Recent Advances
in Modeling Gas-Particle Flows

Luca Mazzei[*]

Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE, UK

Abstract

This chapter is concerned with the mathematical modeling of dense fluidized suspensions, and focuses on the so-called Eulerian or multifluid approach. It introduces newcomers to some of the techniques adopted to model fluidized beds and to the challenges and long-standing problems that these techniques present. After introducing the principal approaches for modeling fluid-solid systems, we focus on the multifluid, overviewing the main averaging techniques that consent to describe granular media as continua. We then derive the Eulerian equations of motion for fluidized powders of a finite number of monodisperse particle classes, employing volume averages. We present the closure problem, and overview constitutive relations for modeling the granular stress and the interaction forces between the phases. To conclude, we introduce the population balance modeling approach, which permits handling suspensions of particles continuously distributed over the size and any other property of interest.

Keywords: Multiphase flows, Fluidization, Multifluid modeling, CFD, Closure problem.

1 Introduction

Fluidization is a well-established technology used in several industrial processes such as coal combustion, biomass gasification, waste disposal and food processing. To design fluidized beds, engineers have resorted for many years to experimental correlations and pilot plants. This practical approach to fluidization is well reflected in the first textbooks on the subject (see for instance Leva, 1959). These correlations, however, lack general validity and can help design only standard units: they cannot tell us how changes in vessel geometry, introduction of internals (like heat exchanger tubes) or feed repartition over various entry points affect fluid dynamics and performance. To answer these and similar questions, and improve the design of conventional units, one needs a theory for predicting how dense fluidized powders behave; pilot plants are not a convenient alternative, being expensive, time-consuming and not always leading to adequate scale up.

When fluidized beds were first employed in the 1920s -1940s, engineers did not appreciate this problem, probably because at the time the required plant performance was either not critical (like in FCC plants) or easily achievable (like in roasting and drying). Nevertheless, when later the problem revealed itself in other and more demanding applications, with some plants falling far short of the expected conversions previously achieved in pilot units, it became clear that this matter had to be addressed thoroughly. Researchers hence endeavored to find more reliable methods to predict the dynamics of fluidized suspensions.

In the 1960s, scientists began to adopt the conservation laws of mass, momentum and energy to analyze nearly any physical and chemical problem. This innovative approach, most probably fostered by the release of the influential textbook *Transport Phenomena* (Bird et al., 1960), led to significant theoretical headway, bolstered the hope to explain theoretically the behavior of fluidized powders and prompted the first trials to develop fluid dynamic models based on transport equations.

---

[*]Email address: l.mazzei@ucl.ac.uk. Tel: +44 (0)20 7679 4328, Fax: +44 (0)20 7383 2348.

Anderson & Jackson (1967) were among the first to model fluidized systems; starting from the continuity and dynamical equations for single-phase, incompressible fluids and the Newtonian equations for rigid-body motion, they derived averaged equations of conservation for the fluid and solid phases by applying a formal mathematical process of volume averaging. Afterwards, several researchers did the same, refer for instance to Whitaker (1969), Drew (1971) and Drew & Segel (1971). Initially, they used these models to understand better the complex behavior of multiphase systems, but without regarding them as a viable way to design real industrial units. Nonetheless, when faster computer processors and advanced numerical methods to integrate partial differential equations became available, they realized that a mathematical theory of multiphase flows could indeed become a useful design tool.

With the further development of new and more rigorous formulations of multiphase equations of motion (Buyevich, 1971; Hinch, 1977; Nigmatulin, 1979; Drew, 1983; Jenkins & Savage, 1983), the late 1970s and early 1980s witnessed the first endeavors to simulate numerically granular flowing systems (Pritchett et al., 1978; Gidaspow & Ettehadieh, 1983; Gidaspow et al., 1986). The promising results of these few pioneering studies generated an increasing interest in computational fluid dynamics (CFD) and multiphase flows, which rapidly started to turn into research areas in their own right.

Nowadays, CFD has become an almost indispensable tool to solve problems of academic and industrial interest. In the field of fluidization, CFD has assisted to understand fluid-solid interactions and has enabled to predict numerous macroscopic phenomena encountered in particulate systems. Similarly, multiphase flows and fluidization dynamics have become topics of interest not only for the scientific community but also for the industrial world. Over the years, many researchers have developed mathematical models to predict the dynamics of dense fluidized suspensions, proposing several approaches and mathematical schemes; we now briefly overview some of them, highlighting their advantages and limitations.

2   An overview of fluidized bed modeling

Fluidized beds can be modeled at various levels of detail. At the most fundamental, the motion of the system is determined by the Newtonian equations for translation and rotation of each particle and the Navier-Stokes transport equations to be satisfied at every point occupied by the interstitial fluid. In this approach, referred to as *Eulerian-Lagrangian*, the flow field of the fluid is modeled at a length scale far smaller than the particle size; one, therefore, is able to determine the pressure and velocity gradient over the surface of each particle, and from there the interaction force between the fluid and the particles (see for instance Pan et al., 2002). No closure problem hence arises for this force. Furthermore, since the particles are considered individually, the solid phase is not modeled as a continuum, retaining its granular nature; the equations describing its motion, consequently, feature no granular stress. Also the closure problem for this term, which arises in macroscopic models, is therefore absent.

This modeling strategy is appealing: it is conceptually quite simple – being probably the most natural for describing the dynamics of particulate systems – and it is the least affected by closure problems. It presents, nonetheless, a few disadvantages. First of all, it is extremely demanding computationally: simulations of this kind have been performed only for systems containing a relatively small number of particles; extending these calculations to dense suspensions in large domains, like those found in industrial fluidized beds, is presently inconceivable. Moreover, even if this were feasible, the information provided by the solution would be much too detailed, and one would have to filter the results to render them useful. Note that such results are of little direct interest to most end-users: the simulations yield the position and velocity of each particle at any given time, but what are the spatial distributions of the observables, such as the granular temperature and pressure, which are of real interest in applications? With the output of Eulerian-Lagrangian simulations one can obtain these distributions (if one knows how the observables of interest are related to the fluid and particle dynamics at the microscopic length scale, a knowledge that is acquired when one derives the averaged equations which characterize continuum models), but a complex calculation is required.

