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A comprehensive probability density function formalism for multiphase flows

MADHUSUDAN G. PAI† AND SHANKAR SUBRAMANIAM‡

Department of Mechanical Engineering, Iowa State University, Ames, IA 50011, USA

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A theoretical foundation for two widely used statistical representations of multiphase flows, namely the Eulerian–Eulerian (EE) and Lagrangian–Eulerian (LE) representations, is established in the framework of the probability density function (p.d.f.) formalism. Consistency relationships between fundamental statistical quantities in the EE and LE representations are rigorously established. It is shown that fundamental quantities in the two statistical representations bear an exact relationship to each other only under conditions of spatial homogeneity. Transport equations for the probability densities in each statistical representation are derived. Exact governing equations for the mean mass, mean momentum and second moment of velocity corresponding to the two statistical representations are derived from these transport equations. In particular, for the EE representation, the p.d.f. formalism is shown to naturally lead to the widely used ensemble-averaged equations for two-phase flows. Galilean-invariant combinations of unclosed terms in the governing equations that need to be modelled are clearly identified. The correspondence between unclosed terms in each statistical representation is established. Hybrid EE–LE computations can benefit from this correspondence, which serves in consistently transferring information from one representation to the other. Advantages and limitations of each statistical representation are identified. The results of this work can also serve as a guiding framework for direct numerical simulations of two-phase flows, which can now be exploited to precisely quantify unclosed terms in the governing equations in the two statistical representations.

1. Introduction

Statistical models of multiphase flow are useful because of the statistical variability inherent in most multiphase flow applications. Moreover, information from a single realization of a multiphase flow contains information that far exceeds the amount required for engineering purposes. Therefore, a statistical description of multiphase flows is of interest to the engineering community. Widely used statistical representations of two-phase flows can be broadly classified as Eulerian–Eulerian (EE) or Lagrangian–Eulerian (LE), depending on the reference frames underlying their formulation. Although, for simplicity, only two phases are considered, the statistical formalism developed in this work can be extended to multiphase flows.

By EE statistical representation we mean a statistical approach where both the continuous and dispersed phases are described in a common Eulerian reference frame as Eulerian random fields. A realization of this flow would correspond to a Navier–Stokes

† Present address: Center for Turbulence Research, Stanford University, Stanford, CA 94305, USA. E-mail address for correspondence: mpai@stanford.edu
‡ E-mail address: shankar@iastate.edu

solution for the flow in the whole domain with boundary conditions imposed at the phase interfaces, and where flow within the dispersed-phase elements (DPEs), two-way coupling and interfacial drag are implicitly treated in an exact manner. Ensemble-averaging several such realizations leads to the so-called two-fluid theory in which the two phases are represented in terms of the phasic means, such as the mean densities, volume fractions, mean momentum and second moment of velocity in each phase, with source terms in their corresponding transport equations representing interphase interactions. This EE representation is different from, and not to be confused with, the derivation of Eulerian moment equations from a distribution function based on a Lagrangian representation of the DPEs. A lucid account of this approach is given by Drew (1983) (see also Drew & Passman 1999) and extensions have been developed by Kataoka & Serizawa (1989). An example of an ensemble-averaged EE implementation for chemically reacting or inert multiphase flows is CFDLib (Kashiwa & Rauenzahn 1994; Kashiwa & Gaffney 2003).

In this work, the LE statistical representation refers to a statistical approach that represents the dispersed phase in a Lagrangian frame by a number density based on the location of DPE centres (in this work, the phrase 'dispersed-phase element' is a generic term used to denote either rigid particles, drops or bubbles). The origin of this representation can be traced back to Williams (1958) who proposed the droplet distribution function (d.d.f.) and derived the spray equation, which is the evolution equation for the d.d.f., from physical principles. In numerical implementations of the LE statistical approach, the spray equation is indirectly solved using Lagrangian particle-based methods. Generally, the two primary components of such a particle-method solution are (i) Lagrangian particles, with modelled drag and vaporization terms, that represent the d.d.f. and (ii) a single-phase Reynolds-averaged Navier–Stokes (RANS) closure for the carrier phase with additional source terms representing the effects of the dispersed phase. An example of such an approach is the KIVA series of codes (Amsden, O'Rourke & Butler 1989; Amsden 1993) used widely in the automotive industry.

It is natural to seek a probability density function (p.d.f.) formalism to describe two-phase flows, given their statistical variability. There have been recent studies by several authors (see, for instance, Pozorski & Minier 1999; Zhu *et al.* 2000; Minier & Peirano 2001; Peirano & Minier 2002) to extend p.d.f. methods, which have been successful in single-phase turbulent reactive flows (Lundgren 1969; O'Brien 1980; Pope 1985), to two-phase flows. Minier & Peirano (2001) used a stochastic process as the starting point for their p.d.f. formalism and derived implied evolution equations for the two-point fluid-dispersed-phase p.d.f., single-point fluid and dispersed-phase p.d.f.'s, and implied mean equations. Zhu *et al.* (2000) derived an evolution equation for the Eulerian joint p.d.f. for velocity and radius in the dispersed phase, and posited that this is identical to the evolution of the joint p.d.f. of velocity and radius in Williams' spray-equation formalism. The so-called 'kinetic equation' formalism for the p.d.f. of the dispersed-phase velocity has been studied by several researchers (see, for instance, Derevich & Zaichik 1988; Zaichik 1999; Reeks 1992). Reeks (1992) used the p.d.f. kinetic equation formalism to arrive at continuum equations that describe the dispersed phase in dilute particle-laden flows. In this approach, the acceleration term in the p.d.f. kinetic equation is simplified by assuming Stokes drag and the resulting unclosed phase space 'diffusion current' (Reeks 1991) is modelled (see Mashayek & Pandya 2003 for a review of the techniques used by various researchers to model this diffusion–current term).

Simonin (1996) proposed a kinetic equation for the probable number of particles in an infinitesimal volume in position and velocity phase space that is similar to the spray equation (see also Crowe 2005). He derived mean equations from the transport equation, while assuming that the dispersed-phase volume fraction can be simply related to the number density. Some researchers in the two-phase flow research community refer to these mean equations as 'Eulerian' closures, but this nomenclature is different from what we use in this work. Although the mean equations derived from the spray equation are indeed Eulerian quantities, they originate from a Lagrangian description, whereas there is a distinctly different EE approach to deriving 'Eulerian' mean equations for the two-phase flow.

It is noteworthy that researchers who studied the kinetic equation formalism attempt to make an important connection between kinetic theory and particle-laden flows. However, the several assumptions that the kinetic theory of gases is based upon fail to hold in almost all two-phase flows that are encountered in reality. The following considerations are unique to particle-laden flows and preclude a straightforward extension of kinetic theory to such flows:

(i) Large variation from one realization to another of the number of spray droplets in a macroscopic volume, and finite Knudsen number effects. Classical kinetic theory of molecular gases provides transport coefficients in the low Knudsen number limit where the separation of scales between the molecular mean free path and length scales characterizing macroscopic hydrodynamic variables results in a large number of molecules in a macroscopic volume. In sprays this separation of scales does not exist, and the Knudsen number can be large and vary spatially.

(ii) Non-negligible fluctuations of particle number about the mean,

(iii) Non-independence of particle positions that results in ordering-dependent multiparticle Liouville densities, and

(iv) Need for symmetrization of the multiparticle Liouville p.d.f. to arrive at unique single-particle densities (Subramaniam 2001).

Since the EE and LE statistical representations are essentially the description of a two-phase flow in two reference frames, it is natural to expect that these representations are related. A major challenge in describing two-phase flows, therefore, is to establish the precise relationship between these two modelling approaches. Furthermore, the conditions under which such a relationship holds, and the conditions under which they do not, need to be clearly established.

Establishing the exact form of the relationship between the two statistical representations has far-reaching implications. Subramaniam & O'Rourke (1998) noted that computations of some two-phase applications such as fuel sprays can potentially benefit by using the EE modelling approach in the near-nozzle region, and the LE approach in the dispersed spray region. Figure 1 shows a schematic illustration for a handover from an EE representation to a LE representation in a typical spray. Ning *et al.* (2007) have proposed a new spray model using the Eulerian–Lagrangian Spray and Atomization (ELSA) model after Blokkeel, Borghi & Barbeau (2003) in which an Eulerian description of the spray for the region close to the injector and a Lagrangian description in the dilute regions of the spray is employed. The transfer of information from the Eulerian to the Lagrangian description will require the knowledge of the relationships between corresponding statistics in the two representations. A pertinent question that arises in this context is how can information be transferred from one representation to the other. Clearly, the answer lies in the exact relationship between these two approaches, which will allow a consistent transfer of flow information at the common boundary of the two regions.

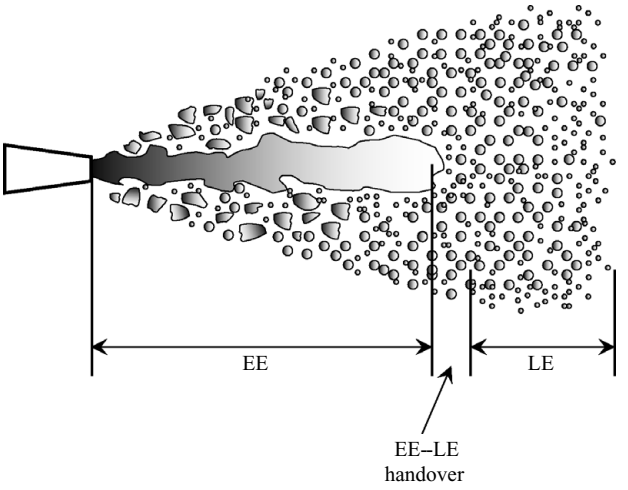

FIGURE 1. Schematic illustration of a typical spray indicating the region where a handover between the EE and the LE descriptions is appropriate. This handover requires consistency conditions to be satisfied between the two statistical representations at the common boundary of the two regions.

More importantly, the exact form of such a relationship also enables us to address several important, but hitherto unresolved, modelling issues such as

(i) How can model predictions from both approaches be compared with one another? If the EE and LE modelling approaches are individually employed to describe the same two-phase flow, then under what conditions can predictions of key two-phase flow statistics from either approach be directly compared?

(ii) How, and under what conditions, are the modelled terms in both approaches related, and how can this relationship be used to guide model development in both approaches?

The primary objective of this work is to address these fundamental issues related to the theoretical foundation for the statistical representation of two-phase flows. In order to achieve this objective, the foundation for the EE and the LE representations is first established in the context of the p.d.f. formalism using fundamental events and corresponding probabilities. It is shown in this work that the EE probabilistic formalism naturally leads to the ensemble-averaged equations of a two-phase flow. Although the LE formalism also results in mean equations, these equations are not identical to the averaged equations in the EE formalism. It is shown in this work that fundamental quantities in the EE and LE representations, such as the dispersed-phase volume fraction in the EE formalism and number density in the LE formalism, bear a simple relationship with each other only under restrictive conditions of spatial uniformity (or statistical homogeneity) of the two-phase flow. This renders the implied relationships between the EE and the LE statistical representations in the work of Simonin (1996) and Zhu *et al.* (2000) applicable only to a restricted class of two-phase flows. This work also identifies the correspondence between unclosed terms (by unclosed term we mean any term that is not directly expressible in terms of the unknowns of the governing equation, and therefore needs to be modelled; for instance, the interphase transfer of momentum is not directly expressible in terms of the phasic velocities without modelling the interphase force in terms of the slip velocity between the phases) in the phasic governing equations for the mean mass, mean momentum and

second moment equations in the two representations. This correspondence enables one to transfer information seamlessly from one representation to the other. The relationship between modelled terms is also useful in constructing improved models for the unclosed terms using data from direct numerical simulations (DNS) of two-phase flows. An important contribution of this work is the identification of Galilean-invariant (GI) combinations of unclosed interphase interaction terms that need to be modelled. The precise form of the unclosed terms is derived, thereby establishing a framework for appraising existing two-phase models and guiding future modelling efforts.

As noted earlier, some researchers have employed the Fokker–Planck (FP) equation as a starting point to derive a 'modelled' p.d.f. formalism for two-phase flows (Minier & Peirano 2001; Peirano & Minier 2002). The FP equation and the corresponding Langevin-like stochastic differential equation are attractive since they automatically guarantee realizability and boundary conditions are straightforward to impose. However, our goal in this work is to derive a model-free exact p.d.f. formalism for two-phase flows. We do recognize that ultimately the closure problem for the unclosed terms that arises in an exact p.d.f. formalism naturally lends itself to FP and Langevin-like closures. Nevertheless for the purposes of this study, we do not consider the modelled p.d.f. equation as an appropriate starting point.

The rest of the paper is organized as follows. The foundation for the EE statistical representation of a two-phase flow is established in § 2 by identifying fundamental events and corresponding probabilities. An important highlight of this section is the definition of the p.d.f. of instantaneous velocity conditional on the presence of a particular phase in a two-phase flow. The basis for the LE statistical representation is also presented and key results that are useful in the rest of the work are summarized in the same section. Relationships between fundamental quantities in the EE and LE statistical representations are developed in § 3. Evolution equations corresponding to the p.d.f. of instantaneous velocity conditional on the presence of each phase in the EE representation, and the droplet distribution function in the LE representation are derived in § 4. In § 5, these evolution equations are used to derive governing equations for the mean mass, mean momentum and second moment of velocity in each representation. In the same section, the correspondence between various unclosed terms in the governing equations is identified. GI forms of the unclosed terms in the governing equations which need to be modelled are also identified. Advantages and limitations of each approach in terms of the information content in each statistical representation are discussed in § 6. Section 7 summarizes the principal achievements and conclusions of this work.

2. Statistical representation of two-phase flows

The statistical representation of a two-phase flow using the EE and LE approaches is described. In the EE approach, the two-phase flow field is represented as a *random field* (Drew 1983; Zhang & Prosperetti 1994) while in the LE approach the dispersed phase is represented as a *marked point process* (Edwards & Marx 1996; Subramaniam 2001) imbedded in a carrier flow. While the ensemble-averaged equations in the EE representation have been reported in literature (Drew 1983), this work provides insight into the underlying p.d.f. framework. Fundamental events and corresponding probabilities associated with a two-phase flow in the EE and LE framework are developed in this section.

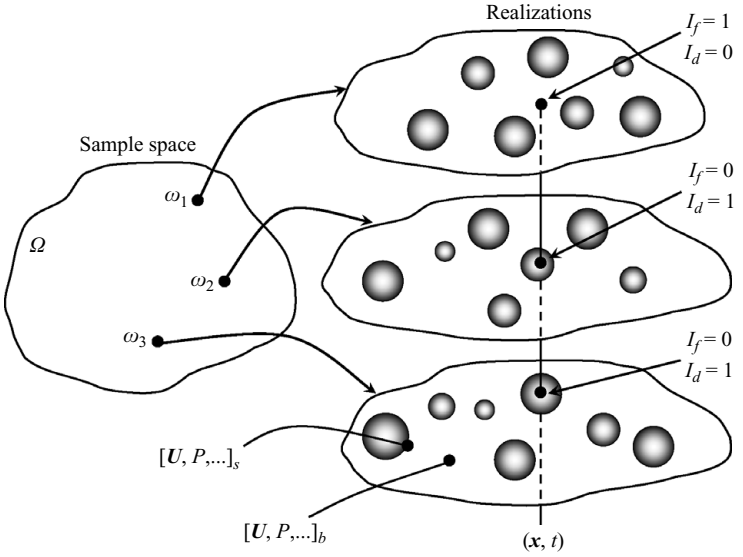

FIGURE 2. Schematic illustration of the sample space Ω of all possible realizations of a two-phase flow from which three realizations $\{\omega_1, \omega_2, \omega_3\}$ are shown. The indicator function $I_\beta(\boldsymbol{x}, t)$ at a point $(\boldsymbol{x}, t)$, where $\beta = \{f, d\}$, as defined in § 2.1 is shown for each of the three realizations. Also, primitive variables $\boldsymbol{U}$: velocity and P : pressure at the DPE surface (subscript s) and in the bulk (subscript b) are shown. As discussed in § 4, a single-point statistical representation cannot distinguish between these two locations in a two-phase flow.

2.1. *Random-field representation*

Consider a realization of a two-phase flow with two distinct thermodynamic phases: a carrier phase and a dispersed phase. Furthermore, for simplicity, the phrase 'two-phase flow' will refer to an isothermal two-phase flow with no scalars or reactions. Each realization can be thought of as an element of a sample space Ω, which is the space of all possible realizations (see figure 2). In a single realization, and at a single space–time location, the phases are distinguished using an indicator function $I_\beta(\boldsymbol{x}, t)$ for the βth phase, defined as

$$I_\beta(\boldsymbol{x}, t) = \begin{cases} 1 & \text{if } \boldsymbol{x} \text{ is in phase } \beta \text{ at time } t \\ 0 & \text{if } \boldsymbol{x} \text{ is not in phase } \beta \text{ at time } t. \end{cases} \tag{2.1}$$

In two-phase flows, the phase indicator functions satisfy the relation

$$\sum_{\beta=\{f,d\}} I_\beta(\boldsymbol{x}, t) = 1, \tag{2.2}$$

where f represents the carrier phase and d represents the dispersed phase, for all $(\boldsymbol{x}, t)$. The instantaneous two-phase velocity field $\boldsymbol{U}(\boldsymbol{x}, t)$, which is defined in both phases, is a vector field that is defined at each point $\boldsymbol{x}$ in the flow domain in physical space $\mathscr{D}$. Similarly $\rho(\boldsymbol{x}, t)$ is the thermodynamic mass density field that is defined in both phases. It is assumed that (i) the density difference between the two phases is sufficiently large so that the density field can be used to distinguish between the two phases (i.e. the thermodynamic state of the fluid is not close to the critical point) and (ii) the characteristic length scale of the interface over which this density change occurs is so small that in a continuum description the density changes discontinuously

at the interface. Since the phases are distinguished only by the indicator function, no information on shape or number of DPEs is available in this approach.

Different events can be used to characterize the state of a two-phase flow at a single space–time location $(\boldsymbol{x}, t)$, and each leads to different probabilities and p.d.f.'s. A complete Eulerian single-point p.d.f. description of the two-phase flow will require the knowledge of the event

$$E_1 = [\boldsymbol{U} \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}), I_f(\boldsymbol{x}, t) = 1], \tag{2.3}$$

which is the event corresponding to the joint occurrence of $\boldsymbol{U}$ falling in the range $(\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})$ at a point $\boldsymbol{x}$ and the fluid phase being present at the same point. Here, $\boldsymbol{u}$ is the sample space variable corresponding to the random variable $\boldsymbol{U}$. Note that $I_f(\boldsymbol{x}, t) = 1$ automatically precludes the occurrence of the dispersed phase at that same point (i.e. $I_d(\boldsymbol{x}, t) = 0$ at the same point $\boldsymbol{x}$). It is noteworthy that Sundaram & Collins (1994*a*,*b*) have explored the simultaneous two-point description of a two-phase flow in the random-field representation. We focus on the single-point representation in this study since single-point models are more tractable, although there is a loss of scale information when moving from the two-point to the single-point description.

Corresponding to the joint event E_1, two marginal events are

$$E_2 = [\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})] \tag{2.4}$$

$$E_3^{(\beta)} = [I_\beta(\boldsymbol{x}, t) = 1], \tag{2.5}$$

where E_2 is the event that $\boldsymbol{U}(\boldsymbol{x}, t)$ belongs to $(\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})$ regardless of whether the phase β is located at $\boldsymbol{x}$, while $E_3^{(\beta)}$ is the event that phase β exists at $\boldsymbol{x}$. Two conditional events are also important

$$E_4 = [\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}) | I_\beta = 1] \tag{2.6}$$

$$E_5 = [I_\beta(\boldsymbol{x}, t) = 1 | \boldsymbol{U} = \boldsymbol{u}], \tag{2.7}$$

where E_4 is the event that $\boldsymbol{U}(\boldsymbol{x}, t)$ belongs to $(\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})$ conditional on the presence of phase β at location $\boldsymbol{x}$, while E_5 is the event that the location $\boldsymbol{x}$ is occupied by phase β conditional on $\boldsymbol{U} = \boldsymbol{u}$ at the same location.

Let the Eulerian p.d.f. of $\boldsymbol{U}$ be denoted as $f_U(\boldsymbol{u}; \boldsymbol{x}, t)$, where $\boldsymbol{x}$ and t are parameter space variables. The probabilities corresponding to each of the above events are

$$P[E_2] = P[\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})] = f_U(\boldsymbol{u}; \boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{u} \tag{2.8}$$

$$P[E_5] = P[I_\beta(\boldsymbol{x}, t) = 1 | \boldsymbol{U} = \boldsymbol{u}] = p_\beta(\boldsymbol{x}, t | \boldsymbol{u}) \tag{2.9}$$

$$\begin{aligned} P[E_1] &= P[I_\beta(\boldsymbol{x}, t) = 1 | \boldsymbol{U} = \boldsymbol{u}]\, P[\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u})] \\ &= p_\beta(\boldsymbol{x}, t | \boldsymbol{u}) f_U(\boldsymbol{u}; \boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{u} \end{aligned} \tag{2.10}$$

$$P\left[E_3^{(\beta)}\right] = \int P[I_\beta = 1 | \boldsymbol{U} = \boldsymbol{u}] f_U(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = \int p_\beta f_U(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u} = \alpha_\beta(\boldsymbol{x}, t) \tag{2.11}$$

$$P[E_4] = P[\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}) | I_\beta = 1] = \frac{p_\beta f_U(\boldsymbol{u}; \boldsymbol{x}, t)}{\alpha_\beta(\boldsymbol{x}, t)}\,\mathrm{d}\boldsymbol{u}, \tag{2.12}$$

where $p_\beta(\boldsymbol{x}, t | \boldsymbol{u})$ is a phase probability function. Also, $\alpha_\beta(\boldsymbol{x}, t)$ is the volume fraction at $(\boldsymbol{x}, t)$. Note that the probability $P[E_3^{(\beta)}]$ defines a probability *field* $\alpha_\beta(\boldsymbol{x}, t)$

$$\alpha_\beta(\boldsymbol{x}, t) \equiv P[I_\beta(\boldsymbol{x}, t) = 1]. \tag{2.13}$$

It is important to note that $\alpha_\beta(\boldsymbol{x}, t)$ is *not* a probability density in $\boldsymbol{x}$. However, α_β is a probability mass function in I_β, which takes values $\{0, 1\}$. Another property of I_β is that $P[I_\beta(\boldsymbol{x}, t) = 1] = \langle I_\beta \rangle$.

