMS-COFERA. Centre d'Etudes du Bouchet, Vert-le-Petit, 2 déc, Proceedings, 1987.

[3] Gouesbet G, Desjonquères P, Berlemont A. Eulerian and Lagrangian approaches to turbulent dispersion of particles, International seminar on transient phenomena. In: Afgan NH, editor. Multiphase flow, organized by the International Center For Heat and Mass Transfer, Dubrovnik, 24–30 May 1987. Hemisphere, 1988:247–271.

[4] Gouesbet G, Berlemont A, Desjonquères P. Prediction and simulation of the behaviour of discrete particles transported by turbulent flows. Chemical Reactivity in Liquids: Fundamental Aspects. 42nd International meeting of the société de Chimie Physique, Paris, 7–11 September 1987. New York: Plenum, 1988:607–616.

[5] Berlemont A, Simonin O, Sommerfeld M. Validation of inter particle collision models based on large eddy simulation. ASME/JSME Int. Conf. on Gas-Solid Flows, Hilton Head, SC, 13–18 August, Proceedings FED. Vol. 228, 1995:359–369.

[6] Yeung PK, Pope SB. Lagrangian statistics from direct numerical simulations of istotropic turbulence. J Fluid Mech 1989:207.

[7] Elghobashi SE, Truesdell GC. On the two-way interaction between homogeneous turbulence and dispersed solid particles. I: Turbulence modification. Phys Fluids A 1993;5:1790–1801.

[8] Wang LP, Maxey MR. Settling velocity and concentration distribution of heavy particles in homogeneous isotropic turbulence. J Fluid Mech 1993;256:27–68.

[9] Eaton JK, Fessler JR. Preferential concentration of particles by turbulence. Int J Multiphase Flow 1994;20:169–209.

[10] Squires KD, Eaton JK. Particle response and turbulence modification in isotropic turbulence. Phys Fluids A 1990;2:1191–1203.

[11] Deutsch E, Simonin O. Large eddy simulation applied on the modelling of particulate transport coefficients in turbulent two phase flows. 8th Symp. on turbulent Shear Flows, 9–11 September, Munich, Germany, 1991.

[12] Wang Q, Squires KD. Large eddy simulation of particle laden turbulent channel flow. Phys Fluids 1996;8:1207–1223.

[13] Berlemont A, Gouesbet G. Prediction of the turbulent round free jet, including velocities correlations, by means of a simplified second-order closure scheme. Letters to Heat and Mass Transfer 1981;8:207–217.

[14] Berlemont A, Gouesbet G. The dispersion of a cloud of particles released in a fully developed pipe flow, using the code DISCO-1. Letters in Heat and Mass Transfer 1982;9:11–19.

[15] Berlemont A, Picart A, Gouesbet G. Prediction of turbulence fields and particles dispersion using the code DISCO-2. In: Taylor C, Johnson JA, Smith WR, editors. Computational techniques for fluid flow, 5th volume in the series on recent advances in numerical methods in fluids. Pineridge Press, 1986:281–313.

[16] Picart A, Berlemont A, Gouesbet G. Modelling and predicting turbulence fields and the dispersion of discrete particles transported by turbulent flows. International Journal of Multiphase Flows 1986;12:237–261.

[17] Gouesbet G, Berlemont A. Prediction of turbulence fields, including fluctuating velocities correlations and approximate spectra by means of a simplified second-order closure scheme: the round free jet and developing pipe flow. Numerical methods in laminar and turbulent flows conferences, Venice, 13–16 July. Proceedings. Pineridge Press, 1981:205–216.

[18] Gossman AD, Ideriah PJK. Teach-T. London: Department of Mechanical Engineering, Imperial College of Science and Technology, 1976.

[19] Rodi W. Turbulence models for environmental problems. Prediction methods for turbulent flows. Von Karman Institute for Fluids Dynamics. Lecture Series 1979-2, 15–19 January 1979.

[20] Berlemont A, Gouesbet G. Prediction of turbulence characteristics including fluctuating velocity variances, by use of a (k–ε) model and second-order closure relations with the aid of general tensor calculus: the fully developed pipe flow and the round free jet. Internal Report TTI/BG/80/01/II 1980.

[21] Picart A. Le code DISCO-2 pour la prédiction du comportement de particules dans un écoulement turbulent. Thèse de 3ème cycle, Rouen, 1984.

[22] Hinze JO. Turbulence, 2nd ed. New York: McGraw-Hill, 1975.

[23] Frenkiel FN. Etude statistique de la turbulence—fonctions spectrales et coefficients de corrélation. Rapport technique, ONERA 34, 1948.