These observations suggest that it might be convenient to formulate equations of change governing the evolution of these observables directly. In this approach, we renounce to capture the details described above,

satisfying ourselves with a far reduced description of the flow. Although there exists no guarantee that these simplified equations can be really obtained – in closed form, that is – several studies have been conducted in such a pursuit (Anderson & Jackson, 1967; Whitaker, 1969; Drew, 1971; Drew & Segel, 1971; Drew, 1983; Drew & Lahey, 1993; Gidaspow, 1994; Zhang & Prosperetti, 1994; Enwald et al., 1996; Jackson, 1997, 1998, 2000). Owing to the complexity of the problem, one does not aim to derive the general exact averaged multiphase equations of motion; the intent is merely to formulate models which may describe satisfactorily phenomena of interest for industrial applications.

Various mathematical techniques yield such equations, and several claims have been advanced as to the superiority of each form of averaging versus the others. However, the resulting transport equations are very similar and present many common features. Two are the most significant. First, they are all written in terms of mean variables defined over the entire physical domain; so, they resemble those that one would write for a set of imaginary fluids which interpenetrate one other and occupy simultaneously the same physical volume. The model, known as *Eulerian-Eulerian* or *multifluid*, thus takes the form of coupled differential equations subjected to initial and/or boundary conditions assigned only on the boundaries of the domain containing the mixture, and no longer on the surface of the particles, as in Eulerian-Lagrangian models. Second, the process of averaging generates a number of indeterminate terms unrelated to the averaged variables, but associated with details of the motion at the particle (that is, microscopic) length scale. These are key terms, represented by the fluid and solid stress tensors and by the interaction forces exchanged by the phases. A closure problem hence arises, which one cannot usually solve analytically; in fact, there is no guarantee that a solution exists. So, one has to resort to empirical relations, this being the main shortcoming of the method.

Besides these two approaches, there is a third that can be regarded as a hybrid between them. Averaged equations of motion are used for the fluid phase, but rigid-body Newtonian equations are solved for every particle of the system. These do not interact with the fluid through its microscopic velocity field – as is the case in Eulerian-Lagrangian models – but with the averaged value of the latter. For instance, the overall force exerted by the fluid on each particle is not computed by integrating over the particle surface the local traction arising from the fluid velocity gradients: the force is instead calculated in terms of slip velocity between the average fluid velocity and the velocity of the particle center of mass and by resorting to empirical relations. This strategy, called *discrete particle modeling* (DPM), is significantly less demanding computationally than the Eulerian-Lagrangian and has met with resounding success (Tsuji et al., 1993; Hoomans et al., 1996; Xu & Yu, 1997; Ouyang & Li, 1999; Kafui et al., 2002; Lu et al., 2005; Zhu et al., 2008; Di Renzo et al., 2011; He et al., 2012; Wang et al., 2013; Deen et al., 2014).

To describe particle collisions, modelers use two approaches: hard and soft sphere. In the first, particles interact via binary, instantaneous, pointwise collisions. Their velocities after an encounter are computed by requiring that linear and angular momentum are conserved in the collision. This approach was pioneered by Allen & Tildesley (1990). Since their publication many authors have found it useful to model the collision dynamics in granular systems. Hoomans et al. (1996) used it in their model for gas-fluidized beds; it was the first time that the technique had been applied to a dense system. Many authors have since published papers with this strategy (see for instance Ouyang & Li, 1999). The soft sphere model for fluidized beds was instead pioneered by Tsuji et al. (1993), who developed their approach on the basis of earlier work done by Cundall & Strack (1979). Here, during an encounter, particles overlap slightly and the contact forces are calculated from the deformation history of the solids using a linear spring-dashpot model. This has been employed by Xu & Yu (1997), Pandit et al. (2005), Ye et al. (2005) and several other researchers.

Among the three modeling approaches discussed, the second is often preferred for its valuable feature of being computationally less demanding. Due to the number of particles present in industrial plants, Eulerian (continuum) modeling is unlikely to be replaced by its Lagrangian (discrete) counterparts in the near future; furthermore, Eulerian models appeal more to end-users, because they provide information of direct interest. The role of discrete modeling is yet paramount. The method, to be considered more as an effective research tool than a practical design instrument, by yielding information about the dynamics of multiphase systems at the microscopic length scale, may significantly help to develop and improve continuous models through the derivation of accurate closure relations. Eulerian-Lagrangian and DPM simulations are to multiphase flows what direct numerical simulations are to turbulent flows. This multiscale modeling strategy is represented in
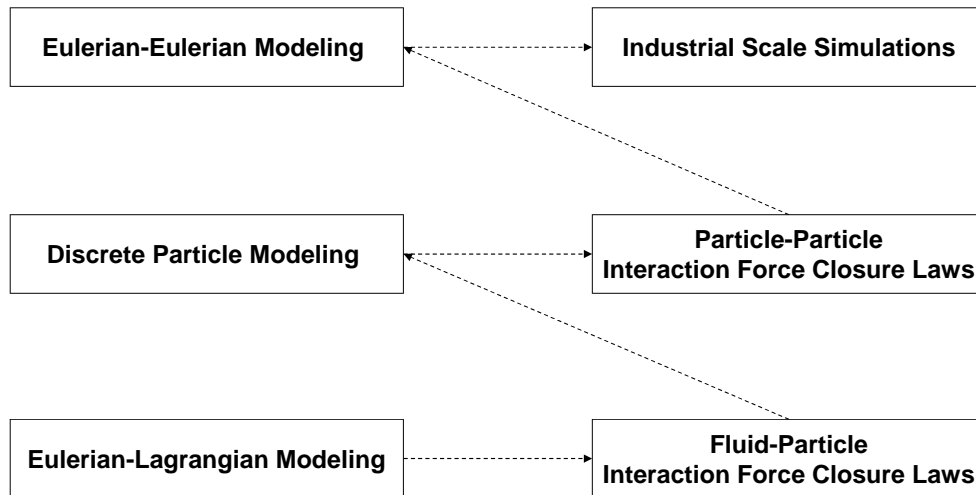
Figure 1: Multiscale modeling strategy.