Since f_U is a p.d.f. it has to satisfy the normalization condition

$$\int f_U(\boldsymbol{u};\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{u} = 1. \tag{2.14}$$

Also, let the probability $P[E_4]$ be denoted by $f_{U|I_\beta}\,\mathrm{d}\boldsymbol{u}$, so that the Eulerian p.d.f. of velocity conditioned on the presence of phase β at $\boldsymbol{x}$, $f_{U|I_\beta}$ is given as

$$f_{U|I_\beta} = \frac{p_\beta f_U(\boldsymbol{u})}{\alpha_\beta(\boldsymbol{x},t)}. \tag{2.15}$$

The mixture mean velocity field $\langle \boldsymbol{U}\rangle$ is defined as

$$\langle \boldsymbol{U}\rangle(\boldsymbol{x},t) = \int \boldsymbol{u} f_U\,\mathrm{d}\boldsymbol{u}, \tag{2.16}$$

while the phasic mean velocity $\langle \boldsymbol{U}^{(\beta)}\rangle$ is defined as

$$\langle \boldsymbol{U}^{(\beta)}\rangle = \int \boldsymbol{u} f_{U|I_\beta}\,\mathrm{d}\boldsymbol{u}. \tag{2.17}$$

The two mean velocities are related as

$$\langle \boldsymbol{U}\rangle = \alpha_f\langle \boldsymbol{U}^{(f)}\rangle + \alpha_d\langle \boldsymbol{U}^{(d)}\rangle. \tag{2.18}$$

Since only one of the phases can exist at a single space–time location, the following relations hold:

$$P[I_f = 1] + P[I_d = 1] = 1 \tag{2.19}$$

$$\alpha_f + \alpha_d = 1 \tag{2.20}$$

$$p_f(\boldsymbol{x},t|\boldsymbol{u}) + p_d(\boldsymbol{x},t|\boldsymbol{u}) = 1. \tag{2.21}$$

It is interesting to note that the phase probability function p_β and the p.d.f. of instantaneous two-phase velocity f_U can be expressed in terms of the volume fraction field α_β and the phasic velocity p.d.f. $f_{U|I_\beta}$ as

$$p_f(\boldsymbol{x},t|\boldsymbol{u}) = \frac{\alpha_f(\boldsymbol{x},t) f_{U|I_f}}{\alpha_f(\boldsymbol{x},t) f_{U|I_f} + \alpha_d(\boldsymbol{x},t) f_{U|I_d}} \tag{2.22}$$

$$f_U(\boldsymbol{u};\boldsymbol{x},t) = \alpha_f(\boldsymbol{x},t) f_{U|I_f} + \alpha_d(\boldsymbol{x},t) f_{U|I_d}. \tag{2.23}$$

This shows that the knowledge of one of α_f or α_d and the phasic probability p.d.f.'s $f_{U|I_\beta}$ for $\beta = \{f, d\}$ is sufficient for a complete single-point description of a two-phase flow. This description corresponds to the *minimal* and *complete single-point Eulerian description* of the two-phase flow (Subramaniam 2005). This, however, does not imply that this single-point statistical description is adequate, or is a unique characterization of a two-phase flow. It simply suggests that all single-point quantities can be expressed in terms of these fundamental quantities.

2.2. *Point-process representation*

The starting point for the point process or the LE description of a two-phase flow is the d.d.f. proposed by Williams (1958). The spray equation, which is the evolution equation of the d.d.f., can be rigorously derived starting from the Lagrangian evolution equations of droplet position, velocity and radius (Subramaniam 2001). Although the d.d.f. was initially conceived to describe a fuel spray in internal combustion engines (and hence the name 'droplet' distribution function), it can be used to describe any two-phase flow where the dispersed phase can be modelled as a collection of

discrete entities. A popular implementation used in the internal combustion engine industry that is based on the LE statistical representation is the KIVA family of codes (Amsden *et al.* 1989; Amsden 1993). While the salient aspects of this statistical description that are relevant to the current discussion are given here, details may be found in Subramaniam (2000, 2001).

Here, we consider the DPEs to be droplets, although the discussion is equally valid for other DPEs. Consider a two-phase flow in a finite flow domain $\mathscr{D}$ in physical space as an ensemble of droplets. It is assumed that one can associate a characteristic length scale with each droplet, which is the radius in the case of spherical droplets. If the droplet is non-spherical, then one may employ the radius of an equivalent sphere that has the same volume as the non-spherical droplet. One could also use the volume of the droplet directly as a phase space variable. However, either choice does not inherently alter the derivation of the spray equation, nor does it provide any further insight into the nature of the unclosed terms in the spray equation and the moment equations derived thereof. Thus, we retain the radius as the characteristic length scale for the size phase space.

At time t the total number of droplets $N(t)$ is a non-negative integer-valued random variable which is finite with probability 1. The ith DPE is characterized by its position vector $\boldsymbol{X}_{(i)}(t)$ (which is defined as the centre of mass of the droplet), its velocity vector $\boldsymbol{V}_{(i)}(t)$ and its radius $R_{(i)}(t)$ ($R_{(i)}(t) > 0$). The position, velocity and radius of a droplet are called the droplet properties, and the droplet property vector associated with each droplet is a seven-dimensional random vector in this representation. Additional droplet properties may be included as required, but they do not fundamentally alter the formulation, other than increasing the dimension of the space of droplet properties. The properties associated with the ith droplet evolve by the following equations:

$$\frac{\mathrm{d}\boldsymbol{X}_{(i)}}{\mathrm{d}t} = \boldsymbol{V}_{(i)} \tag{2.24}$$

$$\frac{\mathrm{d}\boldsymbol{V}_{(i)}}{\mathrm{d}t} = \boldsymbol{A}_{(i)} \tag{2.25}$$

$$\frac{\mathrm{d}R_{(i)}}{\mathrm{d}t} = \Theta_{(i)}, \tag{2.26}$$

where $\boldsymbol{A}_{(i)}$ is the acceleration experienced by the droplet, and $\Theta_{(i)}$ is the rate of radius change due to vaporization (or interphase mass transfer, in general). This initial physical description for the LE approach assumes that the velocity field inside the droplet is uniform, and hence the motion of the ith droplet can be described by the motion of its centre of mass $\boldsymbol{X}_{(i)}$.

The ensemble of droplets is characterized in the seven-dimensional position–velocity–radius space $[\boldsymbol{x}, \boldsymbol{v}, r]$ by its Klimontovich (Nicholson 1992) fine-grained density function f', which is defined as

$$f'(\boldsymbol{x}, \boldsymbol{v}, r, t) \equiv \sum_{i=1}^{N(t)} f'_{(i)} = \sum_{i=1}^{N(t)} \delta(\boldsymbol{x} - \boldsymbol{X}_{(i)}(t))\delta(\boldsymbol{v} - \boldsymbol{V}_{(i)}(t))\delta(r - R_{(i)}(t)). \tag{2.27}$$

Note that $[\boldsymbol{X}_{(i)}, \boldsymbol{V}_{(i)}, R_{(i)}]$ are the Lagrangian coordinates of the ith droplet, whereas $[\boldsymbol{x}, \boldsymbol{v}, r]$ are the measure-space (or sample-space) coordinates. The Klimontovich fine-grained density function f' represents the density of droplets in a seven-dimensional $[\boldsymbol{x}, \boldsymbol{v}, r]$ space. The summation of the product of delta functions in the above equation represents a single realization of the two-phase flow. Thus, the above summation

represents a realization of the two-phase flow in which the ith DPE whose centre of mass $\boldsymbol{X}_{(i)}$ is at location $\boldsymbol{x}$ in position phase space, whose centre of mass velocity $\boldsymbol{V}_{(i)}$ is at location $\boldsymbol{v}$ in velocity phase space and whose radius $R_{(i)}$ is at location r in radius phase space.

If the number of droplets in any region B_+ in $[\boldsymbol{x}, \boldsymbol{v}, r_+]$ space (since droplets with only non-zero radius belong to the spray system, if for convenience of notation we denote r_+ to be the positive r-axis ($r > 0$), then it is sufficient to integrate over regions only in $[\boldsymbol{x}, \boldsymbol{v}, r_+]$ space) is denoted by $N(B_+; t)$, it is obtained by integrating f' over the region B_+ such that

$$N(B_+; t) = \int_{B_+} f'(\boldsymbol{x}, \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}r. \tag{2.28}$$

Since f' is composed of delta functions it is not a smooth function in $[\boldsymbol{x}, \boldsymbol{v}, r]$ space.

The statistical description of a spray in terms of f' contains far more information than is necessary for engineering calculations. In order to obtain information concerning the average properties of the spray, it is advantageous to consider the ensemble average of f'. The ensemble average of f' is denoted by $f(\boldsymbol{x}, \boldsymbol{v}, r, t)$, and it defines the d.d.f. as

$$f(\boldsymbol{x}, \boldsymbol{v}, r, t) \equiv \langle f'(\boldsymbol{x}, \boldsymbol{v}, r, t)\rangle = \left\langle \sum_{i=1}^{N(t)} \delta\big(\boldsymbol{x} - \boldsymbol{X}_{(i)}(t)\big)\delta\big(\boldsymbol{v} - \boldsymbol{V}_{(i)}(t)\big)\delta\big(r - R_{(i)}(t)\big) \right\rangle. \tag{2.29}$$

The expectation $\langle\cdot\rangle$ above represents an ensemble average of possibly infinite realizations of the two-phase flow. Details on the use of the delta function to represent a realization of a single-phase flow and its ensemble average can be found, for instance, in Pope (2000). It is important to note that the expectation operator cannot be brought inside the summation for a general spray; if done, then the implications of such an operation needs to be understood carefully (see Subramaniam 2000 for a detailed discussion).

Since the d.d.f. is defined to be the ensemble average of f' (cf. (2.29)), it follows that if the expected number of droplets in a region B_+ of $[\boldsymbol{x}, \boldsymbol{v}, r_+]$ space is denoted as $\langle N(B_+; t)\rangle$, it is obtained by integrating the d.d.f. $f(\boldsymbol{x}, \boldsymbol{v}, r, t)$ over the region B_+ such that

$$\langle N(B_+; t)\rangle = \int_{B_+} f(\boldsymbol{x}, \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}r. \tag{2.30}$$

The d.d.f. is the fundamental quantity in the Lagrangian statistical representation. If $\langle N(t)\rangle$ represents the expected total number of spray droplets at time t, then the droplet distribution function $f(\boldsymbol{x}, \boldsymbol{v}, r, t)$ when integrated over the entire $[\boldsymbol{x}, \boldsymbol{v}, r_+]$ space, must yield $\langle N(t)\rangle$, such that

$$\int_{[\boldsymbol{x}, \boldsymbol{v}, r_+]} f(\boldsymbol{x}, \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}r = \langle N(t)\rangle. \tag{2.31}$$

It is noteworthy that f does not possess the normalization property of a p.d.f., since it does not integrate to unity over the space on which it is defined.

If the droplet distribution function is integrated over only $[\boldsymbol{v}, r_+]$ space, the density (in physical space) of the expected number of spray droplets $n(\boldsymbol{x}; t)$ is obtained as

follows:

$$n(\boldsymbol{x};t) \equiv \int_{[\boldsymbol{v},r_+]} f(\boldsymbol{x},\boldsymbol{v},r,t)\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}r. \tag{2.32}$$

If the multiphase flow is modelled as a marked point process, then the theory of point processes (Daley & Vere-Jones 2003) can be used to express the d.d.f. as the product of the number density in physical space $n(\boldsymbol{x};t)$ and $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$, the joint probability density function (j.p.d.f.) of velocity and radius conditional on physical location $\boldsymbol{x}$, such that (Subramaniam 2001)

$$f(\boldsymbol{x},\boldsymbol{v},r,t) = n(\boldsymbol{x};t)\; f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t). \tag{2.33}$$

Unlike the d.d.f., $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$ is a p.d.f. and integrates to unity when integrated over $[\boldsymbol{v},r_+]$ space. In $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$ the superscript c stands for a p.d.f. 'conditional' on $\boldsymbol{x}$, in this case, and the subscript $\boldsymbol{V}\ R$ implies that $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$ is a j.p.d.f. of velocity and radius.

In the LE approach one cannot meaningfully associate a probability density with each droplet in the spray, since information about individual droplets is lost in the course of the derivation of the d.d.f. (Subramaniam 2001). However, the d.d.f. can be related to single-particle densities associated with 'surrogate' droplets as (Subramaniam 2000)

$$f(\boldsymbol{x},\boldsymbol{v},r,t) = \sum_{k\geqslant 1} q_{(k)}\; f^{(k)}(\boldsymbol{x},\boldsymbol{v},r;t) = \sum_{k\geqslant 1} k\; q_{(k)}\; f^{(k)}_{1s}(\boldsymbol{x},\boldsymbol{v},r;t), \tag{2.34}$$

where k is the integer value that $N(t)$ takes with probability $q_{(k)} = P[N(t)=k]$, $f^{(k)}$ is the density of expected number of droplets in phase space, conditional on the event $[N(t)=k]$, i.e. conditional on there being a total of k droplets in the ensemble and $f^{(k)}_{1s}(\boldsymbol{x},\boldsymbol{v},r;t)$ is the single-particle density of identically distributed surrogate droplets, conditional on the event $[N(t)=k]$. The single-particle density of identically distributed surrogate droplets $f^{(k)}_{1s}(\boldsymbol{x},\boldsymbol{v},r;t)$ is related to the droplet properties by the relation

$$f^{(k)}_{1s}(\boldsymbol{x},\boldsymbol{v},r;t) = \frac{1}{k} f^{(k)}(\boldsymbol{x},\boldsymbol{v},r,t) = \frac{1}{k}\left\langle \sum_{i=1}^{k} \delta\big(\boldsymbol{x}-\boldsymbol{X}_{(i)}(t)\big)\delta\big(\boldsymbol{v}-\boldsymbol{V}_{(i)}(t)\big)\delta\big(r-R_{(i)}(t)\big)\right\rangle. \tag{2.35}$$

It is impossible to characterize events associated with a *single* droplet in the LE approach. This is primarily because here one is dealing with a d.d.f. that is the superposition of several surrogate-droplet densities (cf. (2.34)). Nevertheless, even in the LE representation one can characterize number-weighted statistical moments of the particle ensemble, and write conservation equations for mean mass and momentum in a Eulerian reference frame (cf. § 5).

It is useful to review the nature of the j.p.d.f. $f^c_{V\ R}(\boldsymbol{v},r|\boldsymbol{x},t)$ in the LE statistical representation here. In p.d.f. modelling of constant-density turbulent flows the Lagrangian j.p.d.f. of fluid particle position $\boldsymbol{X}^+(t)$ and velocity $\boldsymbol{U}^+(t)$ can be related to the Eulerian j.p.d.f. of the Eulerian velocity field $\boldsymbol{U}(\boldsymbol{x},t)$ by using a conditioning argument as shown by Dreeben & Pope (1997). There the conditioning is on the position of the fluid particle being at the field location $\boldsymbol{x}$, i.e. the conditioning is on the Eulerian event $[\boldsymbol{X}^+(t)=\boldsymbol{x}]$. On the other hand, the j.p.d.f. $f^c_{V\ R}(\boldsymbol{v},r|\boldsymbol{x},t)$ corresponds to a number- and probability-weighted sum of j.p.d.f.s of position, velocity and radius of a single-surrogate droplet, conditioned on the number- and probability-weighted

sum of position p.d.f.s of the single-surrogate droplet (Subramaniam 2000),

$$f^c_{V\,R}(\boldsymbol{v}, r|\boldsymbol{x}, t) = \frac{\sum_{k\geqslant 1} q_{(k)} k f^{(k)}_{1s}(\boldsymbol{x}, \boldsymbol{v}, r; t)}{\sum_{k\geqslant 1} q_{(k)} k f^{(k)}_{1s}(\boldsymbol{x}; t)} \tag{2.36}$$

In other words, the j.p.d.f. $f^c_{VR}(\boldsymbol{v}, r|\boldsymbol{x}; t)$ does not correspond to conditioning on the event that a droplet's position is at the field location $\boldsymbol{x}$. So, the j.p.d.f. $f^c_{VR}(\boldsymbol{v}, r|\boldsymbol{x}; t)$ is not a 'Eulerian' j.p.d.f. since it does not characterize the probability of a Eulerian event, in the sense of $\boldsymbol{U}(\boldsymbol{x}, t)$ being a Eulerian event in a random-field model of turbulent flow.

We have now established the foundation for the EE and LE statistical representations and defined the necessary relations required in the rest of this work. We now proceed to establish a relationship between the two approaches.

3. Relationship between the Eulerian–Eulerian and Lagrangian–Eulerian description

In order to establish a relationship between the two representations, we consider *single-point* quantities of the random-field (Eulerian) and point-process (Lagrangian) statistical descriptions of a two-phase flow. 'Single-point' refers to quantities that are defined at a single space–time location. Two-point quantities (also known as 'second-order' quantities in point-process literature, see for instance Stoyan, Kendall & Mecke 1995), which simultaneously characterize the state of a system at two different space–time locations, such as the pair-correlation function are not considered in this work. The volume fraction $\alpha_d(\boldsymbol{x}, t)$ and the phasic velocity p.d.f.s $f_{\boldsymbol{U}|I_\beta}$ correspond to the minimal and complete single-point description of the velocity field in a two-phase flow in the EE representation (cf. (2.23)). So, we seek a relationship between these quantities and corresponding quantities in the LE representation.

If we assume spherical DPEs, then we can relate $\alpha_d(\boldsymbol{x}, t)$ to the fundamental description as follows:

$$\begin{aligned}\alpha_d(\boldsymbol{x}, t) &= \sum_{k\geqslant 1} q_{(k)}\, k \int_{\mathscr{X}_{\mathscr{R}}} \int_{\boldsymbol{v}} f^{(k)}_{1s}(\boldsymbol{x}', \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}\boldsymbol{x}'\, \mathrm{d}r \\ &= \sum_{k\geqslant 1} q_{(k)} \int_{\mathscr{X}_{\mathscr{R}}} \int_{\boldsymbol{v}} \left\langle \sum_{i=1}^{k} \delta\big(\boldsymbol{x}' - \boldsymbol{X}_{(i)}(t)\big)\delta\big(\boldsymbol{v} - \boldsymbol{V}_{(i)}(t)\big)\delta\big(r - R_{(i)}(t)\big) \right\rangle \mathrm{d}\boldsymbol{v}\, \mathrm{d}\boldsymbol{x}'\, \mathrm{d}r,\end{aligned} \tag{3.1}$$

where the region of integration $\mathscr{X}_{\mathscr{R}} = [\boldsymbol{x}', r : \boldsymbol{x}' \in b(\boldsymbol{x}, r)]$. Here, $b(\boldsymbol{x}, r)$ is the ball of radius r centred at $\boldsymbol{x}$ (see figure 3). The above equation states that the event $E^{(d)}_0 = P[I_d(\boldsymbol{x}, t) = 1]$ can arise from all possible combinations of DPE location and radius that result in $\boldsymbol{x}$ being covered by the DPE.

For a constant number of N DPEs in the system, $q_{(k)} = 1$ for $k = N$, and zero otherwise. With the additional assumption of identically distributed monodispersed DPEs, the above expression simplifies to

$$\alpha(\boldsymbol{x}, t) = \sum_{i=1}^{N} \left\langle H\left(\frac{\sigma}{2} - |\boldsymbol{x} - \boldsymbol{X}_{(i)}(t)|\right)\right\rangle, \tag{3.2}$$

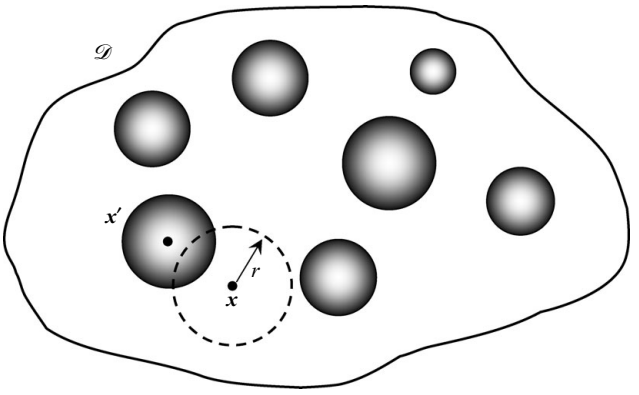

FIGURE 3. A schematic illustration of the region of integration in (3.1) given by $[\boldsymbol{x}', r : \boldsymbol{x}' \in b(\boldsymbol{x}, r)]$. The point $\boldsymbol{x}$ is the location where the volume fraction α_d is desired, $\boldsymbol{x}'$ is the centre of the DPE under consideration and r is the radius of the ball centred at $\boldsymbol{x}$. Note that for the configuration shown, the DPE at $\boldsymbol{x}'$ does not contribute to the volume fraction at $\boldsymbol{x}$ since the location $\boldsymbol{x}'$ does not satisfy $[\boldsymbol{x}' : \boldsymbol{x}' \in b(\boldsymbol{x}, r)]$. However, if the DPE at $\boldsymbol{x}'$ overlaps the location $\boldsymbol{x}$ such that $[\boldsymbol{x}' : \boldsymbol{x}' \in b(\boldsymbol{x}, r)]$, then this DPE contributes to the volume fraction at $\boldsymbol{x}$.

where $H(\boldsymbol{x})$ is the Heaviside function defined as

$$H(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \geqslant 0 \\ 0 & \text{if } \boldsymbol{x} < 0, \end{cases} \tag{3.3}$$

and σ is the diameter of the DPE. Equation (3.2) is identical to the expression for the expectation of the indicator function available in literature (see, for instance, Sundaram & Collins 1994*a*; Zhang & Prosperetti 1994). Equation (3.1) is more general compared to (3.2) because in the former (*a*) the total number of DPEs is assumed to be a random variable (an assumption that extends previous analyses to physical problems in which the expected total number of DPEs can change in time), (*b*) the important effect of polydispersity is considered, and (*c*) the effects of statistical inhomogeneity are also considered.

It is convenient to express $\alpha_d(\boldsymbol{x}, t)$ in (3.1) in terms of the d.d.f. using (2.34) as

$$\alpha_d(\boldsymbol{x}, t) = \int_{[\boldsymbol{x}', r \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} \int_{\boldsymbol{v}} f(\boldsymbol{x}', \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}\boldsymbol{x}'\, \mathrm{d}r. \tag{3.4}$$

Using the decomposition in (2.33), expressing

$$f^c_{VR}(\boldsymbol{v}, r|\boldsymbol{x}; t) = f^c_{V\,|\,R}(\boldsymbol{v}|r, \boldsymbol{x}; t)\; f^c_R(r|\boldsymbol{x}; t),$$

and noting that $f^c_{V\,|\,R}(\boldsymbol{v}|r, \boldsymbol{x}; t)$ integrates to unity over all velocity space, we find as expected that $\alpha_d(\boldsymbol{x}, t)$ depends only on the number density and the radius p.d.f.

$$\alpha_d(\boldsymbol{x}, t) = \int_{[\boldsymbol{x}', r \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} n(\boldsymbol{x}'; t)\, f^c_R(r \mid \boldsymbol{x}', t)\, \mathrm{d}\boldsymbol{x}'\, \mathrm{d}r. \tag{3.5}$$

Later, we consider special cases where assumptions of statistical homogeneity in $n(\boldsymbol{x}; t)$ and f^c_R result in simpler forms of (3.5).