[24] Gouesbet G, Berlemont A, Picart A. On the Tchen's theory of discrete particles dispersion: can dense discrete particles

disperse faster than fluid particles?. Letters in Heat and Mass Transfer 1982;9:407–419.
[25] Basset AB. A treatise on hydrodynamics. Cambridge: Deighton, Bell and Co, 1984 (originally published by George Bell and Sons, London, 1888.
[26] Gouesbet G, Desjonquères P, Berlemont A. On the equation of motion of discrete particles in fluids. Basset's work revisited. Internal Report MADO/GDB/9/84/IX 1984.
[27] Boussinesq J. Théorie analytique de la chaleur. Paris, 1903.
[28] Gouesbet G, Julien B, Desjonquères P, Berlemont A. On the equation of motion of discrete particles in fluids. Boussinesq's work revisited. Internal Report MADO/GJDB/12/84/XII, 1984.
[29] Oseen CW. Neuer methoden and engebnisse inder hydodynamic. Leipzig: Acad. Verglasgesellschaft, 1927.
[30] Stokes GG. On the effect of the inertial friction of fluids on the motion of pendulums. Trans Cambridge Phil Soc 1851;9.
[31] Tchen CM. Mean value and correlation problems connected with the motion of small particles suspended in a turbulent fluid. Ph.D. University of Delft–Martinus Nijhoff, The Hague, 1947.
[32] Corrsin S, Lumley J. On the equation of motion for a particle in turbulent fluid. Appl Sci Res 1991;6:114–116.
[33] Buevich AY. Motion resistance of a particle suspended in a turbulent medium. Fluid Dynamics 1966:1119.
[34] Maxey MR, Riley JJ. Equation of motion of a small rigid sphere in a nonuniform flow. Phys Fluids 1983;26:883–889.
[35] Riley JJ. Ph.D. Thesis, The Johns Hopkins University, Baltimore, MD, 1971.
[36] Gatignol R. The Faxén formulae for a rigid particle in an unsteady non-uniform Stokes flow. Journal de Mécanique Théorique et Appliquée 1983;1:143–160.
[37] Clift R, Grace JR, Weber ME. Bubbles, drops and particles. New York: Academic Press, 1978.
[38] Odar F, Hamilton WS. Forces on a sphere accelerating in a viscous fluid. J Fluid Mech 1964;18:302–314.
[39] Minier JP, Pozorski J. Analysis of existing Lagrangian models and new propositions for particle dispersion in homogeneous stationary turbulence. LNH/EDF, HE44/92.29 1992.
[40] Stokes DE. Particle dispersion in turbulent gas flows. Proceedings of the 2nd Int. Conf. on Multiphase Flows '95. Kyoto, PL2-1-PL2-13, 1995.
[41] Rubinow SI, Keller JB. The transverse force on a spinning sphere moving in a viscous fluid. J Fluid Mechanics 1961;11:447–459.
[42] Julien B, Gouesbet A, Desjonquères P, Berlemont A, On the equation of motion of discrete particles in fluids. Rubinow, Keller and Saffman's work revisited. Internal Report GCA/JGDB:5/85/IV, 1985.
[43] Saffman PG. The lift on a small sphere in a slow shear flow. J Fluid Mech 1965;22:358–398.
[44] Bretherton FP. The motion of rigid particles in a shear flow at low Reynolds number. J Fluid Mech 1982;14:284.
[45] Saffman PG. The lift on a small sphere in a slow shear flow (corrigendum). J Fluid Mech 1968;31:624.
[46] Arnason G. Measurements of particle dispersion in turbulent pipe flow. Ph.D. Thesis, Washington State University, 1982.
[47] Desjonquères P, Gouesbet G, Berlemont A, Picart A. Dispersion of discrete particles by continuous turbulent motion. New results and discussions. Physics of Fluids 1986;29:2147–2151.