Figure 1. The goal of the strategy is clear, but how to link the models and extract from each the information needed by those higher up in the hierarchy is an open challenge.

3 An overview of averaging theory

In the present section, we focus on three techniques that one can adopt to derive averages of point variables: statistical, volume and time averaging.

3.1 Statistical averaging

As previously mentioned, predicting the dynamics of fluidized suspensions may appear conceptually simple: one has to solve the Newtonian equations of motion for each particle and the Navier-Stokes equations for the fluid. In practice, doing so is extremely demanding, because the number of particles is quite large; however, one could argue that this is only a practical and temporary issue, which future generations of computers will certainly overcome. There is, nevertheless, a more fundamental problem: to integrate the equations, one has to know the initial positions and velocities of all the particles. For large particle numbers, this information is impossible to obtain. The problem, therefore, cannot be addressed deterministically: a statistical approach is necessary. To clarify this concept, let us be more definite.

Consider a fluidized suspension of ν identical, spherical, smooth particles, and let $\boldsymbol{x}_s(t)$ and $\boldsymbol{v}_s(t)$ be the position vector and linear velocity of the sth particle center, respectively. Initially, the sth particle is located in the point $\bar{\boldsymbol{x}}_s$ with velocity $\bar{\boldsymbol{v}}_s$. If $\boldsymbol{F}_s(t)$ denotes the unit mass force acting on the particle, as time advances the latter moves obeying the equations:

$$\dot{\boldsymbol{x}}_s(t) = \boldsymbol{v}_s(t) \quad ; \quad \dot{\boldsymbol{v}}_s(t) = \boldsymbol{F}_s(t) \quad ; \quad \boldsymbol{x}_s(0) = \bar{\boldsymbol{x}}_s \quad ; \quad \boldsymbol{v}_s(0) = \bar{\boldsymbol{v}}_s \tag{3.1}$$

Consequently, *if we know the initial conditions for each particle* and the functional expression of the overall force acting on each particle, by integrating the above differential equations we may predict, with certainty, the particle positions and velocities at any future time. For a realistic number of particles, knowing the initial positions and velocities of the particles appears to be impossible even in principle.

For systems comprising a great number of particles, therefore, we cannot know the initial state of every particle; in consequence, we cannot assign the initial conditions deterministically, as we did in Eq. 3.1. What we usually know are solely *macroscopic* – and therefore *measurable* – properties of the system, such as its local density, temperature or mean velocity. But there are infinite system configurations yielding the same

macroscopic properties, each with a certain probability of occurrence. So, we must replace the deterministic initial conditions above with probabilistic initial conditions. To this end, we introduce a probability density function (PDF) defined so that:

$$\pi_\nu(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\nu, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_\nu; t) d\boldsymbol{x}_1 \ldots d\boldsymbol{x}_\nu d\boldsymbol{v}_1 \ldots d\boldsymbol{v}_\nu \tag{3.2}$$

gives the joint probability that at time t the first particle has position and velocity in the ranges $d\boldsymbol{x}_1$ and $d\boldsymbol{v}_1$ about the real-space point $\boldsymbol{x}_1$ and the velocity-space point $\boldsymbol{v}_1$, the second particle has position and velocity in the ranges $d\boldsymbol{x}_2$ and $d\boldsymbol{v}_2$ about the real-space point $\boldsymbol{x}_2$ and the velocity-space point $\boldsymbol{v}_2$, and so on up to the last particle forming the particulate system. If we let:

$$\boldsymbol{r} \equiv (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_\nu, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_\nu) \tag{3.3}$$

we can regard $\boldsymbol{r}$ as the position point identifying the state of the entire particulate system in an abstract phase space of 6ν dimensions. Then $\pi_\nu(\boldsymbol{r}; t) d\boldsymbol{r}$ is the probability that at time t the configuration of the particulate system lies in the range $d\boldsymbol{r}$ about the phase-space point $\boldsymbol{r}$. We refer to the function $\pi_\nu(\boldsymbol{r}; t)$ as the ν-particle joint PDF or master joint PDF. At any given time, we do not know the exact configuration of the system, but the master joint PDF states how probable each configuration is. $\pi_\nu(\boldsymbol{r}; 0) d\boldsymbol{r}$, in particular, is the probability that the initial configuration lies in the range $d\boldsymbol{r}$ about $\boldsymbol{r}$. No determinism is present: *the system can be in any configuration*, but for each one the PDF tells us the probability of occurrence. Knowing the master joint PDF means having complete statistical knowledge of the population of particles.

Another useful function is the one-particle marginal PDF, which gives the probability of finding *a single particle* in a differential neighborhood of a given state – independently of the states of all the other particles. For a system in which the particles are identical, and consequently indistinguishable, the ν-particle joint PDF is symmetrical with respect to the particle state variables and the one-particle marginal PDF is equal for all the particles. Let $\pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t)$ denote the latter (for the real-space and velocity-space variables the subscript is unimportant; the one reported has been selected only for convenience). By definition, $\pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t) d\boldsymbol{x}_1 d\boldsymbol{v}_1$ is the probability of finding at time t a particle – any particle of the population, not just the first particle – in the ranges $d\boldsymbol{x}_1$ and $d\boldsymbol{v}_1$ about the points $\boldsymbol{x}_1$ and $\boldsymbol{v}_1$. The one-particle marginal PDF contains significantly less information about the particulate system than the master joint PDF; however, as we shall see, in most cases of real interest this is all the information that is truly required.

We reduce the ν-particle joint PDF to the one-particle marginal PDF by integrating out the state variables of every particle but the first one:

$$\pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t) \equiv \int_{\Omega_x} \cdots \int_{\Omega_x} \int_{\Omega_v} \cdots \int_{\Omega_v} \pi_\nu(\boldsymbol{r}; t) \prod_{s=2}^{\nu} d\boldsymbol{x}_s d\boldsymbol{v}_s \tag{3.4}$$

where Ω_x and Ω_v represent the ranges of variation of the particle positions and velocities, respectively; the former coincides with the region of physical space enclosed by the vessel containing the suspension, whereas the latter is unbounded and coincides with $\mathbb{R}^3$.