Next we relate the Eulerian p.d.f. arising in the EE description with the conditional j.p.d.f. of velocity and radius arising from the d.d.f. description of the spray. To this

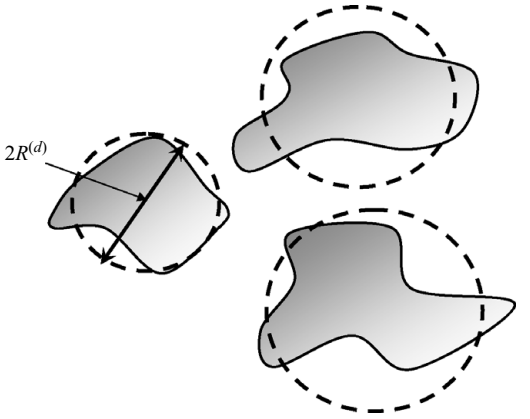

FIGURE 4. Schematic illustration of a representative spherical DPE (dashed line) with radius $R^{(d)}$ corresponding to the dispersed phase (shaded) in the EE representation.

end, we write the event E_2 as

$$E_2 = \left[\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)}(\boldsymbol{x}, t) \in (r, r + \mathrm{d}r)\right],$$

where the event has been augmented with an additional radius phase space $R^{(d)}$ to allow for a consistent comparison with the LE approach. It is implicitly assumed that the dispersed phase is represented as equivalent spherical DPEs (see figure 4). The phasic velocity p.d.f. conditional on the presence of phase β, $f_{\boldsymbol{U}|I_\beta}$ (cf. (2.15)) is now written as $f^E_{\boldsymbol{U}R|I_\beta}$ such that

$$P\left[\,\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)}(\boldsymbol{x}, t) \in (r, r + \mathrm{d}r) \mid I_\beta(\boldsymbol{x}, t) = 1\,\right] = f^E_{\boldsymbol{U}R|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)\ \mathrm{d}\boldsymbol{u}\,\mathrm{d}r, \quad (3.6)$$

where $f^E_{\boldsymbol{U}R|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ represents the Eulerian conditional j.p.d.f. of velocity and radius. For the carrier phase where R is always defined to be zero, this essentially reduces to a p.d.f. of velocity, i.e. $f^E_{\boldsymbol{U}R|I_f}(\boldsymbol{u}, r; \boldsymbol{x}, t) = f^E_{\boldsymbol{U}|I_f}(\boldsymbol{u}; \boldsymbol{x}, t) \cdot \delta(r)$. An additional E superscript has been included compared to (2.15) to denote explicitly in the subsequent comparisons with the LE approach that $f^E_{\boldsymbol{U}R|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ arises from the EE representation. The joint probability of the event $[\boldsymbol{U} \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)} \in (r, r + \mathrm{d}r),\, I_d(\boldsymbol{x}, t) = 1]$, which is essentially the intersection of the events E_2 and $E_3^{(d)}$, can be written in terms of the single-point surrogate density as

$$P\left[E_2 \bigcap E_3^{(d)}\right] = P\left[\,\boldsymbol{U}(\boldsymbol{x}, t)\ \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)}(\boldsymbol{x}, t) \in (r, r + \mathrm{d}r),\, I_d(\boldsymbol{x}, t) = 1\right]$$
$$= \sum_{k \geqslant 1} k\ q_{(k)} \int_{[\boldsymbol{x}' \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} f^{(k)}_{1s}(\boldsymbol{x}', \boldsymbol{v}, r; t)\,\mathrm{d}\boldsymbol{x}'. \quad (3.7)$$

In order to obtain the j.p.d.f. of velocity and radius conditional on $I_d(\boldsymbol{x}, t) = 1$, we use the definition of conditional probability and write

$$P\left[\,\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)}(\boldsymbol{x}, t) \in (r, r + \mathrm{d}r) \mid I_d(\boldsymbol{x}, t) = 1\,\right] = \frac{P\left[\,\boldsymbol{U}(\boldsymbol{x}, t) \in (\boldsymbol{u}, \boldsymbol{u} + \mathrm{d}\boldsymbol{u}),\, R^{(d)}(\boldsymbol{x}, t) \in (r, r + \mathrm{d}r),\, I_d(\boldsymbol{x}, t) = 1\,\right]}{P\left[\,I_d(\boldsymbol{x}, t) = 1\,\right]}. \quad (3.8)$$

Therefore the Eulerian j.p.d.f. of velocity and radius conditional on the dispersed phase, $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ is given by

$$f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u}, r; \boldsymbol{x}, t) = \frac{1}{\alpha_d(\boldsymbol{x}, t)} \int_{[\boldsymbol{x}' \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} f(\boldsymbol{x}', \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{x}'$$
$$= \frac{1}{\alpha_d(\boldsymbol{x}, t)} \int_{[\boldsymbol{x}' \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} n(\boldsymbol{x}'; t) f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r \mid \boldsymbol{x}'; t)\, \mathrm{d}\boldsymbol{x}', \qquad (3.9)$$

which clearly shows that in general it is different from the j.p.d.f. of velocity and radius $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}; t)$ obtained in the Lagrangian approach (cf. (2.33)). The relationships given by (3.5) and (3.9) form the two fundamental equalities that relate two-phase flow quantities across the EE and LE statistical representations.

3.1. *Simplified relations under special conditions*

In this subsection, we consider special conditions under which simple relations between the EE and LE descriptions exist. This involves determining the conditions under which a simple relationship between $\alpha_d(\boldsymbol{x}, t)$ and $n(\boldsymbol{x}; t)$, and between $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ and $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}; t)$ exist, and conditions under which such relationships are precluded. The simplest problem where these relationships can be studied is a *statistically homogeneous* two-phase flow. In two-phase flows there are two sources of statistical inhomogeneity. This is implicit in the decomposition expressed in (2.33), which shows that spatial inhomogeneity of the d.d.f. has two different sources: namely, inhomogeneity can arise from either $n(\boldsymbol{x}; t)$ in physical space, or from $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}; t)$. It is clear from (3.5) that only the statistical properties of the radius p.d.f. $f^c_R(r|\boldsymbol{x}; t)$ affect the relation between $\alpha_d(\boldsymbol{x}, t)$ and the point-process quantities, whereas (3.9) shows that the relationship between $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ and $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}; t)$ also depends on the statistical properties of the j.p.d.f. $f^c_{\boldsymbol{V}\,|\,R}(\boldsymbol{v}|r, \boldsymbol{x}; t)$.

With this in mind, simplifications that result from a statistically homogeneous number density with statistically homogeneous radius p.d.f. and velocity–radius j.p.d.f. are considered here, details of which are given in Appendix C. The principal findings from these simplifications are summarized below. Also given in Appendix C are considerations required to extend these relations to inhomogeneous number density, radius and velocity–radius j.p.d.f.

3.1.1. *Statistically homogeneous cases*

The simplified relationships arising from the cases corresponding to the statistically homogeneous cases are shown in Table 1. Two-phase flows with monodisperse DPEs are included as a special subset of the homogeneous radius p.d.f. case. The principal findings are as follows:

(i) The relation between $\alpha_d(\boldsymbol{x}, t)$ and $n(\boldsymbol{x}; t)$ for the case of statistically homogeneous number density and statistically homogeneous radius p.d.f. is

$$\alpha_d(\boldsymbol{x}, t) = n(t)\, \overline{\mathscr{V}}_D(t) = n(t) K_D\, \langle R^D \rangle(t), \qquad (3.10)$$

where $K_1 = 2$, $K_2 = \pi$ and $K_3 = 4\pi/3$. The above expression reveals that $\alpha_d(\boldsymbol{x}, t)$ depends on the dimensionality D of the physical space through its dependence on r^D (see Appendix C.1.1 for details), while $n(t)$ does not explicitly contain such a dependence. Also, see the example that illustrates this fact in § 3.3. This fact alone clearly shows that the LE and EE statistical representations contain different information.

(ii) For the statistically homogeneous number density and statistically homogeneous $f^c_R(r|\boldsymbol{x}; t)$ the following simplified relation between the EE and LE

Statistically homogeneous number density $n(t)$ and point-process radius p.d.f. $f_R^c(r;t)$	
Monodisperse	Polydisperse
$\alpha_d(t) = n(t) K_D r_0^D$	$\alpha_d(t) = n K_D \langle R^D(t) \rangle$
$f^E_{R\,\vert\, I_d}(r) = f_R^c(r) = \delta(r - r_0)$	$f^E_{R\,\vert\, I_d}(r;t) = r^D \dfrac{f_R^c(r;t)}{\langle R^D \rangle(t)}$
Statistically homogeneous $f^c_{V\,\vert\, R}(\boldsymbol{v} \mid r;t)$	
$f^E_{UR\,\vert\, I_d}(\boldsymbol{v}, r;t) = f^c_{VR}(\boldsymbol{v}, r;t)$	$f^E_{UR\,\vert\, I_d}(\boldsymbol{v}, r;t) = \dfrac{r^D f^c_{VR}(\boldsymbol{v}, r;t)}{\langle R^D(t) \rangle}$

TABLE 1. Relationship between first-order statistics and velocity–radius j.p.d.f.s of EE and LE representations for the statistically homogeneous cases. $K_1 = 2; K_2 = \pi; K_3 = 4\pi/3$.

radius p.d.f.s results:

$$f^E_{R\,\vert\, I_d}(r;t) = \frac{r^D f_R^c(r;t)}{\langle R^D \rangle(t)}. \tag{3.11}$$

(iii) If $f^c_{V\,\vert\, R}(\boldsymbol{v}|r, \boldsymbol{x};t)$ is also statistically homogeneous then the velocity–radius j.p.d.f.'s satisfy the following relation:

$$f^E_{UR\,\vert\, I_d}(\boldsymbol{v}, r;t) = \tilde{f}^c_{VR}(\boldsymbol{v}, r;t) \equiv \frac{r^D f^c_{VR}(\boldsymbol{v}, r;t)}{\langle R^D(t) \rangle}, \tag{3.12}$$

where $\tilde{f}^c_{VR}(\boldsymbol{v}, r;t)$ is the volume-weighted p.d.f. corresponding to $f^c_{VR}(\boldsymbol{v}, r;t)$.

(iv) For a monodisperse size distribution with DPEs of radius r_0, these relations further simplify to

$$\alpha_d(\boldsymbol{x}, t) = n(t) K_D\, r_0^D \tag{3.13}$$

$$f^E_{UR\,\vert\, I_d}(\boldsymbol{v}, r;t) = f^c_{VR}(\boldsymbol{v}, r;t) = f^c_{V\,\vert\, R}(\boldsymbol{v} \mid r;t)\, \delta(r - r_0). \tag{3.14}$$

It was noted earlier that the velocity–radius j.p.d.f in each representation are not equal in general. Zhu *et al.* (2000) derive an evolution equation for $f^c_{VR}(\boldsymbol{v}, r|\boldsymbol{x};t)$ from the transport equation for $f^E_{UR|I_d}(\boldsymbol{v}, r;\boldsymbol{x}, t)$ under an assumption that these two quantities are equal for a general spray. However, it is shown here that only under rather restrictive assumptions of spherical monodisperse DPEs and a statistically isotropic and homogeneous point process does a simple relationship between $f^c_{VR}(\boldsymbol{v}, r;t)$ and $f^E_{UR\,\vert\, I_d}(\boldsymbol{v}, r;t)$ exist (cf. (3.14)).

3.2. *Validity of assumptions necessary for exact relations*

The exact equalities between first-order quantities in the LE and EE approach that were derived in the earlier section hold only under certain conditions and assumptions. These conditions can restrict the applicability of the exact equalities in general two-phase flows.

3.2.1. *Spatial inhomogeneities in the two-phase flow*

Spatial inhomogeneities in $n(\boldsymbol{x};t)$ and $f_R^c(r|\boldsymbol{x};t)$ that exist either at initial time or develop as a two-phase flow evolves could preclude the validity of the exact equalities. Two examples of such flows are

(*a*) Fuel sprays: In the near-nozzle region of the fuel spray injector, the dispersed-phase number density $n(\boldsymbol{x};t)$ can have steep gradients. Also, $f_R^c(r|\boldsymbol{x};t)$ can be spatially

inhomogeneous due to a spatially varying size distribution of the dispersed phase. Under such conditions, even assumptions of local homogeneity (for details on the notion of local homogeneity, the reader is directed to Appendix C.2.) may cease to hold. Furthermore, in regions close to the injector, $n(\boldsymbol{x};t)$ and $f_R^c(r|\boldsymbol{x};t)$ may remain inhomogeneous even as time evolves. Under such conditions, the relationship between the EE and LE representations have to be interpreted only as approximate relations.

(*b*) Particle-laden mixing layers: Particle-laden mixing layers form an important class of canonical problems studied by researchers through multiphase DNS and experiments (see, for example, Lázaro & Lasheras 1992*a*,*b*; Okong'o & Bellan 2004). Consider a particle-laden mixing layer with two monodispersed streams of particles, with each stream having a different particle radius. The particle positions in the two streams are such that the initial number density is statistically homogeneous. The region near the centreline of the mixing layer will have a locally inhomogeneous $f_R^c(r|\boldsymbol{x};t)$. Once the flow starts to evolve, the number density may develop inhomogeneities as well. Again under such conditions, the equalities presented in the earlier section between the EE and LE representations have to be interpreted only as approximate relations.

3.2.2. *Spherical shape assumption*

An important assumption of spherical DPEs has been made in the development of the exact equalities (see Appendix C). This is implicit in the assumption of an isotropic point process for the DPE positions that result in (C 1). In general however, the DPE locations need not form an isotropic point process and thus the exact equalities may fail to hold.

3.2.3. *Internal circulation in a droplet*

As noted in § 2.2, the initial physical description for the LE statistical representation assumes a uniform velocity field inside a DPE (see (2.24) and (2.25)). In other words, the form of the Eulerian j.p.d.f. of velocity and radius expressed in terms of the point-process representation given by (3.9) assumes that the two-phase flow is composed of rigid DPEs, or DPEs in which the internal velocity field is uniform. However, if the dispersed phase is a fluid (as in droplets or bubbles) then the velocity field internal to the DPE need not be constant because of internal circulation effects. Under these conditions, the Eulerian j.p.d.f. as defined in its general form by (3.6) is capable of representing such internal circulation effects. However, its form in (3.9) as derived from the point-process representation will not be equal to that given by (3.6) when the velocity field is non-uniform inside the DPEs.

Although this may seem to be a trivial observation given an initial physical description in the LE statistical representation that assumes a uniform velocity field inside the DPE, the implications of this assumption will become evident in § 5 where a correspondence between unclosed terms in the governing equations across the two statistical representations is established. If the two-phase flow is composed of spherical DPEs with internal circulation, then this correspondence may not hold.

3.3. *Example to show relationship between statistical representations*

The difference between $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u},r;\boldsymbol{x},t)$ in the EE representation and $f^c_{\boldsymbol{V}R}(\boldsymbol{v},r|\boldsymbol{x};t)$ in the LE representation is illustrated by means of a simple example. Also, a comparison between the information contained in the number density $n(\boldsymbol{x};t)$ and $\alpha_d(\boldsymbol{x},t)$ is presented.

Consider an idealized two-phase flow comprising of spherical DPEs in the unit interval along the x-coordinate as shown in figure 5. The total number of DPEs N in

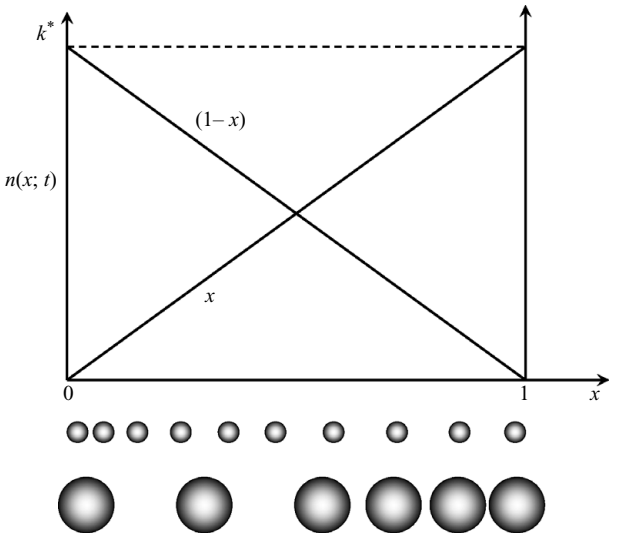

FIGURE 5. Variation of number density with position shown for an idealized two-phase flow composed of two streams of droplets. Droplets with radius r_0 have a position p.d.f. which decreases linearly from unity to zero, while droplets with radius $10r_0$ have a position p.d.f. which increases linearly from zero to unity. The resulting number density is homogeneous and equal to k^*.

the unit interval is deterministic and is always equal to k^*, i.e. $q_{(k^*)} = 1$. For simplicity only the position and radius properties of DPEs are considered. The two-phase flow can be interpreted as being composed of two streams of DPEs: one stream has DPEs of radius r_0, and the p.d.f. of their position decreases linearly from unity to zero with increasing x in the unit interval; while the other stream has DPEs of radius $10r_0$, and the p.d.f. of their position increases linearly from zero to unity with increasing x in the same unit interval. The single-particle density for this example problem is given by (cf. (2.35))

$$f_{1s}^{(k^*)}(x, r; t) = \delta(r - 10r_0)x + \delta(r - r_0)(1 - x). \tag{3.15}$$

Using (2.34) the d.d.f. corresponding to this idealized problem is

$$f(x, r, t) = k^* \left[\delta(r - 10r_0)x + \delta(r - r_0)(1 - x)\right] \tag{3.16}$$

Integrating the d.d.f. over all r_+ space, results in a statistically homogeneous number density

$$n(x; t) = k^* \left\{x + (1 - x)\right\} = k^*, \tag{3.17}$$

which was the intent in constructing this example.

In the LE approach, the p.d.f. of radius conditional on physical location as obtained from the d.d.f. is

$$f_R^c(r|\boldsymbol{x}; t) \ = \delta(r - 10r_0)x + \delta(r - r_0)(1 - x), \tag{3.18}$$

which is a simple linear combination of the two droplet streams. For instance at the mid-point of the unit interval, it is composed of two delta functions at r_0 and $10r_0$ each weighted by 0.5, i.e. on a number-basis there is equal probability of finding a droplet of radius r_0 or $10r_0$.

In the EE representation, the probability that the dispersed phase is located at x as obtained from its relationship (3.1) (or, from (3.4)) is given by

$$\alpha_d(x,t) = k^* \;\; 2r_0 \;\; (9x+1). \tag{3.19}$$

The limit $[x', r : x' \in b(x,r)]$ in (3.1) can be decomposed into two double integrals; one with limits $r = [0,\infty)$ and $x' = [x, x-r]$, and the other with limits $r = [0,\infty)$ and $x' = [x+r, x]$.

The above expression reveals that the probability of being in the liquid phase increases with x because the larger DPEs are occurring more frequently. Substituting the above expressions for $\alpha_d(x,t)$ and $f_R^c(r \mid x;t)$ into (3.9), the Eulerian p.d.f. of radius conditional on the liquid phase, $f^E_{R\,|I_d}(r;x,t)$ is found to be

$$f^E_{R\,|I_d}(r;x,t) = \frac{\{\delta(r-10r_0)10x + \delta(r-r_0)(1-x)\}}{(1+9x)}. \tag{3.20}$$

Clearly this Eulerian p.d.f. of radius is different from its Lagrangian counterpart (3.18). For instance at the midpoint of the unit interval it evaluates to

$$f^E_{R\,|I_d}(r;x,t) = \{0.91\,\delta(r-10r_0) + 0.09\,\delta(r-r_0)\}\,,$$

which reveals that the larger droplets are considerably more probable at that point. This simple example illustrates, as noted earlier, that $\alpha_d(\boldsymbol{x},t)$ and $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{v},r;\boldsymbol{x},t)$ depends on the dimensionality of the physical space defining the flow domain (one-dimensional in this example), whereas the radius p.d.f. in the Lagrangian approach $f^c_{\boldsymbol{V}R}(\boldsymbol{v},r|\boldsymbol{x};t)$ does not.

A related problem widely studied using two-phase DNS is that of monodispersed DPEs whose number density can vary in space. A linear dependence of $n(x;t)$ on x is the simplest form of inhomogeneity that can occur in two-phase flows. Assuming that the dispersed phase is composed of DPEs of size r_0, and the number density is varying as a function of x as $n(x;t) = k^*x$, then the single-particle density is given by

$$f_{1s}^{(k^*)} = \delta(r-r_0)x,$$

and the corresponding d.d.f. is

$$f(x,r,t) = k^*\delta(r-r_0)x.$$

The p.d.f. of radius conditional on location in the LE approach is

$$f_R^c(r \mid x;t) = \delta(r-r_0).$$

Following the same procedure as earlier, the volume fraction α_d corresponding to the inhomogeneous number density is

$$\alpha_d(x,t) = k^* \; 2r_0 \; x,$$

which shows that the volume fraction is also linear in x (and thus, inhomogeneous). The above expression also shows that for simple analytically integrable forms of the inhomogeneity in number density (cf. (3.5)) and invoking simplifying assumptions on the radius p.d.f., exact expressions for the volume fraction can be derived. However, if the number density variation in space is not an analytically integrable function of x, then the volume fraction cannot be expressed in terms of a simple function of number density. Finally, the Eulerian p.d.f. of radius $f^E_{R\,|I_d}(r;x,t)$ can be derived as

$$f^E_{R\,|I_d}(r;x,t) = \delta(r-r_0).$$

Note that for a linear number density and monodispersed size distribution, the p.d.f. f_R^c in the LE approach is the same as the Eulerian p.d.f. $f^E_{R\,|I_d}(r;x,t)$ in the EE approach.

Having established a clear foundation for the EE and the LE statistical representations, along with an understanding of the relationship between the two representations, we now derive the evolution equations corresponding to the probability densities in each approach.

4. Evolution equations for the probability densities

The primary objective of this section is to derive the evolution equations for densities $f_{\boldsymbol{U}|I_\beta}$ and $f(\boldsymbol{x},\boldsymbol{v},r,t)$ that were introduced in § 2 corresponding to the EE and LE statistical representations. Evolution equations for the densities developed in this section form the basis for the derivation of the phasic governing equations for the mean mass, mean momentum and second moment of velocity in the two statistical representations.