[48] Gouesbet G, Berlemont A. A three dimensional dispersion model for the behaviour of vaporizing particles in a turbulent fluid. Sixth Biennial Symposium on Turbulence, 8–10 Oct. University of Missouri, Rolla, MO, 1979.
[49] Gouesbet G, Berlemont A. Une approche dispersive pour la modélisation du comportement de particules dans un champ turbulent. C R Acad Sci A 1979; 242B.
[50] Gouesbet G, Berlemont A, Picart A. On the dispersion of discrete particles by continuous turbulent motions. Extensive discussion of the Tchen's theory, using a two-parameter family of Lagrangian correlation functions. Physics of Fluids 1984;27:827–837.
[51] Gouesbet G, Picart A, Berlemont A. Dispersion of discrete particles by turbulent continuous motions using a Frenkiel's family of Lagrangian correlation functions, in the non-discrete approach. Proceedings of the Third International Conference on Numerical Methods in Laminar and Turbulent Flow, 8–11 August, The University of Washington, Seattle, WA, 1983.
[52] Batchelor GK. Diffusion in a field of homogeneous turbulence I. Eulerian analysis. Austr J Sci Res 1949;2:437–450.
[53] Taylor GI. Diffusion by continuous movement. Proc London, Math Soc 1921;20:196.
[54] Taylor GI. Statistical theory of turbulence. J Math and Phys Sci 1935;421–478.
[55] Kampé de Fériet MJ. Les fonctions aléatoires stationnaires et la théorie statistique de la turbulence homogène. J Ann Soc Sci Bruxelles, Ser I 1939;59:145.
[56] Picart A, Berlemont A, Gouesbet G. De l'influence du terme de Basset sur la dispersion de particules discrètes dans le cadre de la théorie de Tchen. C R Acad Sci, Paris, Série II, 1982:305–308, T 295.
[57] Yudine MI. Physical considerations on heavy-particle dispersion. Advances in Geophysics 1959;6:185–191.
[58] Csanady GT. Turbulent diffusion of heavy particles with atmosphere. J Atmos Sci 1963;20:201–208.
[59] Wells MR, Stock DE. The effects of crossing trajectories on the dispersion of particles in a turbulent fow. J Fluid Mech 1983;136:31–36.
[60] Berlemont A, Gouesbet G. Prediction of the behaviour of a cloud of discrete particles released in a fully developed turbulent pipe flow, using a dispersive approach. Proceedings of a Conference on Numerical Methods in Laminar and Turbulent Flow, 13–16 July, Venice, 1981.
[61] Berlemont A, Picart A, Gouesbet G. The code DISCO-2 for predicting the behaviour of discrete particles in turbulent flows, and its comparisons against the code DISCO-1, and experiments. Third International Conference on Numerical Methods in Laminal and Turbulent Flow, 8–11 August. The University of Washington, Seattle, WA, 1983:963–973.
[62] Reeks MW. On the continuum equation for dispersed particles in non uniform flows. Phys. Fluids A 1992;4.
[63] Simonin O. Combustion and turbulence in two phase flows: continuum modelling of dispersed two phase flows. Lecture series 1996-02, Von Karman Institute for Fluid Dynamics, 1996.
[64] Simonin O, Deutsch E, Minier JP. Eulerian prediction of the fluid/particle correlated motion in turbulent two phase flows. Applied Scientific Research 1993;51:275–283.
[65] Reeks MW. On a kinetic equation for the transport of particles in turbulent flows. Phys Fluids A 1991;3.