Knowing the master joint PDF allows calculating any average associated with the population of particles. Take a function $b(\boldsymbol{r})$ that associates a scalar value with the state of the particulate system. This is referred to as *dynamical function* (Balescu, 1975). If the system changes configuration (that is, the value of $\boldsymbol{r}$ changes), the value of the function changes. The observable $\langle b \rangle_s$ associated with the function b is the average value of the latter over all the system configurations; therefore, it is:

$$\langle b \rangle_s(t) \equiv \int_{\Omega_r} b(\boldsymbol{r}) \pi_\nu(\boldsymbol{r}; t) d\boldsymbol{r} \tag{3.5}$$

where Ω_r represents the range of variation of $\boldsymbol{r}$. In the integral above, we are summing all the values that the dynamical function can take, each one weighted by the probability of occurrence of the system configuration to which that value refers. Being macroscopic variables, observables do not depend on the microscopic state of the system, but can be functions of the time, real-space and velocity-space coordinates; in the expression

above $\langle b \rangle_s$ is only a function of time, for b does not depend on real-space and velocity-space coordinates; in general, however, this dependence will be present. Eq. 3.5 suggests that to calculate any kind of macroscopic property of the system one needs to know the master joint PDF (that is, one has to have complete knowledge of the system). In general this is true, but fortunately this is not always the case.

A class of dynamical functions of particular theoretical importance is given by functions which take the following mathematical form:

$$b(\boldsymbol{r}) = \sum_{s=1}^{\nu} b_1(\boldsymbol{x}_s, \boldsymbol{v}_s) \tag{3.6}$$

where b_1 is an arbitrary function of the phase-space state *of one particle*. This dynamical function depends on the state of the entire system, but the state of each particle is taken one at a time. An example is given by the total kinetic energy of the system, in which case $b_1 \equiv m(\boldsymbol{v}_s \cdot \boldsymbol{v}_s)/2$, where m is the particle mass. For this class of dynamical functions, we can write:

$$\langle b \rangle_s(t) = \sum_{s=1}^{\nu} \left[\int_{\Omega_r} b_1(\boldsymbol{x}_s, \boldsymbol{v}_s) \pi_\nu(\boldsymbol{r}; t) d\boldsymbol{r} \right]$$

$$= \nu \int_{\Omega_x} \int_{\Omega_v} b_1(\boldsymbol{x}_1, \boldsymbol{v}_1) \pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t) d\boldsymbol{x}_1 d\boldsymbol{v}_1 = \int_{\Omega_x} \int_{\Omega_v} b_1(\boldsymbol{x}_1, \boldsymbol{v}_1) f_1(\boldsymbol{x}_1, \boldsymbol{v}_1, t) d\boldsymbol{x}_1 d\boldsymbol{v}_1 \tag{3.7}$$

where it is:

$$f_1(\boldsymbol{x}_1, \boldsymbol{v}_1, t) \equiv \nu \pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t) \tag{3.8}$$

Here we have exploited the symmetry properties of the ν-particle PDF, which hold insofar as all the particles are identical. Thus, for this class of dynamical functions, to calculate the observables one needs to know only the one-particle marginal PDF, or equivalently the scalar function $f_1(\boldsymbol{x}_1, \boldsymbol{v}_1, t)$.

Known as *number density function* (NDF), the latter arises naturally from the passages shown above, but has as well an important physical interpretation: $f_1(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{x} d\boldsymbol{v}$ represents the average number of particles present at time t in the range (or infinitesimal volume) $d\boldsymbol{x}$ around the real-space point $\boldsymbol{x}$ with velocity in the range $d\boldsymbol{v}$ around the velocity-space point $\boldsymbol{v}$ (we have removed the subscript from the arguments of the NDF for convenience). $f_1(\boldsymbol{x}, \boldsymbol{v}, t)$, in other words, is an observable representing the mean particle number density in the six-dimensional phase space formed by the union of the real space Ω_x and velocity space Ω_v. To prove this, we must show that the NDF is the mean value of the number density of particles present in the real-space point $\boldsymbol{x}$ with velocity $\boldsymbol{v}$. This density has this expression:

$$\varphi_1(\boldsymbol{r}; \boldsymbol{x}, \boldsymbol{v}) \equiv \sum_{s=1}^{\nu} \delta(\boldsymbol{x}_s - \boldsymbol{x}, \boldsymbol{v}_s - \boldsymbol{v}) \tag{3.9}$$

This is because if no particle is located in $\boldsymbol{x}$ with velocity $\boldsymbol{v}$ the density is zero, whilst if a particle is therein located the density diverges (assuming that the volume of the particles is negligibly small compared with the macroscopic volumes of interest). Notice that $\varphi_1(\boldsymbol{r}; \boldsymbol{x}, \boldsymbol{v})$ belongs to the special class of dynamical functions defined by Eq. 3.6. Thus, we have:

$$\langle \varphi_1 \rangle_s(\boldsymbol{x}, \boldsymbol{v}, t) = \nu \int_{\Omega_x} \int_{\Omega_v} \delta(\boldsymbol{x}_1 - \boldsymbol{x}, \boldsymbol{v}_1 - \boldsymbol{v}) \pi_1(\boldsymbol{x}_1, \boldsymbol{v}_1; t) d\boldsymbol{x}_1 d\boldsymbol{v}_1 = \nu \pi_1(\boldsymbol{x}, \boldsymbol{v}; t) \tag{3.10}$$

This differs from the NDF defined in Eq. 3.8 merely in notation. Because of the important physical meaning that the NDF possesses, one usually favors the latter over the one-particle marginal PDF; knowledge of either function, however, permits calculating observables associated with dynamical functions of the class defined by Eq. 3.6. Of course, to determine observables of this kind, one needs to know how the NDF evolves in each phase-space point; this, as we shall see at the end of this chapter, is extremely challenging.