4.1. *Random-field statistical representation*

Although the transport equation for the p.d.f. can be obtained starting from the unweighted p.d.f. $f_{\boldsymbol{U}|I_\beta}$, it is convenient to work with mass-weighted or Favre quantities, as is done in single-phase flows (Pope 1985). The Favre fine-grained mass density conditional on the phase β is defined as

$$\mathscr{F}'_{\boldsymbol{U}|I_\beta}(\boldsymbol{u},\boldsymbol{x},t)=\rho(\boldsymbol{x},t)\,I_\beta(\boldsymbol{x},t)\delta(\boldsymbol{U}(\boldsymbol{x},t)-\boldsymbol{u}).$$

Here, ρ is the instantaneous thermodynamic density of the two-phase flow at $\boldsymbol{x}$. The expectation of $\mathscr{F}'_{\boldsymbol{U}|I_\beta}$ defines the Favre mass density conditional on phase β:

$$\mathscr{F}_{\boldsymbol{U}|I_\beta}\equiv\langle\mathscr{F}'_{\boldsymbol{U}|I_\beta}\rangle, \tag{4.1}$$

where the angled brackets $\langle\cdot\rangle$ represent an expectation over all possible realizations in the $\boldsymbol{u}$ space. Since the fundamental events defined in § 2.1 are in terms of $f_{\boldsymbol{U}}$, the following relations establish the connection between $\mathscr{F}_{\boldsymbol{U}|I_\beta}$ and the fundamental events (note that the dependence on $\boldsymbol{x}$ is implicit in the following development):

$$\begin{aligned}\mathscr{F}_{\boldsymbol{U}|I_\beta}=\langle\rho I_\beta\delta(\boldsymbol{U}-\boldsymbol{u})\rangle&=\int\langle\rho I_\beta\delta(\boldsymbol{U}-\boldsymbol{u})|\boldsymbol{U}=\boldsymbol{u}'\rangle\,f_{\boldsymbol{U}}(\boldsymbol{u}')\,\mathrm{d}\boldsymbol{u}'\\&=\int\delta(\boldsymbol{u}'-\boldsymbol{u})\,\langle\rho I_\beta|\boldsymbol{U}=\boldsymbol{u}'\rangle\,f_{\boldsymbol{U}}(\boldsymbol{u}')\,\mathrm{d}\boldsymbol{u}'\\&=\langle\rho I_\beta|\boldsymbol{U}=\boldsymbol{u}\rangle\,f_{\boldsymbol{U}}(\boldsymbol{u}).\end{aligned} \tag{4.2}$$

Integrating $\mathscr{F}_{\boldsymbol{U}|I_\beta}$ over all velocity space results in

$$\int_{\boldsymbol{u}}\mathscr{F}_{\boldsymbol{U}|I_\beta}(\boldsymbol{u},\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{u}=\langle\rho I_\beta\rangle(\boldsymbol{x},t).$$

The relationship between the mass density and the mass-weighted phasic velocity p.d.f. is given by $\mathscr{F}_{\boldsymbol{U}|I_\beta}=\langle\rho I_\beta\rangle\tilde{f}_{\boldsymbol{U}|I_\beta}$. Density-weighted means can be defined as

$$\langle\widetilde{Q(\boldsymbol{U})}\rangle(\boldsymbol{x},t)=\frac{1}{\langle\rho I_\beta\rangle}\int Q(\boldsymbol{u})\mathscr{F}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u}=\int Q(\boldsymbol{u})\tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u}, \tag{4.3}$$

where $\tilde{f}_{\boldsymbol{U}|I_\beta}$ is analogous to the phasic p.d.f. $f_{\boldsymbol{U}|I_\beta}$ defined in § 2.1. Likewise, unweighted means can also be defined as

$$\langle Q(\boldsymbol{U})\rangle(\boldsymbol{x},t) = \int Q(\boldsymbol{u}) f_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u} = \int Q(\boldsymbol{u})\frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\,\mathrm{d}\boldsymbol{u}. \tag{4.4}$$

The evolution equation for the fine-grained mass density is obtained by forming the substantial derivative of $\mathscr{F}'_{\boldsymbol{U}|I_\beta}$ as

$$\frac{\mathrm{D}}{\mathrm{D}t}\mathscr{F}'_{\boldsymbol{U}|I_\beta} = \frac{\partial}{\partial t}\mathscr{F}'_{\boldsymbol{U}|I_\beta} + U_k\frac{\partial}{\partial x_k}\mathscr{F}'_{\boldsymbol{U}|I_\beta}, \tag{4.5}$$

where $\boldsymbol{U}$, the instantaneous two-phase flow velocity, is the convective velocity of the fine-grained mass density in $\boldsymbol{x}$-space. Using a standard procedure of differentiating delta functions (Pope 2000), the temporal and spatial derivatives of $\mathscr{F}'_{\boldsymbol{U}|I_\beta}$ can be derived from the corresponding fine-grained density, resulting finally in

$$\frac{\mathrm{D}}{\mathrm{D}t}\mathscr{F}'_{\boldsymbol{U}|I_\beta} = -\frac{\partial}{\partial u_k}\left[\left(\frac{\partial U_k}{\partial t} + U_j\frac{\partial U_k}{\partial x_j}\right)\right]\mathscr{F}'_{\boldsymbol{U}|I_\beta} + \frac{\mathscr{F}'_{\boldsymbol{U}|I_\beta}}{\rho I_\beta}\left(\frac{\partial(\rho I_\beta)}{\partial t} + U_k\frac{\partial(\rho I_\beta)}{\partial x_k}\right). \tag{4.6}$$

The convective part of $\mathrm{D}\mathscr{F}'_{\boldsymbol{U}|I_\beta}/\mathrm{D}t$ in (4.5) can be written as

$$\begin{aligned} U_k\frac{\partial}{\partial x_k}\mathscr{F}'_{\boldsymbol{U}|I_\beta} &= \frac{\partial}{\partial x_k}\left(U_k\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right) - \mathscr{F}'_{\boldsymbol{U}|I_\beta}\frac{\partial U_k}{\partial x_k} \\ &= u_k\frac{\partial}{\partial x_k}\left(\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right) - \mathscr{F}'_{\boldsymbol{U}|I_\beta}\frac{\partial U_k}{\partial x_k}, \end{aligned} \tag{4.7}$$

where the instantaneous two-phase velocity is not assumed to be solenoidal. The random variable U_k in the first equality can be replaced by the sample space variable u_k due to the sifting property of the delta function in $\mathscr{F}'_{\boldsymbol{U}|I_\beta}$.

We will now show that the last term on the right-hand side of (4.6) represents a contribution due to interphase mass transfer. The term $\mathscr{F}'_{\boldsymbol{U}|I_\beta}\partial U_k/\partial x_k$ on the right-hand side of (4.7) can be combined with the last term on the right-hand side of (4.6) to give

$$\begin{aligned} \frac{\partial\mathscr{F}'_{\boldsymbol{U}|I_\beta}}{\partial t} + u_k\frac{\partial}{\partial x_k}\left(\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right) = -\frac{\partial}{\partial u_k}\left[\left(\frac{\partial U_k}{\partial t} + U_j\frac{\partial U_k}{\partial x_j}\right)\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right] \\ + \frac{\mathscr{F}'_{\boldsymbol{U}|I_\beta}}{\rho I_\beta}\left(\frac{\partial(\rho I_\beta)}{\partial t} + \frac{\partial(\rho I_\beta U_k)}{\partial x_k}\right). \end{aligned} \tag{4.8}$$

Since the velocity field $\boldsymbol{U}$ is the instantaneous two-phase velocity field in the two-phase flow, it satisfies instantaneous mass conservation in each phase. Thus, on each realization it is true that

$$I_\beta\left[\frac{\partial\rho}{\partial t} + \frac{\partial(\rho U_k)}{\partial x_k}\right] = 0.$$

Using the product rule and rearranging results in

$$\left[\frac{\partial(\rho I_\beta)}{\partial t} + \frac{\partial(\rho I_\beta U_k)}{\partial x_k}\right] = \rho\left[\frac{\partial I_\beta}{\partial t} + U_k\frac{\partial I_\beta}{\partial x_k}\right]. \tag{4.9}$$

The material derivative of I_β on the right-hand side of the above equation can be simplified as

$$\frac{\partial I_\beta}{\partial t} + U_k \frac{\partial I_\beta}{\partial x_k} = \left[\frac{\partial I_\beta}{\partial t} + \left(U_k - U_k^{(I)} + U_k^{(I)}\right)\frac{\partial I_\beta}{\partial x_k}\right] = \left[\frac{\partial I_\beta}{\partial t} + U_k^{(I)}\frac{\partial I_\beta}{\partial x_k}\right] + \left(U_k - U_k^{(I)}\right)\frac{\partial I_\beta}{\partial x_k},$$

where $\boldsymbol{U}^{(I)}$ is the velocity of the phasic interface, with the additional observation that the topological equation (Drew 1983) holds

$$\frac{\partial I_\beta}{\partial t} + U_k^{(I)}\frac{\partial I_\beta}{\partial x_k} = 0. \tag{4.10}$$

Thus, instantaneous mass conservation at any location in the two-phase flow implies

$$\left[\frac{\partial(\rho I_\beta)}{\partial t} + \frac{\partial(\rho I_\beta U_k)}{\partial x_k}\right] = \rho\left[\left(U_k - U_k^{(I)}\right)\frac{\partial I_\beta}{\partial x_k}\right]. \tag{4.11}$$

The above development shows that the instantaneous mass conservation in each phase (4.11) has a source term due to the difference between the interface velocity and the instantaneous two-phase velocity, which occurs in two-phase flows with interphase mass transfer, e.g. vaporization. An interesting observation from (4.9) is that in flows with zero interphase mass transfer, the indicator function behaves like a non-diffusive conserved scalar

$$\frac{\mathrm{D}}{\mathrm{D}t} I_\beta = \frac{\partial I_\beta}{\partial t} + U_k \frac{\partial I_\beta}{\partial x_k} = 0.$$

With the above simplifications, (4.8) becomes

$$\frac{\partial \mathscr{F}'_{\boldsymbol{U}|I_\beta}}{\partial t} + u_k \frac{\partial}{\partial x_k}\left(\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right) = -\frac{\partial}{\partial u_k}\left[\left(\frac{\partial U_k}{\partial t} + U_j\frac{\partial U_k}{\partial x_j}\right)\mathscr{F}'_{\boldsymbol{U}|I_\beta}\right] + \frac{\mathscr{F}'_{\boldsymbol{U}|I_\beta}}{\rho I_\beta}\left[\rho\left(U_k - U_k^{(I)}\right)\frac{\partial I_\beta}{\partial x_k}\right], \tag{4.12}$$

where the last term accounts for the change in the fine-grained density $\mathscr{F}'_{\boldsymbol{U}|I_\beta}$ due to interphase mass transfer. Taking the expectation of (4.12) and using the definition (4.1) leads to the evolution equation for the phasic mass density in each phase β

$$\frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial t} + u_k \frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial x_k} = -\frac{\partial}{\partial u_k}\left[\left\langle \rho I_\beta \frac{\mathrm{D}U_k}{\mathrm{D}t}\middle| \boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right] + \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\left\langle \rho\left(U_k - U_k^{(I)}\right)\frac{\partial I_\beta}{\partial x_k}\middle|\boldsymbol{u}\right\rangle \tag{4.13}$$

where $\langle\cdot|\boldsymbol{U} = \boldsymbol{u}\rangle$ is abbreviated as $\langle\cdot|\boldsymbol{u}\rangle$. The description of each term in the above equation is as follows: the two terms on the left-hand side represent the unsteady and convective derivative of the phasic mass density; on the right-hand side, the first term represents the transport in velocity space and the second term represents a source in the transport equation due to a regressing interface (in case of evaporating sprays). This term leads to the interphase mass transfer source term in the phasic mean mass conservation (see (5.1)), the contribution to the mean momentum due to interphase mass transfer (see (5.13) and (5.15)) and the contribution to the phasic Reynolds stresses due to interphase mass transfer (see (5.29)).

The terms representing transport in velocity space and the mass source in (4.13) are unclosed, i.e. they are not known in terms of the phasic mass density. Since the mass density transport equation is a one-point description of the two-phase flow, the unclosed terms are also evaluated at a single location in space–time coordinates. However, closures for such terms are almost always non-local in the sense that information at a particular location can depend on the state at other locations in the two-phase flow. For instance, as discussed in § 5.3, the drag experienced by a DPE depends on the pressure and state of fluid stress at its surface. Such information is absent in the mass density transport equation (4.13), since non-local information cannot be captured in a one-point description of the two-phase flow. In fact, a one-point description cannot distinguish between a location on the surface of a DPE and one in the bulk (see schematic illustration in figure 2). To distinguish the two locations one would require, at a minimum, a two-point description of the system.

In order to gain insight into (4.13) in terms of the decomposition $\mathscr{F}_{\boldsymbol{U}|I_\beta} = \langle \rho I_\beta \rangle \tilde{f}_{\boldsymbol{U}|I_\beta}$, we form

$$\langle \rho I_\beta \rangle \frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial t} = \frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial t} - \tilde{f}_{\boldsymbol{U}|I_\beta} \frac{\partial \langle \rho I_\beta \rangle}{\partial t},$$

to derive the evolution of $\tilde{f}_{\boldsymbol{U}|I_\beta}$. The second term on the right-hand side is the evolution equation of $\langle \rho I_\beta \rangle$ obtained by integrating (4.13) over all velocity space (see (5.1) in § 5). Substituting (4.13) and (5.1) into the above equation and rearranging results in

$$\begin{aligned} \frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial t} + u_k \frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial x_k} = &- \frac{\partial}{\partial u_k} \left[\left\langle \rho I_\beta \frac{\mathrm{D}U_k}{\mathrm{D}t} \middle| \boldsymbol{u} \right\rangle \frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta | \boldsymbol{u} \rangle} \right] \\ &+ \frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta | \boldsymbol{u} \rangle} \left\langle \rho \left(U_k - U_k^{(I)} \right) \frac{\partial I_\beta}{\partial x_k} \middle| \boldsymbol{u} \right\rangle - \tilde{f}_{\boldsymbol{U}|I_\beta} \frac{\mathrm{D}}{\mathrm{D}t} \ln \langle \rho I_\beta \rangle, \end{aligned} \tag{4.14}$$

where

$$\frac{\mathrm{D}}{\mathrm{D}t} \langle \rho I_\beta \rangle = \frac{\partial}{\partial t} \langle \rho I_\beta \rangle + u_k \frac{\partial \langle \rho I_\beta \rangle}{\partial x_k}.$$

Defining the acceleration conditional on velocity in phase β as

$$\langle \boldsymbol{A}^{(\beta)} | \boldsymbol{u} \rangle = \frac{1}{\langle \rho I_\beta | \boldsymbol{u} \rangle} \left\langle \rho I_\beta \frac{\mathrm{D}\boldsymbol{U}}{\mathrm{D}t} \middle| \boldsymbol{u} \right\rangle,$$

and the source term due to interphase mass transfer conditional on velocity as

$$\left\langle S_\rho^{(\beta)} \middle| \boldsymbol{u} \right\rangle = \left\langle \rho \left(U_k - U_k^{(I)} \right) \frac{\partial I_\beta}{\partial x_k} \middle| \boldsymbol{u} \right\rangle,$$

(4.14) can be rewritten as

$$\frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial t} + u_k \frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial x_k} + \frac{\partial}{\partial u_k} \left\langle A_k^{(\beta)} \middle| \boldsymbol{u} \right\rangle \tilde{f}_{\boldsymbol{U}|I_\beta} = \frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta | \boldsymbol{u} \rangle} \left\langle S_\rho^{(\beta)} \middle| \boldsymbol{u} \right\rangle - \tilde{f}_{\boldsymbol{U}|I_\beta} \frac{\mathrm{D}}{\mathrm{D}t} \ln \langle \rho I_\beta \rangle. \tag{4.15}$$

One may verify using (4.15) that the source term on the right-hand side involving the material derivative of $\ln \langle \rho I_\beta \rangle$ ensures that $\tilde{f}_{\boldsymbol{U}|I_\beta}$ retains its normalization property for all time (see Appendix A). An interesting analogy exists between the evolution equation for $\tilde{f}_{\boldsymbol{U}|I_\beta}$ above, and that for f_{VR}^c in the LE approach (see the discussion following (4.21)).

4.2. *Lagrangian statistical representation*

Starting from the Klimontovich fine-grained density (2.27), and using the droplet evolution equations (2.24)–(2.26), an evolution equation for the droplet distribution function $f(\boldsymbol{x}, \boldsymbol{v}, r, t)$, also widely known as Williams' spray equation, can be derived (Subramaniam 2001)

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x_j}[v_j f] + \frac{\partial}{\partial v_j}\left[\langle A_j|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle f\right] + \frac{\partial}{\partial r}\left[\langle \Theta|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle f\right] = 0. \tag{4.16}$$

For the sake of brevity, a detailed derivation of the d.d.f. evolution equation is not reproduced here and can be found in Subramaniam (2001). In (4.16), $\langle \boldsymbol{A}|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle$ is the expected acceleration conditional on the location $\boldsymbol{x}$, velocity $\boldsymbol{v}$ and radius r, and $\langle \Theta|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle$ is the expected vaporization rate conditional on location, velocity and radius. These quantities are given as (Subramaniam 2001)

$$\langle \boldsymbol{A}|\ \boldsymbol{x}, \boldsymbol{v}, r; t\rangle = \frac{1}{f(\ \boldsymbol{x}, \boldsymbol{v}, r, t)}\left\{\sum_{k\geqslant 1} q_{(k)}\langle \boldsymbol{A}^{(k)}|\ \boldsymbol{x}, \boldsymbol{v}, r, t)\rangle f^{(k)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)\right\} \tag{4.17}$$

if $f > 0$, and zero otherwise, and

$$\langle \Theta|\ \boldsymbol{x}, \boldsymbol{v}, r; t\rangle = \frac{1}{f(\ \boldsymbol{x}, \boldsymbol{v}, r, t)}\left\{\sum_{k\geqslant 1} q_{(k)}\langle \Theta^{(k)}|\ \boldsymbol{x}, \boldsymbol{v}, r, t)\rangle f^{(k)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)\right\} \tag{4.18}$$

if $f > 0$, and zero otherwise. Furthermore, in the above expressions,

$$\langle \boldsymbol{A}^{(k)}|\ \boldsymbol{x}, \boldsymbol{v}, r; t\rangle = \frac{1}{f^{(k)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)}\left\{\left\langle \sum_{i=1}^{k} \boldsymbol{A}_{(i)} f'_{(i)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)\right\rangle\right\} \tag{4.19}$$

if $f^{(k)} > 0$, and zero otherwise, and

$$\langle \Theta^{(k)}|\ \boldsymbol{x}, \boldsymbol{v}, r; t\rangle = \frac{1}{f^{(k)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)}\left\{\left\langle \sum_{i=1}^{k} \Theta_{(i)} f'_{(i)}(\ \boldsymbol{x}, \boldsymbol{v}, r, t)\right\rangle\right\} \tag{4.20}$$

if $f^{(k)} > 0$, and zero otherwise.

As the above expressions suggest, $\langle \boldsymbol{A}|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle$ is not the acceleration corresponding to a single DPE (cf. $\boldsymbol{A}_{(i)}$ in (4.19)), but is the expected acceleration contribution at location $\boldsymbol{x}$ due to a large ensemble of realizations of the two-phase flow under consideration. Similarly, $\langle \Theta|\boldsymbol{x}, \boldsymbol{v}, r; t\rangle$ is not the vaporization rate corresponding to a single droplet (cf. $\Theta_{(i)}$ in (4.20)), but is the expected vaporization rate contribution at a point $\boldsymbol{x}$ due to a large ensemble of realizations of the same two-phase flow. Note that there are two intermediate stages of averaging performed on the droplet acceleration and vaporization rate (cf. (4.17) and (4.19) for $\boldsymbol{A}_{(i)}$, and (4.18) and (4.20) for $\Theta_{(i)}$). Therefore, $\langle \boldsymbol{A}|\ \boldsymbol{x}, \boldsymbol{v}, r, t\rangle$ and $\langle \Theta|\ \boldsymbol{x}, \boldsymbol{v}, r, t\rangle$ are not the droplet acceleration and the droplet vaporization rate, respectively.

It is noteworthy that using the decomposition $f = n f^c_{VR}$ and using an analogous approach as in §4.1, we can form the transport equation for f^c_{VR} as (cf. (66) in Subramaniam 2001):

$$\frac{\partial f^c_{VR}}{\partial t} + \frac{\partial}{\partial x_k} v_k f^c_{VR} + \frac{\partial}{\partial v_k}\left[\langle A_k|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle f^c_{VR}\right] + \frac{\partial}{\partial r}\left[\langle \Theta|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle f^c_{VR}\right] = -f^c_{VR}\frac{\mathrm{D}}{\mathrm{D}t}\ln n(\boldsymbol{x}; t). \tag{4.21}$$

Analogous to the EE representation, the source term involving the material derivative of $\ln n$ ensures that f^c_{VR} retains its normalization property for all time. Comparing the

two equations (4.15) and (4.21), we note a correspondence between individual terms for the case $\beta = d$

$$u_k \frac{\partial \tilde{f}_{\boldsymbol{U}|I_\beta}}{\partial x_k} \Longleftrightarrow \frac{\partial}{\partial x_k} v_k f^c_{\boldsymbol{V}R} \tag{4.22}$$

$$\frac{\partial}{\partial u_k}\langle A_k^{(\beta)}|\boldsymbol{u}\rangle \tilde{f}_{\boldsymbol{U}|I_\beta} \Longleftrightarrow \frac{\partial}{\partial v_k}\left[\langle A_k|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle f^c_{\boldsymbol{V}R}\right] \tag{4.23}$$

$$-\frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\langle S_\rho^{(\beta)}|\boldsymbol{u}\rangle \Longleftrightarrow \frac{\partial}{\partial r}\left[\langle \Theta|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle f^c_{\boldsymbol{V}R}\right] \tag{4.24}$$

$$\tilde{f}_{\boldsymbol{U}|I_\beta}\frac{D}{Dt}\ln\langle \rho I_\beta\rangle \Longleftrightarrow f^c_{\boldsymbol{V}R}\frac{D}{Dt}\ln n(\boldsymbol{x}, t). \tag{4.25}$$

Since a correspondence exists between terms in the evolution equations for the probability densities in the EE and LE statistical representations, one may expect a similar correspondence to exist between terms in the corresponding moment equations, which are the phasic governing equations for the mean mass, mean momentum and second moment of velocity in the two statistical representations. This correspondence is established in the next section.