[66] Simonin O. Second moment prediction of dispersed phase turbulence in particle laden flows. 8th Symp. on Turbulent Shear Flow, Munich, Germany, 1991.
[67] Gosman AD, Ioannides IE. Aspects of computer simulation of liquid-fuelled combustors. AIAA J 1981;81:0323.
[68] Durst F, Milojevic D, Shönung B. Eulerian and Lagrangian predictions of particulate two-phase flows: a numerical study. Appl Math Modelling 1984;8:101–105.
[69] Sommerfeld M. Particle dispersion in turbulent flow: the effect of particle size distribution. Part Syst Charact 1990;7:209–220.
[70] Graham DI, James PW. Turbulent dispersion of particles using eddy interaction models. Int J Multiphase Flow 1996;22:157–175.
[71] Wang LP, Stock DE. Numerical simulation of heavy particle dispersion: time-step and non linear drag consideration. J Fluids Engng 1992;114:100–106.
[72] Ormancey A. Simulation du comportement de particle dans des écoulements turbulents. Thèse de 3ème cycle, Ecole des Mines de Paris, 1984.
[73] Ormancey A, Martinon A. Prediction of particle dispersion in turbulent flows. Physico-Chemical Hydrodynamics 1984;5:229–244.
[74] Zhou Q, Leschziner MA. A Lagrangian particle dispersion model based on a time-correlated approach. FED Gas Solid Flows ASME 1991;121:255–260.
[75] Desjonquères P, Berlemont A, Gouesbet G. A Lagrangian approach for the prediction of particle dispersion in turbulent flows. J Aerosol Sci 1988;19:99–103.
[76] Desjonquères P, Berlemont A, Gouesbet G. Lagrangian simulation of a two-phase turbulent round jet. Proceedings of the Sixth Symposium on Turbulent Shear Flows, 7–9 September Toulouse, France, 1987:21-3-1/21-3-5.
[77] Berlemont A, Gouesbet G, Desjonquères P. Lagrangian simulation of particle dispersion. Lecture Notes in Engineering 1987;40:815–823.
[78] Berlemont A, Desjonquères P, Gouesbet G. Particle Lagrangian simulation in turbulent flows. International Journal of Multiphase Flows 1990;16:19–34.
[79] Berlemont A, Desjonquères P, Gouesbet G. Lagrangian simulation of turbulence modifications in three particle laden turbulent round jets. Proceedings of the ASME International Symposium on Turbulence Modifications in Dispersed Multiphase Flows, 9–12 July, San Diego, CA, 1989.
[80] Berlemont A, Desjonquères P, Gouesbet G. 3D turbulent dispersion in non-homogeneous magnetic field. Proceedings of an International Conference on Mechanics of Two-phase Flows, 12–15 June, Taipei, Taiwan, 1989:19–23.
[81] Berlemont A, Desjonquères P, Gouesbet G. Particle turbulent dispersion in 3D magnetic fields using a Lagrangian approach. Particle and Particle Systems Characterization 1991;8:151–158.
[82] Modarress D, Tan H, Elgobashi S. Two-component LDA measurement in a two-phase turbulent jet. AIAA J 1984;22:624.
[83] Shuen JS, Solomon ASP, Zhang QF, Faeth GM. Structure of particle-laden jets: measurements and predictions. Report AIAA 84-0038, 1985.
[84] Hishida K, Kaeneko K, Maeda M. Turbulence structure of a gas-solid two phase circular jet. Trans JSME Ser B 1985;51:2330–2337.
[85] Yuan Z, Michaelides E. Turbulence modulation in particle flows. A theoretical approach. Int J Multiphase Flow 1992;18:779–785.
[86] Hanjalic K, Launder BE, Shiestel R. Multiple time scale concepts in turbulent transport modelling. 2nd Turbulent Shear Flows. Berlin: Springer, 1980:36–49.
[87] Gore RA, Crowe CT. Effect of particle size on modulating turbulent intensity. Int J Multiphase Flow 1989;86:491–511.
[88] Sato Y. Turbulence structure and modelling of dispersed two phase flows. Ph.D. thesis, Dept. Mech. Engng, Keio University, Japan, 1996.
[89] Crowe CT, Sharma MP, Stock DE. The particle source in cell (PSI-cell) method for gas-droplet flows. J Fluid Engng 1977;99:325–332.
[90] Kohnen G, Rüger M, Sommerfeld M. Convergence behaviour for numerical calculations by the Euler/Lagrange method for strongly coupled phases. ASME Symposium on Numerical Methods in Multiphase Flows FED 1994;185:191–202.
[91] Milojevic D, Bôrner T, Wenneberg D, Berlemont A, Desjonqueres P, Avila R. A comparison of six two phase flow models for the prediction of turbulent gas particle flows in jets and channels. In: Afgan NH, editor. International Seminar on Transient Phenomena in Mult. Flow, Int. Center for Heat and Mass Transfer, Dubrovnik, Hemisphere, 1988:823–840.
[92] Spalding DB. Combustion and Mass Transfer. Oxford: Pergamon Press, 1979.
[93] Linan A. Theory of droplet vaporisation and combustion. Ecole d'été sur les problèmes non linéaires appliqués. Lecture in CEA-INRIA-EDF, 1985.
[94] Prakash S, Sirignano WA. Theory of convective droplet vaporization with unsteady heat transfer in the circulation liquid phase. Int J Heat Mass Transfer 1980;23:253–268.
[95] Aggarwal SK, Tong AY, Sirignano WA. A comparison of vaporization models in spray combustion. AIAA J 1984;22:10.
[96] Renksizbulut M, Haywood RJ. Transient droplet evaporation with variable properties in an internal circulation at intermediate Reynolds numbers. Int J Multiphase Flow 1988;14:189–202.
[97] Berlemont A, Grancher MS, Gouesbet G. On the Lagrangian simulation of turbulence influence on droplet evaporation. Int J Heat and Mass Transfer 1991;34:2805–2812.
[98] Grancher MS, Gouesbet G, Berlemont A. Lagrangian simulation of heat and mass transfer in dispersed two-phase flows. In: Rodi, G, editor. Engineering turbulence modelling and experiments. Amsterdam: Elsevier, 1990:867–875.
[99] Berlemont A, Grancher MS, Gouesbet G. Heat and mass transfer coupling between vaporizing droplets and turbulence using a Lagrangian approach. Int J Heat and Mass Transfer 1995;38:3023–3034.
[100] Crowe CT. On the relative importance of particle particle collisions in gas particle flows. Proc. Conf on Gas Borne Particle, paper C78/81, 1981:135–137.
[101] Laviéville J, Deutsch E, Simonin O. Large eddy simulation of interaction between colliding particles and a homogeneous isotropic turbulence field. 6th Symp. on Gas–Solid Flows ASME FED 288, 1995.
[102] Laviéville J. Simulation numérique et modélisation des interactions entre l'entraînement par la turbulence et les collisions