To conclude this section, we present three examples of observables that are particularly significant: mass, linear momentum and energy density. The dynamical functions with which these macroscopic quantities are associated take the following expressions:

$$b_M(\boldsymbol{r};\boldsymbol{x}) \equiv m\sum_{s=1}^{\nu}\delta(\boldsymbol{x}_s - \boldsymbol{x}) \quad ; \quad b_L(\boldsymbol{r};\boldsymbol{x}) \equiv m\sum_{s=1}^{\nu}\boldsymbol{v}_s\delta(\boldsymbol{x}_s - \boldsymbol{x})$$

$$b_E(\boldsymbol{r};\boldsymbol{x}) \equiv (m/2)\sum_{s=1}^{\nu}(\boldsymbol{v}_s \cdot \boldsymbol{v}_s)\delta(\boldsymbol{x}_s - \boldsymbol{x}) \tag{3.11}$$

Eq. 3.7 then gives:

$$\langle b_M\rangle_s(\boldsymbol{x},t) = mn(\boldsymbol{x},t) \quad ; \quad \langle b_L\rangle_s(\boldsymbol{x},t) = mn(\boldsymbol{x},t)\langle\boldsymbol{v}\rangle_s(\boldsymbol{x},t)$$

$$\langle b_E\rangle_s(\boldsymbol{x},t) = (m/2)n(\boldsymbol{x},t)\langle\boldsymbol{v}\cdot\boldsymbol{v}\rangle_s(\boldsymbol{x},t) \tag{3.12}$$

where n represents the expected number of particles per unit real-space volume, or equivalently the expected number density of particles in real space, $\langle\boldsymbol{v}\rangle_s$ the expected particle velocity and $\langle\boldsymbol{v}\cdot\boldsymbol{v}\rangle_s$ twice the expected kinetic energy per particle unit mass. Mathematically, their expressions are:

$$n(\boldsymbol{x},t) \equiv \int_{\Omega_v} f_1(\boldsymbol{x},\boldsymbol{v},t)d\boldsymbol{v} \quad ; \quad \langle\boldsymbol{v}\rangle_s(\boldsymbol{x},t) \equiv \frac{1}{n(\boldsymbol{x},t)}\int_{\Omega_v}\boldsymbol{v}f_1(\boldsymbol{x},\boldsymbol{v},t)d\boldsymbol{v}$$

$$\langle\boldsymbol{v}\cdot\boldsymbol{v}\rangle_s(\boldsymbol{x},t) \equiv \frac{1}{n(\boldsymbol{x},t)}\int_{\Omega_v}(\boldsymbol{v}\cdot\boldsymbol{v})f_1(\boldsymbol{x},\boldsymbol{v},t)d\boldsymbol{v} \tag{3.13}$$

In this section, to simplify the treatment, we have assumed that the state of each particle is identified only by position in real space and velocity. Additional coordinates can be introduced, such as the particle size, but the concepts presented do not change. For a more general treatment of this subject, we refer to the literature, in particular to the recent textbook by Marchisio & Fox (2013).

3.2 Volume averaging

Another method of deriving observables relies on volume averages; these are computed over spatial domains that are large enough to contain a statistically-significant number of particles, but which are small compared with the length scale of variation of the observables.

There are two kinds of volume averages: hard and soft. In the former, a volume V_x bounded by a surface S_x is attached to every spatial point $\boldsymbol{x}$; within this volume, one averages the property of interest by using the mean value theorem of integral calculus. The values of the property within V_x are accounted for and ascribed the same weight in the average, whilst those outside V_x are ignored. Soft averages are based on an alternative technique, more elegant and convenient from a mathematical viewpoint, that uses radial weighting functions. These are continuous, monotone, decreasing functions of the radial distance from the spatial point in which the average is evaluated. This mathematical device ascribes a weight to the property values within the whole physical domain; however, the length scale over which the weighting function decays significantly (referred to as weighting function radius) identifies a spherical volume around the point of average $\boldsymbol{x}$ outside which the property values affect the average negligibly. The two averaging schemes, accordingly, are not as different as they may appear. For mathematical convenience, in what follows we favor soft averages.

Volume-averaged variables might appear to depend on the specific choice of volume V_x or of weighting function (in particular on its radius). The larger the ratio between the smallest length scale of variation of the observables and the particle size, the more such a dependence dwindles provided that the weighting function radius is properly chosen. If this radius is denoted by r_2, the particle radius by r_1 and the macroscopic length scale by r_3, the local average is expected not to depend on the particular form of weighting function provided

that the condition $r_1 \ll r_2 \ll r_3$ is satisfied. In such a case, there is said to exist *separation of scales* between the macroscopic fluid dynamic problem and the detailed motion at the scale of a single particle. Only in this instance the volume-averaged variables have an unambiguous physical meaning.

In multiphase systems, made up of one continuous phase (the fluid) and one or more discrete phases (the particles), one can employ volume averages to obtain mean properties for each phase. We now first introduce formally the weighting functions and then report how such averages are defined.

3.2.1 Weighting functions

Weighting functions are characterized by the following mathematical properties:

1) The weighting function ψ is a scalar function of r defined for $r > 0$, where r denotes the distance of a point $\boldsymbol{z}$ from a point $\boldsymbol{x}$ in Euclidean space:

$$\psi = \psi(r) \quad , \quad r \equiv |\boldsymbol{x} - \boldsymbol{z}| \tag{3.14}$$

2) $\psi(r)$ is positive for any value of r, decreases monotonically with r and possesses continuous derivatives of any order. In other words, it is a function of class C^∞.

3) $\psi(r)$ is normalized so that, if Ω_x denotes the spatial domain occupied by the system of interest (assumed here to stretch out to infinity), it is:

$$\int_{\Omega_x} \psi(|\boldsymbol{x} - \boldsymbol{z}|)\,d\boldsymbol{z} = 4\pi \int_0^\infty \psi(r)r^2\,dr = 1 \tag{3.15}$$

In the integral on the left-hand side, $\boldsymbol{z}$ is the spatial variable of integration, while $\boldsymbol{x}$ is the spatial position in which the volume average is computed. The radius of the weighting function is defined as the scalar r_2 that satisfies the following equation:

$$4\pi \int_0^{r_2} \psi(r)r^2\,dr = 4\pi \int_{r_2}^\infty \psi(r)r^2\,dr = \frac{1}{2} \tag{3.16}$$

The weighting function radius is thus a measure of the linear size of the spherical neighborhood of $\boldsymbol{x}$ in which the spatial points have appreciable weight in the averaging process.