Transport equations for the probability densities in the EE and LE statistical representations have been derived. It is now straightforward to derive the governing equations for the mean mass, mean momentum and the second moment of velocity in each statistical representation from these transport equations.

5. Governing equations for a two-phase flow

5.1. *Mean mass conservation*

5.1.1. *Random field statistical representation*

As noted earlier, integrating (4.13) over $\boldsymbol{u}$ space results in the mean mass conservation in each phase

$$\frac{\partial \alpha_\beta \langle \rho|I_\beta = 1\rangle}{\partial t} + \frac{\partial}{\partial x_k}\left(\alpha_\beta\langle \rho|I_\beta = 1\rangle\widetilde{\langle U_k^{(\beta)}\rangle}\right) = \langle S_\rho^{(\beta)}\rangle, \tag{5.1}$$

where $\langle S_\rho^{(\beta)}\rangle$ is the unconditional interphase mass transfer term. The term $\langle \rho|I_\beta = 1\rangle$ is the expected value of the thermodynamic density conditional on the indicator function corresponding to phase β being unity at location $\boldsymbol{x}$.

5.1.2. *Number-density based Lagrangian approach*

If a constant thermodynamic density of the dispersed phase ρ_d is assumed, then the mean mass conservation equation implied by the d.d.f. evolution equation is obtained by multiplying (4.16) by $(4/3)\pi r^3 \rho_d$ and integrating over all $[\boldsymbol{v}, r_+]$, to obtain

$$\frac{\partial}{\partial t}\left[\frac{4}{3}\pi\langle R^3\rangle \rho_d\, n\right] + \frac{\partial}{\partial x_k}\left[\frac{4}{3}\pi\langle R^3\rangle\langle \widetilde{V}_k\rangle \rho_d\, n\right]$$
$$= n\frac{4}{3}\pi\rho_d\,\langle R^3\rangle\{3\langle \widetilde{\Omega}\mid \boldsymbol{x}; t\rangle + \langle \widetilde{\Theta}\mid \boldsymbol{x}, r = 0_+; t\rangle f_R^c(r = 0_+|\boldsymbol{x}; t)\}, \tag{5.2}$$

where $\Omega = \Theta/R$ and the volume-weighted average of any smooth function $Q(\boldsymbol{v}, r)$ is defined as

$$\langle \widetilde{Q} \rangle \equiv \frac{\langle R^3 Q \rangle}{\langle R^3 \rangle}.$$

The source term on the right-hand side of (5.2) contains two parts. The part containing Ω corresponds to a loss of mean mass due to evaporation. The other part represents the depletion of number density due to a flux of droplets across the $r = 0_+$ boundary, which corresponds to the smallest radius below which a drop is considered evaporated.

5.1.3. *Correspondence for locally homogeneous flows*

Under conditions of local homogeneity (see Appendix C.2 for details), a correspondence between unclosed terms across the two statistical representations can be established. For statistically homogeneous number density (but inhomogeneous radius p.d.f.), the following relationships hold:

$$\alpha_d(\boldsymbol{x}, t) = n(t)\frac{4}{3}\pi\langle R^3 \rangle(\boldsymbol{x}, t) \tag{5.3}$$

$$f^E_{R|I_d}(r; \boldsymbol{x}, t) = r^3 f^c_R(r|\boldsymbol{x}, t)/\langle R^3 \rangle(\boldsymbol{x}, t), \tag{5.4}$$

where the last equality holds only for two-phase flows with rigid particles, or for two-phase flows with fluid-dispersed phase elements in which the internal fluid motion can be neglected. Using the first of the above relations, (5.2) can be written as

$$\frac{\partial}{\partial t}\left[\alpha_d\ \rho_d\ \right] + \frac{\partial}{\partial x_k}\left[\alpha_d\ \rho_d\ \langle \widetilde{V}_k \rangle\right] = \alpha_d\ \rho_d\ 3\langle \widetilde{\Omega} \mid \boldsymbol{x}; t\rangle + \alpha_d\ \rho_d\ \langle \widetilde{\Theta} \mid \boldsymbol{x}, r = 0_+; t\rangle f^c_R(r = 0_+|\boldsymbol{x}; t). \tag{5.5}$$

If (5.4) holds, then it is true that

$$\langle \widetilde{\boldsymbol{U}^{(d)}} \rangle = \widetilde{\langle \boldsymbol{V} \rangle}. \tag{5.6}$$

Then (5.5) can be directly compared with the phase mass conservation equation (5.1) arising from the random-field approach written for the dispersed phase (i.e. $\beta = d$) and for constant thermodynamic density $\langle \rho | I_d = 1 \rangle = \rho_d$

$$\frac{\partial}{\partial t}[\alpha_d \rho_d] + \frac{\partial}{\partial x_k}\left[\alpha_d \rho_d \langle \widetilde{U^{(d)}_k} \rangle\right] = \langle S^{(d)}_\rho \rangle, \tag{5.7}$$

thereby leading to the correspondence of the terms

$$\langle S^{(d)}_\rho \rangle \Longleftrightarrow \alpha_d\ \rho_d\ \{3\langle \widetilde{\Omega} \mid \boldsymbol{x}; t\rangle + \langle \widetilde{\Theta} \mid \boldsymbol{x}, r = 0_+; t\rangle f^c_R(r = 0_+|\boldsymbol{x}; t)\ \}. \tag{5.8}$$

If the number density retains spatial homogeneity as the flow evolves, then the above correspondence becomes an equality. However, if the number density develops spatial inhomogeneities as the flow evolves, then relation given by (5.3) no longer holds, and the correspondence given above should be treated only as an approximation.

5.2. *Mean momentum conservation*

5.2.1. *Random-field statistical representation*

Multiplying (4.13) by u_i and integrating over $\boldsymbol{u}$ space results in

$$\frac{\partial \langle \rho I_\beta \rangle \widetilde{\langle U^{(\beta)}_i \rangle}}{\partial t} + \frac{\partial}{\partial x_j}\langle \rho I_\beta \rangle \widetilde{\langle U_i U_j \rangle} = \left\langle \rho I_\beta \frac{\mathrm{D}U_i}{\mathrm{D}t} \right\rangle + \left\langle \rho U_i \left(U_j - U^{(I)}_j\right) \frac{\partial I_\beta}{\partial x_j} \right\rangle. \tag{5.9}$$

If the fluctuation with respect to the Favre-averaged phasic velocity is defined as $\boldsymbol{u}''^{(\beta)} = \boldsymbol{U} - \langle \widetilde{\boldsymbol{U}^{(\beta)}} \rangle$, then the above expression can be simplified as

$$\frac{\partial \langle \rho I_\beta \rangle \langle \widetilde{U_i^{(\beta)}} \rangle}{\partial t} + \frac{\partial}{\partial x_j} \langle I_\beta \rho \rangle \langle \widetilde{U_i^{(\beta)}} \rangle \langle \widetilde{U_j^{(\beta)}} \rangle = -\frac{\partial}{\partial x_j} \left\langle I_\beta \rho \; u_i''^{(\beta)} u_j''^{(\beta)} \right\rangle + \left\langle \rho I_\beta \frac{\mathrm{D}U_i}{\mathrm{D}t} \right\rangle + \left\langle \rho U_i \left(U_j - U_j^{(I)} \right) \frac{\partial I_\beta}{\partial x_j} \right\rangle \quad (5.10)$$

(the reader is cautioned against confusing the fluctuation $\boldsymbol{u}''^{(\beta)}$ with the sample space variable $\boldsymbol{u}$ corresponding to the random variable $\boldsymbol{U}$; the choice of the fluctuating velocity is discussed in § 5.3). The above mean momentum equation is identical to that derived using the indicator function formalism of Drew (1983).

The second term on the right-hand side of (5.10) is equal to the expectation of the divergence of the stress tensor evaluated in the βth phase

$$\left\langle \rho I_\beta \frac{\mathrm{D}U_i}{\mathrm{D}t} \right\rangle = \left\langle I_\beta \frac{\partial \tau_{ji}}{\partial x_j} \right\rangle. \quad (5.11)$$

The mean momentum equations as given by (5.10) are not GI forms; the first term (cf. (5.11)) on the right-hand side of this equation is the only GI term. Note that a Galilean transformation consists of a change of reference frame from $(\boldsymbol{x}, t)$ to $(\boldsymbol{x}^*, t^*)$ by transforming position and time as $\boldsymbol{x}^* = \boldsymbol{x} + \boldsymbol{W}t$ and $t^* = t$, respectively, where $\boldsymbol{W}$ is a constant translational velocity. If a quantity $\boldsymbol{Q}$ is GI, then $\boldsymbol{Q}(\boldsymbol{x}^*, t^*) = \boldsymbol{Q}(\boldsymbol{x}, t)$. The velocity transforms as $\boldsymbol{U}^*(\boldsymbol{x}^*, t^*) = \boldsymbol{U}^*(\boldsymbol{x} + \boldsymbol{W}t, t) = \boldsymbol{U}(\boldsymbol{x}, t) + \boldsymbol{W}$ and is not GI. When constructing models for terms such as interphase mass, momentum and energy transfer, it is useful to model the GI forms of these terms because such models are then frame-invariant with respect to Galilean transformations. If the non-GI forms are modelled, then the resulting models may not be frame-invariant.

One can rewrite (5.10) as

$$\frac{\partial}{\partial t} \left[\alpha_\beta \langle \rho \mid I_\beta = 1 \rangle \langle \widetilde{U_i^{(\beta)}} \rangle \right] + \frac{\partial}{\partial x_j} \left[\alpha_\beta \langle \rho \mid I_\beta = 1 \rangle \langle \widetilde{U_i^{(\beta)}} \rangle \langle \widetilde{U_j^{(\beta)}} \rangle \right] = -\frac{\partial}{\partial x_j} \left[\alpha_\beta \langle \rho \mid I_\beta = 1 \rangle \widetilde{R}_{ij}^{(\beta)} \right] + \left\langle \frac{\partial}{\partial x_j} \left(I_\beta \tau_{ji} \right) \right\rangle + \langle S_{Mi}^{(\beta)} \rangle. \quad (5.12)$$

The Reynolds stress in the βth phase $\widetilde{R}_{ij}^{(\beta)}$ is given by

$$\widetilde{R}_{ij}^{(\beta)} \equiv \frac{\left\langle I_\beta \rho \; u_i''^{(\beta)} u_j''^{(\beta)} \right\rangle}{\langle I_\beta \rho \rangle},$$

while $\langle \boldsymbol{S}_M^{(\beta)} \rangle$ is the interfacial momentum source term.

The term $\langle \boldsymbol{S}_M^{(\beta)} \rangle$ is composed of two parts, one is attributable to the interphase mass transfer arising from phase change $\langle \boldsymbol{S}_M^{(\beta)(PC)} \rangle$, and the other to the interfacial stress $\langle \boldsymbol{S}_M^{(\beta)(IS)} \rangle$, which is non-zero even in the absence of interphase mass transfer. These are defined as

$$\langle S_{Mi}^{(\beta)(PC)} \rangle \equiv \left\langle \rho U_i \left(U_j - U_j^{(I)} \right) \frac{\partial I_\beta}{\partial x_j} \right\rangle \tag{5.13}$$

$$\langle S_{Mi}^{(\beta)(IS)} \rangle \equiv - \left\langle \tau_{ji} \frac{\partial I_\beta}{\partial x_j} \right\rangle. \tag{5.14}$$

The one arising from interfacial stress $\langle S_{Mj}^{(\beta)(IS)} \rangle$ is in GI form, whereas $\langle S_{Mj}^{(\beta)(PC)} \rangle$, the term arising from interfacial mass transfer, is not in GI form.

Substituting the mean mass conservation equation (5.1) into (5.10) results in

$$\alpha_\beta \langle \rho \mid I_\beta = 1 \rangle \frac{\tilde{\mathrm{D}}_\beta \widetilde{\langle U_i^{(\beta)} \rangle}}{\tilde{\mathrm{D}}_\beta t} + \frac{\partial}{\partial x_j} \left[\alpha_\beta \langle \rho \mid I_\beta = 1 \rangle \widetilde{R}_{ij}^{(\beta)} \right] - \left\langle \frac{\partial}{\partial x_j} (I_\beta \tau_{ji}) \right\rangle$$
$$= \langle S_{Mi}^{(\beta)(IS)} \rangle + \{ \langle S_{Mi}^{(\beta)(PC)} \rangle - \widetilde{\langle U_i^{(\beta)} \rangle} \langle S_\rho^{(\beta)} \rangle \}, \tag{5.15}$$

where the operator

$$\frac{\tilde{\mathrm{D}}_\beta}{\tilde{\mathrm{D}}_\beta t} = \frac{\partial}{\partial t} + \widetilde{\langle U_k^{(\beta)} \rangle} \frac{\partial}{\partial x_k}. \tag{5.16}$$

Written in the above form, the material derivative $\tilde{\mathrm{D}}_\beta \widetilde{\langle U_j^{(\beta)} \rangle} / \tilde{\mathrm{D}}_\beta t$ following the Favre-averaged phasic mean velocity is in GI form. Also the other terms on the left-hand side and $\langle S_{Mi}^{(\beta)(IS)} \rangle$ are in GI form. It follows that the term $\{ \langle S_{Mi}^{(\beta)(PC)} \rangle - \widetilde{\langle U_i^{(\beta)} \rangle} \langle S_\rho^{(\beta)} \rangle \}$ on the right-hand side of (5.15) should also be in GI form. Therefore, it is this term that should be modelled in the mean momentum equation for two-phase flows with interphase mass transfer.

5.2.2. *Number-density based Lagrangian approach*

The mean momentum conservation equation implied by the d.d.f. evolution equation (4.16) is obtained by multiplying (4.16) by $(4/3)\pi r^3 \rho_d v_j$ and integrating over all $[\boldsymbol{v}, r_+]$ space, resulting in

$$\frac{\partial}{\partial t} \left[n \frac{4}{3} \pi \rho_d \langle R^3 \rangle \widetilde{\langle V_i \rangle} \right] + \frac{\partial}{\partial x_j} \left[n \frac{4}{3} \pi \rho_d \ \langle R^3 \rangle \widetilde{\langle V_i V_j \rangle} \right] = n \frac{4}{3} \pi \rho_d \ \langle R^3 \rangle \widetilde{\langle A_i \mid \boldsymbol{x}; t \rangle}$$
$$+ n \frac{4}{3} \pi \rho_d \langle R^3 \rangle \{ 3 \widetilde{\langle V_i \Omega \mid \boldsymbol{x}; t \rangle} + \widetilde{\langle V_i \Theta \mid \boldsymbol{x}, r = 0_+; t \rangle} f_R^c (r = 0_+ | \boldsymbol{x}; t) \}, \tag{5.17}$$

where mass-weighted averages have been used as in (5.2). The first term on the right-hand side of the above equation represents the interphase transfer of momentum, while the last term on the right-hand side corresponds to a loss of mean momentum due to evaporation, and the depletion of mean momentum due to a flux of droplets across the $r = 0_+$ boundary.

Substituting the mean mass conservation equation (5.2) into (5.17) results in

$$
\begin{aligned}
&n\frac{4}{3}\pi\rho_d\langle R^3\rangle\left\{\frac{\partial\langle\widetilde{V}_i\rangle}{\partial t}+\langle\widetilde{V}_j\rangle\frac{\partial\langle\widetilde{V}_i\rangle}{\partial x_j}\right\}\\
&\quad=n\frac{4}{3}\pi\rho_d\ \langle R^3\rangle\langle\widetilde{A}_i\mid\boldsymbol{x};t\rangle-\frac{\partial}{\partial x_j}\left[n\frac{4}{3}\pi\rho_d\ \langle R^3\rangle\langle\widetilde{v_i''v_j''}\rangle\right]\\
&\qquad+n\frac{4}{3}\pi\rho_d\ \langle R^3\rangle\{3\langle\widetilde{V_i\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{V_i\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+|\boldsymbol{x};t)\}\\
&\qquad-n\frac{4}{3}\pi\rho_d\ \langle R^3\rangle\{3\langle\widetilde{V}_i\rangle\langle\widetilde{\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{V}_i\rangle\langle\widetilde{\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+|\boldsymbol{x};t)\},
\end{aligned}
\tag{5.18}
$$

where

$$
\langle\widetilde{v_i''v_j''}\rangle\equiv\int_{[\boldsymbol{v},r_+]}\big(v_i-\langle\widetilde{V}_i\rangle\big)\big(v_j-\langle\widetilde{V}_j\rangle\big)\frac{r^3f_{VR}^c(\boldsymbol{v},r|\boldsymbol{x};t)}{\langle R^3(\boldsymbol{x},t)\rangle}\mathrm{d}\boldsymbol{v}\,\mathrm{d}r,
$$

The above equation is in GI form, and from among the unclosed terms, those that specifically correspond to the contribution of interphase mass transfer to the mean momentum are

$$
\{\langle\widetilde{V_i\Omega}\mid\boldsymbol{x};t\rangle-\langle\widetilde{V}_i\rangle\langle\widetilde{\Omega}\mid\boldsymbol{x};t\rangle\},
\tag{5.19}
$$

and

$$
\{\langle\widetilde{V_i\Theta}\mid\boldsymbol{x},r=0_+;t\rangle-\langle\widetilde{V}_i\rangle\langle\widetilde{\Theta}\mid\boldsymbol{x},r=0_+;t\rangle\}.
\tag{5.20}
$$

It is useful to note that Lagrangian particle-method solutions (Amsden *et al.* 1989; Pai & Subramaniam 2006, 2007) to the d.d.f. evolution equation that indirectly model $\langle\boldsymbol{A}|\boldsymbol{x},\boldsymbol{v},r;t\rangle$ and $\langle\Theta|\boldsymbol{x},\boldsymbol{v},r;t\rangle$ automatically guarantee GI modelling of the above terms in the mean momentum equation.

5.2.3. *Correspondence for locally homogeneous flows*

Under the assumptions of local homogeneity of $n(\boldsymbol{x};t)$ and inhomogeneous radius p.d.f., and spherical DPEs, we can substitute $\alpha_d(\boldsymbol{x},t)=n(t)(4/3)\pi\langle R^3\rangle(\boldsymbol{x},t)$ into (5.18) to obtain

$$
\begin{aligned}
&\alpha_d\ \rho_d\ \left[\frac{\partial\langle\widetilde{V}_i\rangle}{\partial t}+\langle\widetilde{V}_j\rangle\frac{\partial\langle\widetilde{V}_i\rangle}{\partial x_j}\right]\\
&\quad=\alpha_d\ \rho_d\ \langle\widetilde{A}_i\mid\boldsymbol{x};t\rangle-\frac{\partial}{\partial x_j}[\alpha_d\ \rho_d\ \langle\widetilde{v_i''v_j''}\rangle]\\
&\qquad+\alpha_d\ \rho_d\ \{3\langle\widetilde{V_i\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{V_i\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+|\boldsymbol{x};t)\ \}\\
&\qquad-\alpha_d\ \rho_d\ \{3\langle\widetilde{V}_i\rangle\langle\widetilde{\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{V}_i\rangle\langle\widetilde{\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+|\boldsymbol{x};t)\}.
\end{aligned}
\tag{5.21}
$$

This equation can be directly compared with (5.15), which is the phasic mean momentum conservation equation arising from the random-field approach written for the dispersed phase $\beta=d$ and constant thermodynamic density

$$
\alpha_d\rho_d\frac{\tilde{\mathrm{D}}_d\langle\widetilde{U_i^{(d)}}\rangle}{\tilde{\mathrm{D}}_\beta t}=\big\langle S_{Mi}^{(d)(IS)}\big\rangle-\frac{\partial}{\partial x_j}\big[\alpha_d\rho_d\widetilde{R_{ij}^{(d)}}\big]+\big\{\big\langle S_{Mi}^{(d)(PC)}\big\rangle-\big\langle\widetilde{U_i^{(d)}}\big\rangle\big\langle S_\rho^{(d)}\big\rangle\big\},
\tag{5.22}
$$

where now the stress term $\langle\partial/\partial x_j(I_\beta\tau_{ji})\rangle$ drops out because the velocity field is uniform in the DPE (being either a rigid DPE, or a fluid DPE with a uniform internal flow field).

A comparison of (5.21) and (5.22) leads to the correspondence of the terms

$$\left\langle S_{Mi}^{(d)(IS)} \right\rangle \Longleftrightarrow \alpha_d \ \rho_d \ \left\langle \widetilde{A}_i \right\rangle \tag{5.23}$$

$$\widetilde{R}_{ij}^{(d)} \Longleftrightarrow \langle \widetilde{v_i'' v_j''} \rangle \tag{5.24}$$

$$\left\langle S_{Mi}^{(d)(PC)} \right\rangle \Longleftrightarrow \alpha_d \ \rho_d \ \{3\langle \widetilde{V_i \Omega} \mid \boldsymbol{x}; t\rangle + \langle \widetilde{V_i \Theta} \mid \boldsymbol{x}, r = 0_+; t\rangle f_R^c(r = 0_+ | \boldsymbol{x}; t)\} \tag{5.25}$$

$$-\langle \widetilde{U}_i^{(d)} \rangle \langle S_\rho^{(d)} \rangle \Longleftrightarrow -\alpha_d \ \rho_d \ \{3\langle \widetilde{V}_i \rangle \langle \widetilde{\Omega} \mid \boldsymbol{x}; t\rangle + \langle \widetilde{V}_i \rangle \langle \widetilde{\Theta} \mid \boldsymbol{x}, r = 0_+; t\rangle f_R^c(r = 0_+ | \boldsymbol{x}; t)\}. \tag{5.26}$$

If the number density retains spatial homogeneity as the flow evolves, then the above correspondence becomes an equality. However, if the number density develops spatial inhomogeneities as the flow evolves, then relation given by (5.3) no longer holds, and the correspondence given above should be treated only as an approximation.

5.3. *Second-moment equations*

5.3.1. *Random-field based Eulerian approach*

Prior to deriving second-moment evolution equations for velocity we need to define the fluctuating velocity field. In single-phase turbulent flow there are two ways in which velocity fluctuations can be defined (i) the fluctuation defined with respect to the mean velocity, (ii) the Favre fluctuation velocity defined with respect to the density-weighted mean. The two fluctuating velocity fields are identical for constant density flows, but for variable density flows the equations are considerably simpler when written in terms of Favre fluctuating velocities and associated second moments (Jones 1979; Libby & Williams 1993). Therefore Favre averaging is the more general averaging approach, and is preferred for variable density flows, in spite of the difficulties encountered in modelling the unclosed terms and comparison with experimentally measured velocity moments.