interparticulaires en écoulements gaz-solide. Thèse de l'Université de Rouen, 1997.
[103] Sommerfeld M. The importance of inter-particle collisions in horizontal gas–solid channel flows. In Stock DE, Tsuji Y, Jurewicz JT, Reeks MW, Gautam M, editors. Gas-solid flows. ASME FED 228, 1995.
[104] Oesterle B, Petitjean A. Simulation of particle-to-particle interaction in gas–solid flows. Int J Multiphase Flow 1993;19:199–211.
[105] Berlemont A, Benoist F, Gouesbet G. Influence of collisions on particle fluctuating velocities using a Lagrangian approach. Int Symp Num Method for Multiphase Flows, ASME, FED 1994;185:23–28.
[106] Chauvin C, Gouesbet G, Berlemont A. Influence of particle interactions on particle dispersion in low turbulence field. In: Rodi W, Martelli F, editors. Proceedings of the 2nd Int. Symp. on Eng. turb. Mod. and Meas., Florence, Italy. Amsterdam: Elsevier, 1993:915–925.
[107] Berlemont A, Chang Z, Gouesbet G. Une approche lagrangienne pour la simulation d'interactions particule/particule en écoulement. La Houille Blanche 1996;1–2:57–63.
[108] Berlemont A, Chauvin C, Gouesbet G. On hydrodynamic interactions between sedimenting spheres. 3rd World Conf. on Exp. Heat Trans., Fluid Mech. and Thermodynamics, November, Honolulu, HI, 1993.
[109] Berlemont A, Desjonquères P, Gouesbet G. Particle tracking in turbulent flows. Proceedings of ASME Gas–Solid Flows Conference, 20–24 June, Washington, DC, Vol. 166, 1993:121–131.
[110] Berlemont A, Simonin O, Sommerfeld M. Validation of inter-particle collision models based on large eddy simulation. ASME/JSME, Int. Conf. on Gas–Solid Flows, 13–18 August, Hilton Head, SC, 1995.
[111] Berlemont A. Euler–Lagrange approach: modelling particle/particle interactions. Numerical modelling and prediction of dispersed two phase flows, Invited paper ERCOFTAC Summer School, 26–29 September, Merseburg, Germany, 1995.
[112] Sawford BL. Reynolds number effects in Lagrangian stochastic models of turbulent dispersion. Phys Fluids A 1991;3.
[113] Tennekes H, Lumley JL. A first course in turbulence. Cambridge, MA: MIT Press, 1972.
[114] Shirolkar JS, Coimbra CFM, McQuay MQ. Fundamental aspects of modeling turbulent particle in dilute flows. Progress in Energy and Comb Sci 1996;22:363.
[115] Snyder WH, Lumley JL. J Fluid Mech 1971;48:41–71.
[116] Gouesbet G, Berlemont A, Desjonqueres P, Gréhan G. On modelling and measurement problems in the study of turbulent two-phase flows with particles. Proceedings of 6th Workshop on Two Phase Flow Prediction. LSTM, University of Erlangen, Germany, 1993.
[117] Faeth GM. Current status of droplet and liquid combustion. Prog. Energy Combustion Science 1977;3:191–224.
[118] Grancher MS. Simulation de l'évaporation de gouttelettes en écoulement turbulent suivant une approche lagrangienne. Thèse de Doctorat, Université de Rouen, 1990.
[119] Hubbard GL, Denny VE, Mills AF. Droplet evaporation: effects of transient and variable properties. Int J Heat Mass Transfer 1975;18:1003–1008.
[120] Jeffrey DJ, Onishi Y. Calculation of the resistance and mobility functions for two unequal rigid spheres in low Reynolds number flow. J Fluid Mech 1984;139:261–290.
[121] Jeffrey DJ, Onishi Y. The forces and couples acting on two nearly touching spheres in low Reynolds number flow. J Applied Math Phys 1984;35:634.
[122] Durlofsky LF, Brady JF, Bossis GJ. Dynamic simulation of hydrodynamically interacting particles. Fluid Mech 1987;80:21–49.