3.2.2 Fluid-phase volume averages

The void fraction, or fraction of space occupied by the fluid, and the fluid-phase volume average of a generic point variable $\zeta(\boldsymbol{x}, t)$ calculated in $\boldsymbol{x}$ at time t are so defined:

$$\varepsilon(\boldsymbol{x}, t) \equiv \int_{\Lambda_e} \psi(|\boldsymbol{x} - \boldsymbol{z}|)\,d\boldsymbol{z} \quad ; \quad \langle \zeta \rangle_e(\boldsymbol{x}, t) \equiv \frac{1}{\varepsilon(\boldsymbol{x}, t)} \int_{\Lambda_e} \zeta(\boldsymbol{z}, t)\psi(|\boldsymbol{x} - \boldsymbol{z}|)\,d\boldsymbol{z} \tag{3.17}$$

In the equations above, Λ_e represents the domain occupied by the fluid phase at time t (we have left out the explicit dependence on t to simplify the notation).

3.2.3 Solid-phase volume averages

In a system with ν solid phases, the volume fraction of the rth phase $\mathscr{S}_r$ and the solid-phase volume average of a generic point variable $\zeta(\boldsymbol{x}, t)$ calculated in $\boldsymbol{x}$ at time t are so defined:

$$\phi_r(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r} \int_{\Lambda_r} \psi(|\boldsymbol{x} - \boldsymbol{z}|)\,d\boldsymbol{z} \quad ; \quad \langle \zeta \rangle_s^r(\boldsymbol{x}, t) \equiv \frac{1}{\phi_r(\boldsymbol{x}, t)} \sum_{\mathscr{S}_r} \int_{\Lambda_r} \zeta(\boldsymbol{z}, t)\psi(|\boldsymbol{x} - \boldsymbol{z}|)\,d\boldsymbol{z} \tag{3.18}$$

where Λ_r is the region of Eulerian space occupied by a generic particle of phase $\mathscr{S}_r$ at time t. The summation is over all the particles of phase $\mathscr{S}_r$. In $\langle\zeta\rangle_s^r$ the subscript s indicates that this is a solid-phase volume average, whilst the superscript r indicates that the average refers to solid phase $\mathscr{S}_r$.

This average, used by several researchers (Enwald et al., 1996; Drew & Passman, 1998), operates on the microscopic properties of the particle material, considering point fields $\zeta(\boldsymbol{x}, t)$ that vary *within the particles*. It is an average which exactly parallels the one given for the fluid. Another approach, advanced by Anderson & Jackson (1967), is based on properties $\zeta_r(t)$ of the particles *as a whole*.

3.2.4 Particle-phase volume averages

Since the particles are rigid, their motion is determined by the translation of their centers of mass and by the rotation of their bodies about instantaneous axes of rotation. Thus, the resultant forces and torques acting on the particles suffice to establish their motion. We can then introduce a different kind of volume average that depends only on properties of the particles as a whole. We define the number density of particles of class $\mathscr{S}_r$ calculated in $\boldsymbol{x}$ at time t as follows:

$$n_r(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r} \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \tag{3.19}$$

$\boldsymbol{z}_r(t)$ being the position occupied at time t by the center of mass of a generic particle of solid phase $\mathscr{S}_r$. The volume fraction $\phi_r(\boldsymbol{x}, t)$ is related to the number density $n_r(\boldsymbol{x}, t)$ as follows:

$$\phi_r(\boldsymbol{x}, t) \approx n_r(\boldsymbol{x}, t) V_r \tag{3.20}$$

in which V_r is the volume of a particle of solid phase $\mathscr{S}_r$. As indicated, this equation is approximate, but it is accurate if the separation-of-scale requirement is met and the weighting function radius is selected correctly; this, as said, must be far larger than the particle radius.

Generalizing the averaging scheme of Jackson (1997), we define the particle-phase volume average for a particle property $\zeta_r(t)$ of solid phase $\mathscr{S}_r$ calculated in $\boldsymbol{x}$ at time t as:

$$\langle\zeta\rangle_p^r(\boldsymbol{x}, t) \equiv \frac{1}{n_r(\boldsymbol{x}, t)} \sum_{\mathscr{S}_r} \Big[\zeta_r(t) \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \Big] \tag{3.21}$$

In $\langle\zeta\rangle_p^r$ the subscript p indicates that this is a particle-phase volume average, whilst the superscript r indicates that the average refers to solid phase $\mathscr{S}_r$.

3.3 Time averaging

The third averaging method available is time averaging. Let us consider a field $\zeta(\boldsymbol{x}, t)$; for any fixed spatial position $\bar{\boldsymbol{x}}$, $\zeta(\bar{\boldsymbol{x}}, t)$ is a function of time that fluctuates irregularly. We denote the time scale that represents these fluctuations as τ_1. In $\bar{\boldsymbol{x}}$, we can obtain a mean value of $\zeta(\boldsymbol{x}, t)$ by time averaging over a large number of fluctuations, considering a time interval τ_2 much larger than the time scale of the fluctuations. Again, we resort to the mean value theorem, this time writing:

$$\langle\zeta\rangle_t(\boldsymbol{x}, t) \equiv \frac{1}{\tau_2} \int_{t-\alpha}^{t+\alpha} \zeta(\boldsymbol{x}, \tau) d\tau \quad , \quad \alpha \equiv \tau_2/2 \tag{3.22}$$

where $\langle\zeta\rangle_t(\boldsymbol{x}, t)$ denotes the time average and τ is a dummy integration variable. Also now, the mean value is expected to be insensitive to the averaging time scale provided that $\tau_1 \ll \tau_2 \ll \tau_3$, where τ_3 represents the time scale of the mean flow variations. That is, there has to be separation of scale (now in the time domain) between the macroscopic motion of the fluid-solid mixture and the microscopic motion of the particles; only in this case the time-averaged variables have an unambiguous physical meaning.