In two-phase flows there are *four* ways in which velocity fluctuations can be defined: (i) the fluctuation defined with respect to the mean velocity of that phase, (ii) the Favre fluctuation velocity defined with respect to the density-weighted mean velocity of that phase, (iii) the fluctuation defined with respect to the mean velocity of the two-phase mixture and (iv) the Favre fluctuation velocity defined with respect to the density-weighted mean velocity of the two-phase mixture. The most useful definition of fluctuating velocity is the Favre fluctuation in phase β

$$u_i''^{(\beta)} \equiv U_i - \widetilde{\langle U_i^{(\beta)} \rangle}, \tag{5.27}$$

as was defined earlier. As in single-phase flows, the equations for the second moments based on the Favre fluctuation velocity are considerably simpler than those based on other definitions.

The Favre-averaged Reynolds stress $\widetilde{R_{ij}^{(\beta)}}$ in phase β is defined in terms of $u_i''^{(\beta)}$ as

$$\widetilde{R}_{ij}^{(\beta)} \equiv \frac{\langle I_\beta \rho \ u_i''^{(\beta)} u_j''^{(\beta)} \rangle}{\langle I_\beta \rho \ \rangle} = \int_{\boldsymbol{u}} v_i''^{(\beta)} v_j''^{(\beta)} \ \mathscr{F}_{\boldsymbol{U}|I_\beta} \, \mathrm{d}\boldsymbol{u}. \tag{5.28}$$

In order to derive the evolution equation for $\tilde{R}_{ij}^{(\beta)}$, we multiply (4.13) by $v_i''^{(\beta)} v_j''^{(\beta)}$ and integrate over $\boldsymbol{u}$ space, along with manipulations as detailed in Appendix B, to

obtain

$$\langle I_\beta \rho\rangle \underbrace{\frac{\tilde{\mathrm{D}}}{\tilde{\mathrm{D}}t}\widetilde{R}_{ij}^{(\beta)}}_{1} + \underbrace{\frac{\partial}{\partial x_k}\left\langle \rho I_\beta u_i''^{(\beta)} u_j''^{(\beta)} u_k''^{(\beta)}\right\rangle}_{2}$$
$$= \underbrace{-\left\{\left\langle \rho I_\beta u_i''^{(\beta)} u_k''^{(\beta)}\right\rangle \frac{\partial\widetilde{\langle U_j^{(\beta)}\rangle}}{\partial x_k} + \left\langle \rho I_\beta u_j''^{(\beta)} u_k''^{(\beta)}\right\rangle \frac{\partial\widetilde{\langle U_i^{(\beta)}\rangle}}{\partial x_k}\right\}}_{3}$$
$$+ \underbrace{\left\langle u_i''^{(\beta)} \frac{\partial(I_\beta \tau_{kj})}{\partial x_k}\right\rangle}_{4} + \underbrace{\left\langle u_j''^{(\beta)} \frac{\partial(I_\beta \tau_{ki})}{\partial x_k}\right\rangle}_{5} + \underbrace{\left\langle u_i''^{(\beta)}\left(S_{Mj}^{(\beta)} - U_j S_\rho^{(\beta)}\right)\right\rangle}_{6}$$
$$+ \underbrace{\left\langle u_j''^{(\beta)}\left(S_{Mi}^{(\beta)} - U_i S_\rho^{(\beta)}\right)\right\rangle}_{7} + \underbrace{\left\langle u_i''^{(\beta)} u_j''^{(\beta)} S_\rho^{(\beta)}\right\rangle - \widetilde{R}_{ij}^{(\beta)}\left\langle S_\rho^{(\beta)}\right\rangle}_{8}. \tag{5.29}$$

Term 1 in (5.29) is the material derivative that convects at the Favre-averaged mean flow velocity, term 2 is the triple velocity correlation, term 3 corresponds to production due to mean flow gradients, terms 4 and 5 correspond to the fluctuating velocity–stress correlations, terms 6 and 7 correspond to the fluctuating velocity–interfacial force correlations and term 8 is the source in Reynolds stress equation due to phase change. The above equation has been written in GI form; in particular, the GI forms of unclosed terms which need to be modelled (note that they are also symmetric in indices i and j) are terms 4 and 5, terms 6 and 7 and term 8.

5.3.2. *Number-density based Lagrangian approach*

In order to derive the second-moment equation in the LE approach, it is instructive to define the volume-weighted d.d.f. (analogous to mass weighting in the Favre average presented earlier) of fluctuating velocity $\tilde{g}(\boldsymbol{x}, \boldsymbol{w}, r, t)$ as

$$\tilde{g}(\boldsymbol{x}, \boldsymbol{w}, r, t) = \tilde{f}(\boldsymbol{x}, \langle \widetilde{\boldsymbol{V}} \mid \boldsymbol{x}; t\rangle + \boldsymbol{w}, r, t) \tag{5.30}$$
$$= r^3 f(\boldsymbol{x}, \boldsymbol{v}, r, t) \tag{5.31}$$
$$= \langle R^3\rangle(\boldsymbol{x}; t) n(\boldsymbol{x}; t)\ \tilde{f}_{VR}^c(\langle \widetilde{\boldsymbol{V}} \mid \boldsymbol{x}; t\rangle + \boldsymbol{w}, r \mid \boldsymbol{x}; t) \tag{5.32}$$
$$= \langle R^3\rangle(\boldsymbol{x}; t) n(\boldsymbol{x}; t)\ \tilde{g}^c(\boldsymbol{w}, r \mid \boldsymbol{x}; t), \tag{5.33}$$

where

$$\boldsymbol{w} = \boldsymbol{v} - \langle \widetilde{\boldsymbol{V}} \mid \boldsymbol{x}; t\rangle, \tag{5.34}$$

where $\tilde{g}^c(\boldsymbol{w}, r|\boldsymbol{x}; t)$ is the r^3-weighted or volume-weighted p.d.f. of fluctuating velocity.

The evolution equation of $\tilde{g}$ can be derived from (4.16) (see Appendix D for a derivation)

$$\frac{\partial \tilde{g}}{\partial t} + (\langle \widetilde{V}_k\rangle + w_k)\frac{\partial \tilde{g}}{\partial x_k} = w_k \frac{\partial \tilde{g}}{\partial w_l}\frac{\partial\langle \widetilde{V}_l\rangle}{\partial x_k}$$
$$-\frac{\partial}{\partial w_l}\left[\langle A_l \mid \boldsymbol{x}, \boldsymbol{v}, r; t)\rangle \tilde{g} - \tilde{g}\frac{\partial\langle \widetilde{V}_l\rangle}{\partial t} - \tilde{g}\langle \widetilde{V}_k\rangle \frac{\partial\langle \widetilde{V}_l\rangle}{\partial x_k}\right]$$
$$-\frac{\partial}{\partial r}\left\{\langle \Theta \mid \boldsymbol{x}, \boldsymbol{v}, r; t\rangle \tilde{g}\right\} + 3\langle \Omega \mid \boldsymbol{x}, \boldsymbol{v}, r; t\rangle \tilde{g}. \tag{5.35}$$

The second-moment equation can be obtained by multiplying the $\tilde{g}$ evolution equation by $w_i w_j$ and integrating over all $[\boldsymbol{w}, r_+]$ space to obtain

$$\underbrace{\kappa n\langle R^3\rangle\left\{\frac{\partial\langle\widetilde{v_i''v_j''}\rangle}{\partial t}+\langle\widetilde{V}_k\rangle\frac{\partial\langle\widetilde{v_i''v_j''}\rangle}{\partial x_k}\right\}}_{1}+\underbrace{\kappa\frac{\partial}{\partial x_k}[n\langle R^3\rangle\langle v_i''\widetilde{v_j''v_k''}\rangle]}_{2}$$

$$=\underbrace{-\kappa n\langle R^3\rangle\left\{\langle\widetilde{v_j''v_k''}\rangle\frac{\partial\langle\widetilde{V}_i\rangle}{\partial x_k}+\langle\widetilde{v_i''v_k''}\rangle\frac{\partial\langle\widetilde{V}_j\rangle}{\partial x_k}\right\}}_{3}$$

$$+\underbrace{\kappa n\langle R^3\rangle\{\langle\widetilde{A_i v_j''}\rangle+\langle\widetilde{A_j v_i''}\rangle\}}_{4}$$

$$+\underbrace{\kappa n\langle R^3\rangle\left[3\langle\widetilde{v_i''v_j''\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{v_i''v_j''\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+\mid\boldsymbol{x},t)\right]}_{5}$$

$$-\underbrace{\kappa n\langle R^3\rangle\langle\widetilde{v_i''v_j''}\rangle\{3\langle\widetilde{\Omega}\mid\boldsymbol{x};t\rangle+\langle\widetilde{\Theta}\mid\boldsymbol{x},r=0_+;t\rangle f_R^c(r=0_+\mid\boldsymbol{x},t)\}}_{6},\quad(5.36)$$

where additionally, the above equation has been multiplied throughout by $\kappa = (4/3)\pi\rho_d$. The description of each term is as follows: term 1 is the material derivative (following the volume-weighted mean flow) of the dispersed-phase Reynolds stress, term 2 is the triple velocity correlation term, term 3 is the production due to mean velocity gradients, term 4 is the fluctuating velocity–acceleration correlation and terms 5 and 6 correspond to the net Reynolds stress change due to interphase mass transfer.

Note that the terms in the above equation are automatically in GI form. The acceleration-fluctuating velocity correlation can be written in terms of $\tilde{g}^c(\boldsymbol{w}, r|\boldsymbol{x};t)$ as

$$\langle\widetilde{A_i v_j''}\rangle=\int_{[\boldsymbol{v},r_+]}\langle A_i|\boldsymbol{x},\boldsymbol{v},r;t\rangle w_j\tilde{g}^c(\boldsymbol{w},r|\boldsymbol{x};t)\,\mathrm{d}\boldsymbol{w}\,\mathrm{d}r,$$

where the expected acceleration $\langle A_i|\boldsymbol{x},\boldsymbol{v},r;t\rangle$ is completely determined by (2.24) and (2.25) and the d.d.f. In homogeneous two-phase flows with neither production nor interphase mass transfer, the only terms that remain in (5.36) are (i) the time derivative of the Reynolds stress and (ii) the acceleration–fluctuating velocity correlations.

5.3.3. *Acceleration–fluctuating velocity correlation*

It is important to recognize that the acceleration–fluctuating velocity correlation $\langle\widetilde{A_i v_j''}\rangle$ is a non-local term. This can be better understood from the expression for the centre-of-mass acceleration of a single DPE. For the ith DPE of radius r_0, the acceleration of the centre-of-mass $\boldsymbol{X}_p^{(i)}$ depends on the state of the stress $\boldsymbol{\tau}$ (for a Newtonian fluid, $\boldsymbol{\tau}(\boldsymbol{y},t) = -p(\boldsymbol{y},t)\boldsymbol{I} + 2\mu\boldsymbol{S}(\boldsymbol{y},t) - (2/3)\mu(\boldsymbol{\nabla}\cdot\boldsymbol{U})\boldsymbol{I}$, where p is the mechanical pressure, $\boldsymbol{I}$ is the identity tensor, μ is the dynamic viscosity of the carrier phase and $\boldsymbol{S}$ is the rate of strain tensor) at the DPE surface $\mathscr{S}$ through the expression (cf. (4.19))

$$\boldsymbol{A}_{(i)}(t)=\frac{1}{m_{(i)}}\int_{\mathscr{S}}\boldsymbol{\tau}(\boldsymbol{y},t)\cdot\boldsymbol{n}(\boldsymbol{y})\,\mathrm{d}A_s,\quad(5.37)$$

where $\boldsymbol{y}=\boldsymbol{x}+\boldsymbol{e}_r r_0$ is a point on the DPE surface, $\boldsymbol{x}=\boldsymbol{X}_p^{(i)}$, $\boldsymbol{e}_r$ is the unit vector directed radially outward from $\boldsymbol{x}$, $\mathrm{d}A_s$ is the differential surface area of the DPE,

$\boldsymbol{n}$ is the unit normal (outwardly directed) to the DPE surface at $\boldsymbol{y}$ and $m_{(i)}$ is the mass of the DPE. This observation has important implications in modelling two-phase flows. In single-phase flows, the non-local nature of the unclosed terms in the Reynolds stress equation requires closures that incorporate two-point information. Near the walls it is known that non-local closures for the conditional acceleration are necessary to take wall effects into account correctly (Dreeben & Pope 1997). In two-phase flows, hydrodynamic interactions among DPEs, and between DPEs and walls, alter the fluid stresses at the DPE surface. Such interactions can also depend on statistics that characterize the spatial configuration of the DPEs, such as the nearest neighbour distance. Therefore, in two-phase flow modelling, not only does one require closures that incorporate two-point information (as a means to characterize the spatial configuration of DPEs), closures for terms such as $\langle A_i v_j'' \rangle$ need to incorporate information on non-local statistics at the surface of the DPE as well.

A widely used single-point closure for the DPE acceleration in particle-method solutions to the spray equation (see, for instance, Amsden *et al.* 1989) is of the form

$$\boldsymbol{A}_p(t) = \frac{\mathrm{d}\boldsymbol{V}_p(t)}{\mathrm{d}t} = \frac{\boldsymbol{U}_f(\boldsymbol{X}_p, t) - \boldsymbol{V}_p}{\tau_p} C_d(Re_p), \tag{5.38}$$

where $\boldsymbol{A}_p$ is a model for $\boldsymbol{A}_{(i)}$ in (2.25), $\boldsymbol{V}_p$ is the modelled dispersed-phase velocity, $\boldsymbol{U}_f$ is the mean carrier-phase velocity evaluated at the particle *centre* $\boldsymbol{X}_p$ (or sometimes referred to as the carrier-phase velocity 'seen' by the particle), τ_p is the particle response time scale and C_d is the drag coefficient which is a function of the particle Reynolds number Re_p. Clearly, such models cannot capture the changing state of the hydrodynamic stress at the DPE surface when the spatial configuration of the physical DPEs is such that $\boldsymbol{U}_f(\boldsymbol{X}_p, t)$ can no longer be considered a good model for the unperturbed carrier-phase velocity field (Maxey & Riley 1983) in the absence of the particle. This makes such models applicable only to a restricted class of flows (primarily, dilute flows) where the point-particle approximation is valid.

5.3.4. *Correspondence for locally homogeneous flows*

Again invoking the assumptions of local homogeneity and the equalities given by (5.3) and (5.4), with constant thermodynamic density, a direct comparison of (5.29) and (5.36) leads to the following correspondence of the terms to be modelled:

$$\frac{\partial}{\partial x_k}\left\langle I_d \rho\, u_i''^{(d)} u_j''^{(d)} u_k''^{(d)} \right\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d \frac{\partial}{\partial x_k}\left[n\langle R^3\rangle \widetilde{\langle v_i'' v_j'' v_k''\rangle}\right] \tag{5.39}$$

$$\left\langle u_i''^{(d)} \frac{\partial (I_d \tau_{kj})}{\partial x_k} \right\rangle + \left\langle u_i''^{(d)} \left(S_{Mj}^{(d)} - U_j S_\rho^{(d)}\right)\right\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \widetilde{\langle A_j v_i''\rangle} \tag{5.40}$$

$$\left\langle u_j''^{(d)} \frac{\partial (I_d \tau_{ki})}{\partial x_k} \right\rangle + \left\langle u_j''^{(d)} \left(S_{Mi}^{(d)} - U_i S_\rho^{(d)}\right)\right\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \widetilde{\langle A_i v_j''\rangle} \tag{5.41}$$

$$\langle u_i''^{(d)} u_j''^{(d)} S_\rho^{(d)} \rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \big[3\langle \widetilde{v_i'' v_j''\Omega} \mid \boldsymbol{x};t\rangle + \langle \widetilde{v_i'' v_j''\Theta} | \boldsymbol{x}, r=0_+;t\rangle f_R^c(r=0_+ \mid \boldsymbol{x},t)\big] \quad (5.42)$$

$$-\widetilde{R}_{ij}^{(d)}\langle S_\rho^{(d)}\rangle \Longleftrightarrow -\frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \langle \widetilde{v_i'' v_j''}\rangle \{3\langle \widetilde{\Omega} \mid \boldsymbol{x};t\rangle + \langle \widetilde{\Theta} \mid \boldsymbol{x}, r=0_+;t\rangle f_R^c(r=0_+ \mid \boldsymbol{x},t)\}. \quad (5.43)$$

This correspondence allows one to compare budgets of the second-moment transport equation from the EE statistical representation with that in the LE statistical representation, or vice versa.

5.3.5. *Turbulent kinetic energy*

For the sake of completeness, the evolution equations for the phasic turbulent kinetic energy (TKE) are derived. The Favre-averaged TKE in phase β is defined as half the trace of the Favre-averaged Reynolds stress in phase β, $\tilde{k}^{(\beta)} \equiv (1/2)\,\widetilde{R}_{ii}^{(\beta)}$.

Using this definition, the evolution equation for the phasic TKE in the random-field representation can be obtained as

$$\langle I_\beta\rho\rangle \frac{\tilde{\mathrm{D}}}{\tilde{\mathrm{D}}t}\tilde{k}^{(\beta)} + \frac{1}{2}\frac{\partial}{\partial x_k}\big\langle \rho I_\beta u_i''^{(\beta)} u_i''^{(\beta)} u_k''^{(\beta)}\big\rangle = -\big\langle \rho I_\beta u_i''^{(\beta)} u_k''^{(\beta)}\big\rangle \frac{\partial \langle \widetilde{U_i^{(\beta)}}\rangle}{\partial x_k} + \left\langle u_i''^{(\beta)} \frac{\partial (I_\beta \tau_{ki})}{\partial x_k}\right\rangle + \big\langle u_i''^{(\beta)}\big(S_{Mi}^{(\beta)} - U_i S_\rho^{(\beta)}\big)\big\rangle + \frac{1}{2}\big\langle u_i''^{(\beta)} u_i''^{(\beta)} S_\rho^{(\beta)}\big\rangle - \tilde{k}^{(\beta)}\big\langle S_\rho^{(\beta)}\big\rangle. \quad (5.44)$$

Similarly, the evolution equation for the dispersed-phase TKE in the point-process representation which is defined as $\tilde{k}_L^{(d)} = (1/2)\langle \widetilde{v_i'' v_i''}\rangle$, where the subscript L informs us that this quantity corresponds to the LE statistical representation, is given as

$$\kappa n\langle R^3\rangle \left\{ \frac{\partial \tilde{k}_L^{(d)}}{\partial t} + \langle \widetilde{V}_k\rangle \frac{\partial \tilde{k}_L^{(d)}}{\partial x_k}\right\} + \frac{1}{2}\kappa \frac{\partial}{\partial x_k}[n\langle R^3\rangle \langle \widetilde{v_i'' v_i'' v_k''}\rangle]$$

$$= -\kappa n\langle R^3\rangle \langle \widetilde{v_i'' v_k''}\rangle \frac{\partial \langle \widetilde{V}_i\rangle}{\partial x_k} + \kappa n\langle R^3\rangle \langle \widetilde{A_i v_i''}\rangle + \frac{1}{2}\kappa n\langle R^3\rangle \big[3\langle \widetilde{v_i'' v_i''\Omega} \mid \boldsymbol{x};t\rangle + \langle \widetilde{v_i'' v_i''\Theta} \mid \boldsymbol{x}, r=0_+;t\rangle f_R^c(r=0_+ \mid \boldsymbol{x},t)\big] - \kappa n\langle R^3\rangle \tilde{k}_L^{(d)}\{3\langle \widetilde{\Omega} \mid \boldsymbol{x};t\rangle + \langle \widetilde{\Theta} \mid \boldsymbol{x}, r=0_+;t\rangle f_R^c(r=0_+ \mid \boldsymbol{x},t)\}, \quad (5.45)$$

Invoking the assumptions of local homogeneity as earlier, the following correspondence between unclosed terms in the dispersed-phase TKE evolution equation across the two statistical representations can be identified:

$$\frac{\partial}{\partial x_k}\big\langle I_d\rho\; u_i''^{(d)} u_i''^{(d)} u_k''^{(d)}\big\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\; \frac{\partial}{\partial x_k}[n\langle R^3\rangle \langle \widetilde{v_i'' v_i'' v_k''}\rangle] \quad (5.46)$$

$$\left\langle u_i''^{(d)} \frac{\partial (I_d \tau_{ki})}{\partial x_k}\right\rangle + \big\langle u_i''^{(d)}\big(S_{Mi}^{(d)} - U_i S_\rho^{(d)}\big)\big\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \langle \widetilde{A_i v_i''}\rangle \quad (5.47)$$

$$\left\langle u_i''^{(d)} u_i''^{(d)} S_\rho^{(d)} \right\rangle \Longleftrightarrow \frac{4}{3}\pi\rho_d\, n\langle R^3\rangle [3\langle \widetilde{v_i'' v_i''\Omega} \mid \boldsymbol{x}; t\rangle + \left\langle \widetilde{v_i'' v_i''\Theta} \mid \boldsymbol{x}, r = 0_+; t\right\rangle f_R^c(r = 0_+ \mid \boldsymbol{x}, t)] \quad (5.48)$$

$$-\tilde{k}^{(d)}\left\langle S_\rho^{(d)}\right\rangle \Longleftrightarrow -\frac{4}{3}\pi\rho_d\, n\langle R^3\rangle \tilde{k}_L^{(d)} \times \{3\langle\widetilde{\Omega} \mid \boldsymbol{x}; t\rangle + \langle\widetilde{\Theta} \mid \boldsymbol{x}, r = 0_+; t\rangle f_R^c(r = 0_+ \mid \boldsymbol{x}, t)\}. \quad (5.49)$$

Again, the above correspondence allows one to compare budgets of the evolution equation of the dispersed-phase TKE across the two statistical representations. The first term on the left-hand side of (5.47) contains a contribution to the dissipation of TKE in the dispersed phase, while the second term represents the interphase transfer of TKE due to momentum and mass transfer. The sum of these two terms corresponds to the acceleration–fluctuating velocity correlation $\langle \widetilde{A_i v_i''}\rangle$ on the right-hand side. The dissipation of TKE can be traced to two sources: a dissipation in the dispersed phase due to viscous sources and a dissipation due to inelastic collisions between DPEs. In the above correspondence, however, note that the velocity field in the DPE is assumed to be uniform. So, the viscous dissipation in the dispersed phase is either zero or negligible. Thus, the dissipation of TKE is solely due to the collisional source. If the collisions are elastic then there is no contribution to dissipation in the above correspondence, and so $\langle \widetilde{A_i v_i''}\rangle$ on the right-hand side of (5.47) corresponds only to the interphase transfer of TKE due to momentum and mass transfer.

6. Comparison of advantages and limitations

The EE and LE probabilistic descriptions of two-phase flows contain different information. In this section, the advantages and limitations of each approach is presented in terms of the information contained in each statistical representation.