3.4   A final remark

Before concluding this section on averaging, we would like to point out that different averaging schemes can lead to different average values. If the values are equal, the system is said to be *ergodic*, but not all systems present this feature. For details, refer, for instance, to Jackson (2000).

4   Averaged equations of motion for fluid-particle systems

We now derive the averaged equations of motion for a generic fluid-particle system of ν solid phases by using volume averages. Similar equations can be obtained with statistical and time averages; refer, for instance, to Gidaspow (1994), Drew & Passman (1998) and Brilliantov & Poschel (2004). Our treatment is an extension of the work of Jackson (2000) and Owoyemi et al. (2007). Below, we adopt Einstein's convention: repeated indices are summed over the values one to three, with the exception of r and s, used as phase indices, and of e and p, used to specify the volume average type.

4.1   Fluid phase

Let us first derive the volume-averaged continuity equation. The starting point is the microscopic continuity equation for the fluid. If we assume that the latter is incompressible, this reads:

$$\partial_a u_a = 0 \tag{4.1}$$

where $\partial_a \equiv \partial/\partial x_a$ and u_a is the ath component of the fluid velocity vector $\boldsymbol{u}(\boldsymbol{x}, t)$ with respect to a generic orthonormal vector basis. Let us multiply both sides by $\psi(|\boldsymbol{x} - \boldsymbol{z}|)$ and integrate over Λ_e with respect to $\boldsymbol{z}$; doing so yields this averaged equation:

$$\varepsilon \langle \partial_a u_a \rangle_e = \int_{\Lambda_e} \left[\partial_a u_a(\boldsymbol{z}, t) \right] \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{z} = 0 \tag{4.2}$$

In this form the equation is not useful, because it is written in terms of averaged derivatives of point variables instead of derivatives of averaged point variables. We may, however, manipulate the equation by using these mathematical relations, whose proof is given in the appendix:

$$\varepsilon \langle \partial_a \zeta \rangle_e = \partial_a \left(\varepsilon \langle \zeta \rangle_e \right) - \sum_{r=1}^{\nu} \sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} \zeta(\boldsymbol{z}, t) k_a(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z \tag{4.3}$$

$$\varepsilon \langle \partial_t \zeta \rangle_e = \partial_t \left(\varepsilon \langle \zeta \rangle_e \right) + \sum_{r=1}^{\nu} \sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} \zeta(\boldsymbol{z}, t) \boldsymbol{u}(\boldsymbol{z}, t) \cdot \boldsymbol{k}(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z \tag{4.4}$$

Here $\partial_t \equiv \partial/\partial t$, $\boldsymbol{k}(\boldsymbol{x}, t)$ is the outward unit normal to the surface $\partial \Lambda_r$ bounding Λ_r, whilst $k_a(\boldsymbol{x}, t)$ is the ath component of the unit vector $\boldsymbol{k}(\boldsymbol{x}, t)$. Setting $\zeta \equiv u_a$ and $\zeta \equiv 1$ in Eqs. 4.3 and 4.4, respectively, and adding the results yields the averaged continuity equation in the form that we sought:

$$\partial_t \varepsilon + \partial_a \left(\varepsilon \langle u_a \rangle_e \right) = 0 \tag{4.5}$$

In this equation, as we should have expected, the fluid volume fraction takes on the role that the fluid density has for single-phase compressible fluids.

Let us go on to derive the volume-averaged linear momentum balance equation for the fluid. The starting point is the corresponding microscopic balance equation:

$$\rho_e \left[\partial_t u_a + \partial_b(u_a u_b) \right] = \partial_b T_{ab} + \rho_e g_a \tag{4.6}$$

where ρ_e is the (constant) fluid density, $T_{ab}(\boldsymbol{x},t)$ is the abth component of the point fluid stress tensor, while g_a is the ath component of the gravitational field. Multiply both sides by $\psi(|\boldsymbol{x}-\boldsymbol{z}|)$ and integrate over Λ_e with respect to $\boldsymbol{z}$. To treat the left-hand side of the averaged equation obtained, write Eqs. 4.3 and 4.4 with $\zeta \equiv u_a u_b$ and $\zeta \equiv u_a$, respectively, whilst to treat the right-hand side, use Eq. 4.3 with $\zeta \equiv T_{ab}$. With these relations, the averaged equation becomes:

$$\rho_e \left[\partial_t \Big(\varepsilon \langle u_a \rangle_e \Big) + \partial_b \Big(\varepsilon \langle u_a u_b \rangle_e \Big) \right]$$

$$= \partial_b \Big(\varepsilon \langle T_{ab} \rangle_e \Big) + \varepsilon \rho_e g_a - \sum_{r=1}^{\nu} \sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} T_{ab}(\boldsymbol{z},t) k_b(\boldsymbol{z},t) \psi(|\boldsymbol{x}-\boldsymbol{z}|) d\boldsymbol{\sigma}_z \tag{4.7}$$

The last term on the right-hand side is the sum over all particle classes of the mean resultant traction forces exerted by the fluid on the particles of each class. The force:

$$\sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} T_{ab}(\boldsymbol{z},t) k_b(\boldsymbol{z},t) \psi(|\boldsymbol{x}-\boldsymbol{z}|) d\boldsymbol{\sigma}_z \tag{4.8}$$

is the sum of the average resultant forces exerted by the fluid on the rth phase particles. To compute this force for each particle, we first weight the differential traction forces acting on each infinitesimal region $d\boldsymbol{\sigma}_z$ of the particle surface using the value of $\psi(|\boldsymbol{x}-\boldsymbol{z}|)$ corresponding to each region, and then we sum the (infinite number of) contributions. The fluid-solid interaction force, defined by Eq. 4.8, couples the linear momentum balance equation of the fluid to that of each particle class.