6.1. *Eulerian–Eulerian*

(*a*) The fundamental description of a two-phase flow in the EE statistical representation starts from a phase probability (or, volume fraction) field $\alpha_\beta(\boldsymbol{x}, t)$ and p.d.f. $f^E_{UR|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$, where $\beta = \{f, d\}$, that are defined in both phases. The governing equations for the mean mass, mean momentum and second moment that are derived from the transport equation for the phasic p.d.f. are also defined in both phases. Thus, in the EE representation, the coupling between the fluid dynamic equations in both phases arises naturally from the instantaneous conservation equations.

(*b*) The complete single-point EE description in terms of phase probability fields and p.d.f. contains no explicit representation of *shape or number* of dispersed-phase elements. This informs us that very different two-phase flows can have the same phase probability fields α_β and p.d.f. $f^E_{UR|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$.

(*c*) The EE representation is valid in each phase regardless of the size of the dispersed-phase element. Internal circulation effects inside a droplet or bubble can be captured by the EE statistical description in terms of (3.6).

(*d*) A noteworthy limitation of the p.d.f. $f^E_{UR|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ is that it is incapable of distinguishing the flow at a point near the dispersed phase surface and the flow in the bulk. This is primarily due to the inability of a single-point p.d.f. to capture spatial gradients (of velocity, for instance), which can be very different close to the particle surface compared to that in the bulk. The reason for this can be traced to the fact

that the velocity gradient cannot be written in terms of a single-point p.d.f. of velocity (see Fox 2003, for instance). In order to capture such velocity gradients, a two-point p.d.f. formalism is necessary at a minimum.

6.2. *Lagrangian–Eulerian*

(*a*) Since the LE representation is primarily a description of the dispersed phase, no information on the carrier phase is directly available in the d.d.f. or the spray equation. The coupling arises through the dependence of $\boldsymbol{A}^{(i)}$ on the carrier phase. One should note that the terms such as $\langle \boldsymbol{A}|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle$ in (4.16) need to be correctly interpreted as the expected acceleration of the dispersed phase conditional on position, velocity and radius and also the state of the carrier phase, where the carrier phase information is assumed to be known.

(*b*) The d.d.f. contains both size and number information of the dispersed-phase elements. However, the shape of the dispersed-phase elements is modelled (such as assuming that a characteristic radius r describes the DPE).

(*c*) The d.d.f. cannot capture internal circulation effects since it assumes that a DPE can be described by a single velocity, usually at the particle centre-of-mass. As such, rigid particles of any size, and drops and bubbles in which internal circulation effects are not important can be modelled using the d.d.f. This implicitly imposes a restriction on the size of droplets or bubbles that the d.d.f. is capable of modelling. For instance, during primary break-up of liquid fuel, the dispersed-phase structures that peel off the liquid core near the fuel injector may not be amenable to a description by the d.d.f. since such structures could have significant internal circulation effects, and may be insufficiently characterized by a single velocity at their centre of mass.

(*d*) The implicit restriction on the size of the DPE (droplet or bubble) in (*c*) should not be misconstrued as a limitation of the d.d.f. to model dense flows. In fact, the d.d.f. does not rely on the assumption of diluteness (or denseness) of a two-phase flow for its definition (Subramaniam 2001). It is the models used in existing EE and LE formulations that invoke the assumption of diluteness. Thus, the LE representation based on the d.d.f. approach is valid to model a dense two-phase flow composed of droplets or bubbles in which (i) the DPEs do not have any internal circulation effects and (ii) the DPEs can be described by a characteristic length scale.

(*e*) For two-phase flows where the LE statistical description is valid, unclosed quantities in the EE governing equations can be estimated using the corresponding unclosed terms in the LE approach. To illustrate this procedure, consider a two-phase flow for which we invoke the following assumptions: (i) the DPE drag is modelled by (5.38) without a correction due to the drag coefficient, (ii) the flow has a constant number of DPEs N, (iii) absence of interphase mass transfer, (iv) a monodispersed size distribution with radius R_0, (v) no body forces such as gravity are considered and (vi) the flow is locally homogeneous. Under these assumptions, we have for the interphase momentum transfer term

$$\left\langle \boldsymbol{S}_M^{(d)} \right\rangle (\boldsymbol{x}, t) = \iint \frac{4}{3}\pi r^3 \rho_d \, \langle \boldsymbol{A}|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle \, f(\boldsymbol{x}, \boldsymbol{v}, r, t) \, \mathrm{d}\boldsymbol{v} \, \mathrm{d}r. \tag{6.1}$$

Here

$$\begin{aligned} \langle \boldsymbol{A}|\boldsymbol{x}, \boldsymbol{v}, r, t\rangle &= \frac{1}{f}\left\langle \sum_{i=1}^{N} \boldsymbol{A}_{(i)} \delta\left(\boldsymbol{x} - \boldsymbol{X}_{p(i)}\right) \delta\left(\boldsymbol{v} - \boldsymbol{V}_{p(i)}\right) \delta(r - R_0) \right\rangle \\ &= \frac{1}{f}\left\langle \sum_{i=1}^{N} \left(\frac{\boldsymbol{U}_f\left(\boldsymbol{X}_{p(i)}, t\right) - \boldsymbol{V}_{p(i)}}{\tau_p} \right) \delta\left(\boldsymbol{x} - \boldsymbol{X}_{p(i)}\right) \delta\left(\boldsymbol{v} - \boldsymbol{V}_{p(i)}\right) \delta(r - R_0) \right\rangle. \end{aligned}$$

Substituting in (6.1) results in

$$\left\langle \boldsymbol{S}_M^{(d)} \right\rangle(\boldsymbol{x}, t) = \iint \frac{4}{3}\pi r^3 \rho_d \left\langle \sum_{i=1}^{N} \left(\frac{\boldsymbol{U}_f\left(\boldsymbol{X}_{p(i)}, t\right) - \boldsymbol{v}}{\tau_p} \right) \delta_{\boldsymbol{X}_{p(i)}} \delta_{\boldsymbol{V}_{p(i)}} \delta_{R_0} \right\rangle \mathrm{d}\boldsymbol{v}\, \mathrm{d}r,$$

where $\delta_{\boldsymbol{X}_{p(i)}} = \delta(\boldsymbol{x} - \boldsymbol{X}_{p(i)})$, $\delta_{\boldsymbol{V}_{p(i)}} = \delta(\boldsymbol{v} - \boldsymbol{V}_{p(i)})$ and $\delta_{R_0} = \delta(r - R_0)$.
Thus,

$$\begin{aligned}
\left\langle \boldsymbol{S}_M^{(d)} \right\rangle(\boldsymbol{x}, t) &= \iint \frac{4}{3}\pi r^3 \rho_d \left\langle \sum_{i=1}^{N} \left(\frac{\boldsymbol{U}_f\left(\boldsymbol{X}_{p(i)}, t\right) - \boldsymbol{v}}{\tau_p} \right) \delta_{\boldsymbol{X}_{p(i)}} \delta_{\boldsymbol{V}_{p(i)}} \delta_{R_0} \right\rangle \mathrm{d}\boldsymbol{v}\, \mathrm{d}r, \\
&= \iint \frac{4}{3}\pi r^3 \rho_d \left(\frac{\langle \boldsymbol{U} \mid \boldsymbol{x}, t\rangle - \langle \boldsymbol{V} \mid \boldsymbol{x}, t\rangle}{\tau_p} \right) f(\boldsymbol{x}, \boldsymbol{v}, r, t)\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}r, \\
&= \iint \frac{4}{3}\pi r^3 \rho_d \left(\frac{\langle \boldsymbol{U} \mid \boldsymbol{x}, t\rangle - \langle \boldsymbol{V} \mid \boldsymbol{x}, t\rangle}{\tau_p} \right) n(\boldsymbol{x}; t) f^c_{V|R} \delta(r - R_0)\, \mathrm{d}\boldsymbol{v}\, \mathrm{d}r, \\
&= \frac{4}{3}\pi R_0^3\ \rho_d\ n(\boldsymbol{x}; t) \left(\frac{\langle \boldsymbol{U} \mid \boldsymbol{x}, t\rangle - \langle \boldsymbol{V} \mid \boldsymbol{x}, t\rangle}{\tau_p} \right), \qquad (6.2)
\end{aligned}$$

where $\langle \boldsymbol{U} \mid \boldsymbol{x}, t\rangle$ and $\langle \boldsymbol{V} \mid \boldsymbol{x}, t\rangle$ are the expected carrier-phase and dispersed-phase velocities, respectively, conditional on location $\boldsymbol{x}$ at time t. Thus, under the assumptions noted earlier, a model for the particle drag in the LE framework implies a model for interphase momentum transfer term in the EE representation. Interestingly, the right-hand side of (6.2) can also be extracted from DNS of particle-laden flows that are performed under the same assumptions (commonly known as the point-particle approximation). This equality suggests that EE models for the interphase momentum transfer term $\left\langle \boldsymbol{S}_M^{(d)} \right\rangle(\boldsymbol{x}, t)$ can be evaluated by comparing with DNS data.

6.3. *Closure at the level of the p.d.f.*

A p.d.f. formalism in the EE statistical representation has been developed. It is shown that the ensemble-averaged EE moment equations can be derived in a straightforward manner from the p.d.f. evolution equation. A p.d.f. formalism in the LE statistical representation starting from the spray equation, which is the evolution equation for the d.d.f., has also been presented. There are significant advantages of seeking a closure at the level of the p.d.f. rather than at the level of the moments. In the LE statistical representation, this fact has been demonstrated in Desjardins, Fox & Villedieu (2008), where they use a two-node quadrature method of moments (QMOM) approximation of the d.d.f. and solve a set of moment equations (indirectly solving for the weights and abscissa corresponding to the two-node quadrature) to capture the crossing of two impinging jets in the limit of infinite Stokes number. In their study, they also show that the moment equations corresponding to a single-node quadrature (or, the averaged equations corresponding to the LE statistical representation) cannot capture the crossing of the impinging jets. The correspondence between the EE and the LE statistical representations that was presented earlier in this work suggests that the EE moment equations do not possess the capability to capture the crossing jets as well. However, it has to be noted that the inability of the EE moment equations (ensemble-averaged equations) to capture the crossing jets must not be misconstrued as an inherent limitation of the EE formalism to capture such phenomena. In this work, we have shown that starting from instantaneous two-phase velocity p.d.f. in the EE statistical representation an EE mass density can be defined. One could use a QMOM approximation of the EE mass density and derive evolution equations for

the weights and abscissa using a procedure analogous to that presented in Desjardins *et al.* (2008). In this way, one can demonstrate that the EE p.d.f. formalism also possesses the capability of capturing the crossing-jets phenomenon.

7. Summary and conclusions

Unlike for a single-phase flow, two distinctly different statistical representations, namely the Eulerian–Eulerian and Lagrangian–Eulerian statistical representations, exist for a two-phase flow. This work clearly shows that the EE and LE probabilistic representations of two-phase flow bear a complicated relationship with each other, unlike the relatively simpler relationship between the Eulerian and Lagrangian descriptions in single-phase flow (Pope 1985, 2000). This work establishes the foundation for the p.d.f. approach to two-phase flows by unifying the EE and LE statistical representations. The principal achievements and conclusions of this work are as follows:

(*a*) Fundamental events and corresponding probabilities associated with a two-phase flow in the EE statistical representation are established. Once this is done, it is then straightforward to derive an evolution equation for the fundamental single-point p.d.f. for the instantaneous velocity conditional on the presence of phase β, where $\beta = \{f, d\}$, for a two-phase flow. Governing equations for the mean mass, mean momentum and second moment that are derived from the evolution equation for the EE mass density are shown to be identical to widely used ensemble-averaged equations for two-phase flows (Drew 1983). To the knowledge of the authors, two-phase flow p.d.f. formulations available in literature have not demonstrated consistency between the Eulerian p.d.f. and the ensemble-averaged two-fluid equations.

(*b*) Fundamental to the LE statistical representation is the droplet distribution function whose evolution equation has been rigorously derived using the theory of point processes (Subramaniam 2000, 2001). Based on the droplet distribution function, the p.d.f. of fluctuating velocity $\tilde{g}$ is proposed in this work. The transport equation for $\tilde{g}$ forms the basis for the derivation of mean mass, mean momentum and second-moment equations for the dispersed phase in the LE representation.

(*c*) Consistency conditions are established between the fundamental quantities in the EE (viz. α_β and $f^E_{\boldsymbol{U}R|I_\beta}(\boldsymbol{u}, r; \boldsymbol{x}, t)$) and the LE (viz. $n(\boldsymbol{x}; t)$ and $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}, t)$) statistical representations. It is noteworthy that these quantities bear a simple relationship with one another only under conditions of statistical homogeneity of number density and radius p.d.f. Examples of two-phase flows where the exact relations between the EE and LE statistical representations fail to hold are enumerated.

(*d*) By comparing unclosed terms in the governing equations for the mean mass, mean momentum and second moment in each statistical representation, correspondence between the unclosed terms is established. GI forms of unclosed terms in the governing equations in both the statistical representations are identified. This work also serves as a framework for comparing existing two-phase flow models with the GI forms of the unclosed terms presented in this work, and also as a guide for proposing new models. The correspondence also aids in estimating unclosed terms in the governing equations in the EE representation using corresponding terms in the LE representation.

(*e*) A comparison between the two statistical representations reveals that the information content in the two approaches is indeed different. The inability of the

d.d.f. to capture internal circulation effects in drops or bubbles imposes a restriction on the class of DPEs that can be modelled by the d.d.f.

DNS studies of particle-laden flows can significantly benefit from the correspondence between the EE and LE representations developed in this work. This work also provides the necessary consistency relations that need to be satisfied in combined EE–LE formulations in which information is handed over from one representation to the other at a common boundary.

Appendix A. Normalization of the mass-weighted phasic velocity p.d.f. in the EE representation

Here, we verify that $\tilde{f}_{\boldsymbol{U}|I_\beta}$ satisfies the normalization property for all time. Integrating both sides of (4.15) over $\boldsymbol{u}$ space, we get

$$\frac{\partial}{\partial t}\int \tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u} + \underbrace{\frac{\partial}{\partial x_i}\int u_i\,\tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u}}_{a} + \underbrace{\int \frac{\partial}{\partial u_i}\langle A_i^{(\beta)}|\boldsymbol{u}\rangle\,\tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u}}_{b} = \underbrace{\int \frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle\rho I_\beta|\boldsymbol{u}\rangle}\langle S_\rho^{(\beta)}\mid\boldsymbol{u}\rangle\,\mathrm{d}\boldsymbol{u}}_{c} - \underbrace{\int \tilde{f}_{\boldsymbol{U}|I_\beta}\frac{\mathrm{D}}{\mathrm{D}t}\ln\langle\rho I_\beta\rangle\,\mathrm{d}\boldsymbol{u}}_{d} \tag{A 1}$$

Term a evaluates to

$$\frac{\partial}{\partial x_i}\int u_i\,\tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u} = \frac{\partial}{\partial x_i}\widetilde{\langle U_i^{(\beta)}\rangle}.$$

Term b evaluates to zero, since the p.d.f. $\tilde{f}_{\boldsymbol{U}|I_\beta}$ has compact support. Term c evaluates to

$$\int \frac{\tilde{f}_{\boldsymbol{U}|I_\beta}}{\langle\rho I_\beta|\boldsymbol{u}\rangle}\langle S_\rho^{(\beta)}\mid\boldsymbol{u}\rangle\,\mathrm{d}\boldsymbol{u} = \langle S_\rho^{(\beta)}\rangle.$$

Term d evaluates to

$$\int \tilde{f}_{\boldsymbol{U}|I_\beta}\frac{\mathrm{D}}{\mathrm{D}t}\ln\langle\rho I_\beta\rangle\,\mathrm{d}\boldsymbol{u} = \frac{\tilde{\mathrm{D}}^{(\beta)}}{\tilde{\mathrm{D}}^{(\beta)}t}\ln\langle\rho I_\beta\rangle.$$

Substituting these simplifications into (A 1) and rearranging results in

$$\frac{\partial}{\partial t}\int \tilde{f}_{\boldsymbol{U}|I_\beta}\,\mathrm{d}\boldsymbol{u} = \langle S_\rho^{(\beta)}\rangle - \frac{\partial}{\partial x_i}\widetilde{\langle U_i^{(\beta)}\rangle} - \frac{\tilde{\mathrm{D}}^{(\beta)}}{\tilde{\mathrm{D}}^{(\beta)}t}\ln\langle\rho I_\beta\rangle. \tag{A 2}$$

The right-hand side of the above equation is the phasic mean mass conservation, which is obtained by integrating (4.13) over $\boldsymbol{u}$ space

$$\frac{\tilde{\mathrm{D}}^{(\beta)}}{\tilde{\mathrm{D}}^{(\beta)}t}\ln\langle\rho I_\beta\rangle + \frac{\partial}{\partial x_i}\widetilde{\langle U_i^{(\beta)}\rangle} - \langle S_\rho^{(\beta)}\rangle = 0.$$

Thus, (A 2) shows that satisfaction of the mean mass conservation ensures that $\tilde{f}_{\boldsymbol{U}|I_\beta}$ retains its normalization property for all time.

Appendix B. Derivation of the second-moment equation from the phasic mass density

In order to derive the evolution equation for $\tilde{R}_{ij}^{(\beta)}$, we multiply (4.13) by $v_i''^{(\beta)}v_j''^{(\beta)}$, where $v_i''^{(\beta)} \equiv u_i - \widetilde{\langle U_i^{(\beta)}\rangle}$, and integrate over $\boldsymbol{u}$ space to obtain

$$\underbrace{v_i''^{(\beta)}v_j''^{(\beta)}\frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial t}}_{1} + \underbrace{v_i''^{(\beta)}v_j''^{(\beta)}u_k\frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial x_k}}_{2} = -\underbrace{v_i''^{(\beta)}v_j''^{(\beta)}\frac{\partial}{\partial u_k}\left[\left\langle \rho I_\beta \frac{\mathrm{D}U_k}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right]}_{3}$$
$$+\underbrace{v_i''^{(\beta)}v_j''^{(\beta)}\frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\left\langle \rho\big(U_k - U_k^{(I)}\big)\frac{\partial I_\beta}{\partial x_k}\middle|\boldsymbol{u}\right\rangle}_{4}. \quad \text{(B 1)}$$

The first term simplifies to

$$v_i''^{(\beta)}v_j''^{(\beta)}\frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial t} = \frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial t} - \mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}}{\partial t}. \quad \text{(B 2)}$$

The second term simplifies to

$$v_i''^{(\beta)}v_j''^{(\beta)}u_k\frac{\partial \mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial x_k} = \frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}u_k\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\partial x_k} - \underbrace{u_k\mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}}{\partial x_k}}_{a}.$$

Taking term a in the above expression

$$u_k\mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}}{\partial x_k} = -u_k\mathscr{F}_{\boldsymbol{U}|I_\beta}\left\{v_i''^{(\beta)}\frac{\partial\langle U_j^{(\beta)}\rangle}{\partial x_k} + v_j''^{(\beta)}\frac{\partial\langle U_i^{(\beta)}\rangle}{\partial x_k}\right\}.$$

Part 3 above simplifies to

$$\begin{aligned}
&v_i''^{(\beta)}v_j''^{(\beta)}\frac{\partial}{\partial u_k}\left[\left\langle \rho\frac{\mathrm{D}U_k}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right]\\
&\quad= \frac{\partial}{\partial u_k}\left[v_i''^{(\beta)}v_j''^{(\beta)}\left\langle \rho I_\beta\frac{\mathrm{D}U_k}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right]\\
&\qquad-\left[\left\langle \rho I_\beta\frac{\mathrm{D}U_k}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right]\frac{\partial}{\partial u_k}\big[v_i''^{(\beta)}v_j''^{(\beta)}\big]\\
&\quad= \frac{\partial}{\partial u_k}\left[v_i''^{(\beta)}v_j''^{(\beta)}\left\langle \rho I_\beta\frac{\mathrm{D}U_k}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle \frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}\right]\\
&\qquad-\left[v_i''^{(\beta)}\left\langle \rho I_\beta\frac{\mathrm{D}U_j}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle + v_j''^{(\beta)}\left\langle \rho I_\beta\frac{\mathrm{D}U_i}{\mathrm{D}t}\middle|\boldsymbol{u}\right\rangle\right]\frac{\mathscr{F}_{\boldsymbol{U}|I_\beta}}{\langle \rho I_\beta|\boldsymbol{u}\rangle}.
\end{aligned}$$

The last term on the right-hand side of (B 2) simplifies to

$$\begin{aligned}
\mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial v_i''^{(\beta)}v_j''^{(\beta)}}{\partial t} &= \mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial}{\partial t}\big[\big(u_i - \widetilde{\langle U_i^{(\beta)}\rangle}\big)\big(u_j - \widetilde{\langle U_j^{(\beta)}\rangle}\big)\big]\\
&= \mathscr{F}_{\boldsymbol{U}|I_\beta}\frac{\partial}{\partial t}\big[u_iu_j - u_j\widetilde{\langle U_i^{(\beta)}\rangle} - u_i\widetilde{\langle U_j^{(\beta)}\rangle} + \widetilde{\langle U_i^{(\beta)}\rangle}\widetilde{\langle U_j^{(\beta)}\rangle}\big]\\
&= \mathscr{F}_{\boldsymbol{U}|I_\beta}\left[-u_j\frac{\partial\widetilde{\langle U_i^{(\beta)}\rangle}}{\partial t} - u_i\frac{\partial\widetilde{\langle U_j^{(\beta)}\rangle}}{\partial t} + \frac{\partial\widetilde{\langle U_i^{(\beta)}\rangle}\widetilde{\langle U_j^{(\beta)}\rangle}}{\partial t}\right].
\end{aligned}$$

When integrated over all $\boldsymbol{u}$ space, the term in square brackets evaluates to zero.

The second-moment equation is then

$$\frac{\partial}{\partial t}\langle I_\beta \rho\rangle \widetilde{R}_{ij}^{(\beta)} + \frac{\partial}{\partial x_k}\langle \rho I_\beta u_i''^{(\beta)} u_j''^{(\beta)} u_k''^{(\beta)}\rangle + \frac{\partial}{\partial x_k}\langle \rho I_\beta\rangle \widetilde{R}_{ij}^{(\beta)} \widetilde{\langle U_k^{(\beta)}\rangle}$$
$$= \left[\langle \rho I_\beta u_i''^{(\beta)} u_k''^{(\beta)}\rangle \frac{\partial \widetilde{\langle U_j^{(\beta)}\rangle}}{\partial x_k} + \langle \rho I_\beta u_j''^{(\beta)} u_k''^{(\beta)}\rangle \frac{\partial \widetilde{\langle U_i^{(\beta)}\rangle}}{\partial x_k}\right]$$
$$+ \left\langle \rho I_\beta u_i''^{(\beta)} \frac{\mathrm{D}U_j}{\mathrm{D}t}\right\rangle + \left\langle \rho I_\beta u_j''^{(\beta)} \frac{\mathrm{D}U_i}{\mathrm{D}t}\right\rangle. \tag{B 3}$$

The second term on the right-hand side can be written as follows:

$$\left\langle \rho I_\beta u_i''^{(\beta)} \frac{\mathrm{D}U_j}{\mathrm{D}t}\right\rangle = \left\langle u_i''^{(\beta)} \frac{\partial (I_\beta \tau_{kj})}{\partial x_k}\right\rangle - \left\langle u_i''^{(\beta)} \tau_{kj} \frac{\partial I_\beta}{\partial x_k}\right\rangle.$$

The same treatment can be applied to the last term on the right-hand side of (B 3). Using the product rule on the temporal derivative and the spatial derivative (third term on left-hand side), rearranging and using the mean mass conservation equation, we obtain (5.29).

Appendix C. Simplified relations between the EE and LE representations

In this section, details of the simplified relationships between $\alpha_d(\boldsymbol{x}, t)$ and $n(\boldsymbol{x}; t)$, and between $f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{u}, r; \boldsymbol{x}, t)$ and $f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r|\boldsymbol{x}; t)$, that were presented in § 3 are provided. Combinations of statistically homogeneous number density, statistically homogeneous radius p.d.f. and statistically homogeneous $f^c_{\boldsymbol{V}|R}(\boldsymbol{v} \mid r, \boldsymbol{x}; t)$ are considered. Two-phase flows with monodisperse DPEs are included as a special subset of the homogeneous radius p.d.f. case. Approximations that are valid in some inhomogeneous cases are considered later.

The assumption of spherical DPEs implies an isotropic point process (non-spherical shapes could still result in an isotropic point process but those are not considered here; see Daley & Vere-Jones 2003 for details) and leads to the following isotropic form of (3.5) that is convenient for simplification under special conditions:

$$\alpha_d(\boldsymbol{x}, t) = \int_{r=0_+}^{\infty} \int_{r'=0}^{r} K'_D\, r'^{D-1} n(\boldsymbol{x} + \boldsymbol{e}\, r'; t)\, f^c_R(r \mid \boldsymbol{x} + \boldsymbol{e}\, r', t)\, \mathrm{d}r'\, \mathrm{d}r, \tag{C 1}$$

where $\boldsymbol{e}$ is the unit vector in the radial direction. The above expression has been written in a general form for D-dimensional space ($1 \leqslant D \leqslant 3$) with $K'_1 = 2$, $K'_2 = 2\pi$ and $K'_3 = 4\pi$.

Similarly, the assumption of an isotropic point process in (3.9) results in the simplification

$$f^E_{\boldsymbol{U}R|I_d}(\boldsymbol{v}, r; \boldsymbol{x}, t) = \frac{1}{\alpha_d(\boldsymbol{x}, t)} \int_{r'=0}^{r} K'_D\, r'^{D-1} n(\boldsymbol{x} + \boldsymbol{e}\, r'; t)\, f^c_{\boldsymbol{V}R}(\boldsymbol{v}, r \mid \boldsymbol{x} + \boldsymbol{e}\, r', t)\, \mathrm{d}r'. \tag{C 2}$$

C.1. *Statistically homogeneous cases*

C.1.1. *Homogeneous number density and homogeneous polydisperse radius p.d.f.*

If the number density is homogeneous ($n(\boldsymbol{x}';t) = n(t)$), and the DPEs have a statistically homogeneous size distribution represented by $f_R^c(r;t)$, then (C 1) simplifies to

$$\begin{aligned}\alpha_d(\boldsymbol{x},t) &= \int_{r=0_+}^{\infty}\int_{r'=0}^{r} K_D'\, r'^{D-1} n(t)\, f_R^c(r;t)\,\mathrm{d}r'\,\mathrm{d}r \\ &= n(t)\, K_D \int_{[r_+]} r^D f_R^c(r;t)\,\mathrm{d}r \\ &= n(t)\,\overline{\mathscr{V}}_D(t), \end{aligned} \tag{C 3}$$

where $\overline{\mathscr{V}}_D(t)$ is the average volume occupied by a DPE in D-dimensional space given by

$$\overline{\mathscr{V}}_D(t) = K_D\,\langle R^D\rangle(t) = K_D \int_{[r_+]} r^D f_R^c(r;t)\,\mathrm{d}r, \tag{C 4}$$

where $\langle R^D\rangle(t)$ is the Dth moment of the radius p.d.f. In the above expression, $K_1 = 2$, $K_2 = \pi$ and $K_3 = 4\pi/3$. In $\mathbb{R}^3$, this reduces to the well-known result

$$\alpha_d(t) = n(t)\frac{4}{3}\pi\langle R^3\rangle(t). \tag{C 5}$$

Although the relation between $\alpha_d(\boldsymbol{x},t)$ and $n(\boldsymbol{x};t)$ only requires assumptions concerning the number density and the radius p.d.f. $f_R^c(r|\boldsymbol{x};t)$ because $\alpha_d(\boldsymbol{x},t)$ does not depend on the statistical properties of the velocity of the DPEs, further assumptions are needed to relate $f^E_{UR|I_d}(\boldsymbol{v},r;\boldsymbol{x},t)$ and $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$. If $f^c_{V\,|\,R}(\boldsymbol{v}\mid r,\boldsymbol{x}';t)$ is also assumed to be statistically homogeneous, then (C 2) simplifies to

$$\begin{aligned} f^E_{U\,R\,|\,I_d}(\boldsymbol{v},r;t) &= \frac{1}{\alpha_d(t)}\int_{r'=0}^{r} K_D'\, r'^{D-1} n(t)\, f_R^c(r;t)\, f^c_{V\,|\,R}(\boldsymbol{v}\mid r;t)\,\mathrm{d}r' \\ &= \frac{1}{\langle R^D\rangle(t)} r^D f^c_{VR}(\boldsymbol{v},r;t) \\ &= \tilde{f}^c_{VR}(\boldsymbol{v},r;t), \end{aligned} \tag{C 6}$$

where the expression for $\alpha_d(\boldsymbol{x},t)$ from (C 3) has been substituted and $\tilde{f}^c_{VR}(\boldsymbol{v},r;t)$ is the (DPE) volume-weighted–p.d.f. corresponding to $f^c_{VR}(\boldsymbol{v},r;t)$ defined as

$$\tilde{f}^c_{VR}(\boldsymbol{v},r;t) \equiv \frac{r^D f^c_{VR}(\boldsymbol{v},r;t)}{\langle R^D(t)\rangle}. \tag{C 7}$$

Integrating both sides of (C 6) over $\boldsymbol{v}$ space results in

$$f^E_{R\,|\,I_d}(r;t) = \frac{1}{\langle R^D(t)\rangle} r^D f_R^c(r;t), \tag{C 8}$$

which provides a relationship between the Eulerian radius p.d.f. conditional on the dispersed phase and the size distribution in the LE approach.

C.1.2. *Homogeneous number density and homogeneous monodisperse radius p.d.f.*

If the number density is homogeneous then $n(\boldsymbol{x}';t) = n(t)$, and if the DPEs are monodispersed then they all have the same radius r_0, so that $f_R^c(r\mid\boldsymbol{x}';t) = \delta(r-r_0)$. Substituting these simplifications into (C 1) results in the following expression for

$\alpha_d(\boldsymbol{x}, t)$:

$$\begin{aligned}\alpha_d(\boldsymbol{x}, t) &= \int_{r=0_+}^{\infty} \int_{r'=0}^{r} K'_D\ r'^{D-1} n(t)\, \delta(r - r_0)\, \mathrm{d}r'\, \mathrm{d}r, \\ &= n(t) \int_{r=0_+}^{\infty} K_D\ r^D \delta(r - r_0)\, \mathrm{d}r \\ &= n(t) K_D\ r_0^D, \end{aligned} \tag{C 9}$$

This yields the result

$$\alpha_d(t) = n(t) \frac{4}{3} \pi r_0^3 \tag{C 10}$$

in $\mathbb{R}^3$. Note that $\alpha_d(\boldsymbol{x}, t)$ in both (C 5) and (C 10) depends on the dimensionality D of physical space through its dependence on r^D. The number density $n(t)$, on the other hand, does not have such an explicit dependence on dimensionality. This alone is evidence that the point-process and random-field statistical representations contain different information. Also see the example given in § 3.3.

If $f^c_{V\,|\,R}(\boldsymbol{v} \mid r, \boldsymbol{x}'; t)$ is assumed to be statistically homogeneous, then (C 2) simplifies to

$$\begin{aligned} f^E_{UR|I_d}(\boldsymbol{v}, r; t) &= \frac{1}{\alpha_d(t)} \int_{r'=0}^{r} K'_D\ r'^{D-1} n(t)\, \delta(r - r_0) f^c_{V\,|\,R}(\boldsymbol{v} \mid r; t)\, \mathrm{d}r' \\ &= \frac{1}{\alpha_d(t)} n(t)\, K_D\ r^D\ f^c_{V\,|\,R}(\boldsymbol{v} \mid r; t)\, \delta(r - r_0) \\ &= \delta(r - r_0) f^c_{V\,|\,R}(\boldsymbol{v} \mid r; t), \end{aligned} \tag{C 11}$$

where the simplified expression for $\alpha_d(\boldsymbol{x}, t)$ given by (C 9) has been substituted above.

Thus, for the case of statistically homogeneous number density and statistically homogeneous radius p.d.f., the following relations hold:

$$\overline{\mathscr{V}}_D = K_D \langle R^D \rangle \tag{C 12}$$

$$\alpha_d(t) = n \overline{\mathscr{V}}_D \tag{C 13}$$

$$f^E_{UR|I_d}(\boldsymbol{u}, r\ ; t) = \frac{r^D}{\langle R^D \rangle} f^c_{VR}(\boldsymbol{v}, r\ ; t) \tag{C 14}$$

$$\alpha_d(t) f^E_{UR|I_d}(\boldsymbol{u}, r\ ; t) = K_D r^D f(\boldsymbol{v}, r, t) \tag{C 15}$$

$$f^E_{UR|I_d}(\boldsymbol{u}, r\ ; t) f^E_X(t) = \frac{r^D}{\langle R^D(t) \rangle \langle N(t) \rangle} f(\boldsymbol{v}, r, t), \tag{C 16}$$

where $f^E_X(t) = \alpha_d(t) / \langle V_d(t) \rangle$ is the Eulerian position p.d.f. of the dispersed phase, $\langle V_d(t) \rangle$ is the mean volume occupied by the dispersed phase and $\langle N(t) \rangle$ is the mean number of DPEs in the domain. Here $f^E_X(t)$ is a constant (or uniform) for the homogeneous case under consideration.

C.2. *Statistically inhomogeneous cases*

Although simplifications are not possible for the general case of statistically inhomogeneous flows, it is possible to exploit a separation of scales where it exists, in order to derive simplified relations that can either be exact or approximate. It is useful to characterize this separation of scales by introducing a property called *local homogeneity*, which is defined as follows. A characteristic radius $r_\epsilon(\boldsymbol{x}, t)$ is defined at every physical location $\boldsymbol{x}$ and time t in terms of the radius p.d.f. $f^c_R(r|\boldsymbol{x}; t)$, such that

the probability of radius at $\boldsymbol{x}$ being larger than r_ϵ is at most ϵ, i.e.

$$r_\epsilon(\boldsymbol{x}, t) \equiv \left\{ r \,:\, \int_{r^*=r}^{\infty} f_R^c(r^* \mid \boldsymbol{x}; t)\, \mathrm{d}r^* \leqslant \epsilon \right\}. \tag{C 17}$$

If the length scale of inhomogeneity in the number density $n(\boldsymbol{x}; t)$ given by $l_n(\boldsymbol{x}, t) = n/|\nabla n|$ is *greater* than the characteristic radius $r_\epsilon(\boldsymbol{x}, t)$ at physical location $\boldsymbol{x}$ and time t, then the flow can be considered *locally homogeneous* with probability $(1-\epsilon)$ at $(\boldsymbol{x}, t)$. If the inequality $l_n(\boldsymbol{x}, t) > r_\epsilon(\boldsymbol{x}, t)$ holds throughout the flow domain (for all time) then the flow is termed *everywhere locally homogeneous* with probability $(1-\epsilon)$.

Simplification to exact relations is possible in the limit when the parameter $\epsilon = 0$; only approximate relations can be established when $\epsilon > 0$. In the limit $\epsilon = 0$ we denote the value of $r_\epsilon(\boldsymbol{x}, t)$ to be $r_{max}(\boldsymbol{x}, t)$, where with probability 1 there are no DPEs with radius larger than $r_{max}(\boldsymbol{x}, t)$ at $(\boldsymbol{x}, t)$, or

$$r_{max}(\boldsymbol{x}, t) \equiv \min_r \left\{ r \,:\, \int_{r^*=r}^{\infty} f_R^c(r^* | \boldsymbol{x}; t)\, \mathrm{d}r^* = 0 \right\}. \tag{C 18}$$

We now consider each source of inhomogeneity and apply the notion of local homogeneity, if applicable, in simplifying the relationship between EE and LE statistical representations.

C.2.1. *Homogeneous number density and inhomogeneous (polydisperse) radius p.d.f.*

If the number density is homogeneous but the DPEs have a statistically *inhomogeneous* size distribution represented by $f_R^c(r \mid \boldsymbol{x}; t)$, then (C 1) simplifies only to

$$\alpha_d(\boldsymbol{x}, t) \;= \int_{[\boldsymbol{x}', r \,:\, \boldsymbol{x}' \in b(\boldsymbol{x}, r)]} n(t)\, f_R^c(r \mid \boldsymbol{x}', t)\, \mathrm{d}\boldsymbol{x}'\, \mathrm{d}r. \tag{C 19}$$

Unlike the previous cases of homogeneous radius p.d.f., the integral of $f_R^c(r \mid \boldsymbol{x}', t)$ over the region $[\boldsymbol{x}' \in b(\boldsymbol{x}, r)]$ of $(\boldsymbol{x}', r)$ space has no simplified form in general. Therefore, for the case of an inhomogeneous radius p.d.f. there is no simple relationship between $\alpha_d(\boldsymbol{x}, t)$ and $n(\boldsymbol{x}; t)$, unless further assumptions are made.

If the weaker assumption of *local homogeneity* of $f_R^c(r \mid \boldsymbol{x}'; t)$ in the disc $b(\boldsymbol{x}, r_\epsilon)$ holds, then the following approximate relation:

$$\alpha_d(\boldsymbol{x}, t) \approx n(t)\, \overline{\mathscr{V}}_D(\boldsymbol{x}, t) \tag{C 20}$$

can be inferred. In the absence of an exact relation between $\alpha_d(\boldsymbol{x}, t)$ and $n(\boldsymbol{x}; t)$, relations between $f_{\boldsymbol{U}R|I_d}^E(\boldsymbol{v}, r; \boldsymbol{x}, t)$ and $f_{\boldsymbol{V}R}^c(\boldsymbol{v}, r|\boldsymbol{x}; t)$ are not explored for this case. If the assumption of local homogeneity of $f_R^c(r|\boldsymbol{x}'; t)$ in the disc $b(\boldsymbol{x}, r_{max})$ holds, then the following relation:

$$\alpha_d(\boldsymbol{x}, t) = n(t)\, \overline{\mathscr{V}}_D(\boldsymbol{x}, t) \tag{C 21}$$

can be inferred. Furthermore, under this assumption the following relation between the radius p.d.f.s in the two statistical representations also holds:

$$f_{R|I_d}^E(r; \boldsymbol{x}, t) = \frac{r^D}{\langle R^D \rangle(\boldsymbol{x}, t)} f_R^c(r|\boldsymbol{x}; t). \tag{C 22}$$

C.2.2. *Inhomogeneous number density and homogeneous monodisperse radius p.d.f.*

In this case (C 1) can be re-written as

$$\begin{aligned}\alpha_d(\boldsymbol{x},t) &= \int_{[\boldsymbol{x}',r\,:\,\boldsymbol{x}'\in b(\boldsymbol{x},r)]} n(\boldsymbol{x}';t)\,\delta(r-r_0)\,\mathrm{d}\boldsymbol{x}'\,\mathrm{d}r \\ &= \int_{r'=0}^{r_0}\int_r K'_D r'^{D-1} n(\boldsymbol{x}+\boldsymbol{e}\,r';t)\,\delta(r-r_0)\,\mathrm{d}r'\,\mathrm{d}r \\ &= K'_D\int_r \delta(r-r_0)\,\mathrm{d}r\int_{r'=0}^{r_0} r'^{D-1} n(\boldsymbol{x}+\boldsymbol{e}\,r';t)\,\mathrm{d}r' \\ &= K'_D\int_{r'=0}^{r_0} r'^{D-1} n(\boldsymbol{x}+\boldsymbol{e}\,r';t)\,\mathrm{d}r'. \end{aligned} \tag{C 23}$$

Again, in the absence of an exact relation between $\alpha_d(\boldsymbol{x},t)$ and $n(\boldsymbol{x};t)$, relations between $f^E_{UR|I_d}(\boldsymbol{v},r;\boldsymbol{x},t)$ and $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$ are not explored for this case. However, it is easy to show that $f^E_{R|I_d}(r;\boldsymbol{x},t)$ is simply $\delta(r-r_0)$ as expected.

If $n(\boldsymbol{x}';t)$ is locally homogeneous in the disk $b(\boldsymbol{x},r_0)$, then the following relationship holds:

$$\alpha_d(\boldsymbol{x},t) = n(\boldsymbol{x};t)K_D\,r_0^D. \tag{C 24}$$

In this case if $f^c_{V\,|\,R}(\boldsymbol{v}|r,\boldsymbol{x}';t)$ is locally homogeneous in the disc $b(\boldsymbol{x},r_0)$ then (C 11) holds.

C.2.3. *Inhomogeneous number density and homogeneous polydisperse radius p.d.f.*

In this case the general relationship given by (C 1) does not even simplify as much as in (C 23). For $n(\boldsymbol{x}';t)$ *locally homogeneous* in the disc $b(\boldsymbol{x},r_{max})$, the following approximate relationship holds:

$$\alpha_d(\boldsymbol{x},t) \approx n(\boldsymbol{x};t)K_D\,\langle R^D(t)\rangle. \tag{C 25}$$

No simple relation exists for the radius p.d.f. as in the monodisperse cases, and relationships between the velocity p.d.f.'s are not explored.

C.2.4. *Inhomogeneous number density and inhomogeneous polydisperse radius p.d.f.*

In this case no simplifications are possible to either (C 1) or (C 2).

C.3. *Summary*

Relationships between first-order quantities in the EE and LE statistical representations were explored. It is observed that only under conditions of statistical homogeneity that exact relationships between $n(\boldsymbol{x},t)$ and $\alpha_\beta(\boldsymbol{x},t)$ and between $f^E_{UR|I_d}(\boldsymbol{u},r;\boldsymbol{x},t)$ and $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$ can be obtained.

One must bear in mind that it is not enough to just define α_d or $f^E_{UR|I_d}(\boldsymbol{u},r;\boldsymbol{x},t)$ independently in terms of $n(\boldsymbol{x},t)$ and $f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)$, respectively, but rather they must jointly form a consistent definition so that quantities like mean momentum in a control volume makes sense. Although one might be tempted to write $\alpha_d(\boldsymbol{x},t) \approx n(\boldsymbol{x};t)\,\overline{\mathscr{V}}_D(\boldsymbol{x},t)$ and $f^E_{UR|I_\beta}(\boldsymbol{u},r;\boldsymbol{x},t) \approx r^D f^c_{VR}(\boldsymbol{v},r|\boldsymbol{x};t)\,/\langle R^D(\boldsymbol{x},t)\rangle$ under conditions of local homogeneity of the number density $l_n > r_{max}$ and radius p.d.f. $l_{f^c_R(r|\boldsymbol{x};t)} > r_{max}$, such relations are only approximate and useful for scaling purposes. They cannot hold as strict equalities simultaneously, and therefore unlike the statistically homogeneous cases presented earlier, they cannot form a consistent basis for comparing the two

statistical representations. In the inhomogeneous cases we must conclude that the two statistical representations are indeed different, and cannot be related.

Appendix D. Evolution equation for the volume-weighted d.d.f. of fluctuating velocity

The evolution equation for the volume-weighted d.d.f. of fluctuating velocity $\tilde{g}$ that was introduced in § 5.3 is derived in this section. Using the chain rule, we first form the time and spatial derivatives of the r^3-weighted d.d.f. $\tilde{f}$

$$\frac{\partial \tilde{f}}{\partial t} = \frac{\partial \tilde{g}}{\partial t} - \frac{\partial \tilde{g}}{\partial w_j}\frac{\partial \widetilde{\langle V_j \rangle}}{\partial t} \tag{D 1}$$

$$\frac{\partial \tilde{f}}{\partial x_k} = \frac{\partial \tilde{g}}{\partial x_k} - \frac{\partial \tilde{g}}{\partial w_j}\frac{\partial \widetilde{\langle V_j \rangle}}{\partial x_k}. \tag{D 2}$$

The above two expressions can be combined as follows:

$$\frac{\partial \tilde{f}}{\partial t} + (\widetilde{\langle V_k \rangle} + w_k)\frac{\partial \tilde{f}}{\partial x_k} = \frac{\partial \tilde{g}}{\partial t} + (\widetilde{\langle V_k \rangle} + w_k)\frac{\partial \tilde{g}}{\partial x_k} - \frac{\partial \tilde{g}}{\partial w_j}\left[\frac{\partial \widetilde{\langle V_j \rangle}}{\partial t} + (\widetilde{\langle V_k \rangle} + w_k)\frac{\partial \widetilde{\langle V_j \rangle}}{\partial x_k}\right]. \tag{D 3}$$

Multiplying (4.16) on both sides by r^3, the evolution equation for $\tilde{f} = r^3 f$ can be derived

$$\frac{\partial \tilde{f}}{\partial t} + v_k \frac{\partial \tilde{f}}{\partial x_k} = -\frac{\partial}{\partial v_k}\left[\langle A_k | \boldsymbol{x}, \boldsymbol{v}, r; t\rangle \tilde{f}\right] - \frac{\partial}{\partial r}\left[\langle \Theta | \boldsymbol{x}, \boldsymbol{v}, r; t\rangle \tilde{f}\right] + 3r^2 \langle \Theta | \boldsymbol{x}, \boldsymbol{v}, r; t\rangle f. \tag{D 4}$$

Note that since v_k is a sample space variable, it can be taken outside the derivative in the second term on the left-hand side. Equating the right-hand sides of (D 3) and (D 4), and rearranging results in the transport equation for the r^3-weighted d.d.f. of fluctuating velocity equation (5.35).

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