For reasons that will be clear later (when we deal with the solid phases), it is convenient to express Eq. 4.8 differently. To do so, we expand the weighting function in a Taylor series about the center $\boldsymbol{z}_r(t)$ of a generic particle of phase $\mathscr{S}_r$, writing:

$$\forall \, \boldsymbol{z} \in \partial \Lambda_r : \psi(|\boldsymbol{x}-\boldsymbol{z}|) \approx \psi(|\boldsymbol{x}-\boldsymbol{z}_r|)$$

$$- \Big[\partial_b \psi(|\boldsymbol{x}-\boldsymbol{z}_r|) \Big] r_r k_b(\boldsymbol{z}) + (1/2) \Big[\partial_{bc}^2 \psi(|\boldsymbol{x}-\boldsymbol{z}_r|) \Big] r_r^2 k_b(\boldsymbol{z}) k_c(\boldsymbol{z}) \tag{4.9}$$

where r_r is the radius of the particles of phase $\mathscr{S}_r$. As the particle radius is far smaller than the radius of the weighting function, we may truncate the Taylor series at the second-order term with acceptably small error. Using this relation, we approximate the force in Eq. 4.8 as:

$$n_r \langle f_a \rangle_p^r - \partial_b \Big(n_r \langle A_{ab} \rangle_p^r \Big) + (1/2) \partial_{bc}^2 \Big(n_r \langle B_{abc} \rangle_p^r \Big) \tag{4.10}$$

where it is:

$$n_r(\boldsymbol{x},t) \langle f_a \rangle_p^r(\boldsymbol{x},t) \equiv \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x}-\boldsymbol{z}_r|) \int_{\partial \Lambda_r} T_{ad}(\boldsymbol{z},t) k_d(\boldsymbol{z},t) d\boldsymbol{\sigma}_z \right] \tag{4.11}$$

$$n_r(\boldsymbol{x},t) \langle A_{ab} \rangle_p^r(\boldsymbol{x},t) \equiv \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x}-\boldsymbol{z}_r|) r_r \int_{\partial \Lambda_r} T_{ad}(\boldsymbol{z},t) k_d(\boldsymbol{z},t) k_b(\boldsymbol{z},t) d\boldsymbol{\sigma}_z \right] \tag{4.12}$$

$$n_r(\boldsymbol{x},t) \langle B_{abc} \rangle_p^r(\boldsymbol{x},t) \equiv \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x}-\boldsymbol{z}_r|) r_r^2 \int_{\partial \Lambda_r} T_{ad}(\boldsymbol{z},t) k_d(\boldsymbol{z},t) k_b(\boldsymbol{z},t) k_c(\boldsymbol{z},t) d\boldsymbol{\sigma}_z \right] \tag{4.13}$$

The quantities defined above are the components of a vector, a second-order tensor and a third-order tensor, respectively. The force in Eq. 4.8 is obtained by first weighting the differential traction forces exerted on the infinitesimal surface elements of the fluid-particle interface, using the values of the weighting function at the locations of the elements, and then by summing such contributions. The force in Eq. 4.11, on the other hand,

is obtained by first calculating the forces acting on the entire surface of each particle, then by weighting them using the values of the weighting function at the particle centers, and finally by summing such contributions. This second average interprets better the fluid-particle interaction force and *fulfills the principle of action and reaction*, as we will see in Section 4.2; this is why we prefer to operate in terms of this average force, and of the additional contributions appearing in Eq. 4.10.

The convective term in Eq. 4.7 features the average of the product of point velocity components. We find it convenient to decompose it into the sum of a product of average velocity components and of an average of velocity fluctuations; thus, we write:

$$\langle u_a u_b \rangle_e \approx \langle u_a \rangle_e \langle u_b \rangle_e + \langle \hat{u}_a \hat{u}_b \rangle_e \tag{4.14}$$

Here hatted variables denote the deviations of point variables from their respective mean values. The relation above is not exact, holding only when there is separation of scale between the microscopic and macroscopic descriptions of the flow. Introducing Eqs. 4.10 and 4.14 into Eq. 4.7 yields:

$$\rho_e \left[\partial_t \Big(\varepsilon \langle u_a \rangle_e \Big) + \partial_b \Big(\varepsilon \langle u_a \rangle_e \langle u_b \rangle_e \Big) \right] = \partial_b \langle S_{ab} \rangle_e - \sum_{r=1}^{\nu} \Big(n_r \langle f_a \rangle_p^r \Big) + \varepsilon \rho_e g_a \tag{4.15}$$

where it is:

$$\langle S_{ab} \rangle_e \equiv \varepsilon \langle T_{ab} \rangle_e + \sum_{r=1}^{\nu} \left[n_r \langle A_{ab} \rangle_p^r - (1/2) \partial_c \Big(n_r \langle B_{abc} \rangle_p^r \Big) \right] - \varepsilon \rho_e \langle \hat{u}_a \hat{u}_b \rangle_e \tag{4.16}$$

This term is the fluid-phase effective stress tensor. Finding an analytical closure for it is extremely complex, but Jackson (1997) did so for the limiting case of diluted, Stokesian, monodisperse suspensions fluidized by Newtonian fluids. We will address the problem of closure, for all the terms featuring on the right-hand side of Eq. 4.15 and of the ν solid-phase averaged dynamical equations, later on in Section 5.

4.2   Solid phases

The volume-averaged continuity equation for the generic solid phase $\mathscr{S}_r$ can be derived quite easily by using this mathematical relation, whose proof is given in the appendix:

$$n_r \langle \dot{\zeta} \rangle_p^r = \partial_t \Big(n_r \langle \zeta \rangle_p^r \Big) + \partial_a \Big(n_r \langle \zeta v_a \rangle_p^r \Big) \tag{4.17}$$

where the dot denotes a total time derivative and $\langle \zeta v_a \rangle_p^r (\boldsymbol{x}, t)$ is the average of the product of $\zeta_r(t)$ and of the ath component of the velocity $\boldsymbol{v}_r(t)$ of the particle center. Setting $\zeta_r \equiv 1$ gives:

$$\partial_t n_r + \partial_a \Big(n_r \langle v_a \rangle_p^r \Big) = 0 \tag{4.18}$$

which is the equation sought. Here the particle number density, or equivalently the volume fraction, takes on the (compressible) fluid density role.

To derive the volume-averaged equation of motion for the generic solid phase $\mathscr{S}_r$, we adopt the equation governing the motion of the generic particle of such phase:

$$\rho_r V_r \dot{v}_{r,a}(t) = \int_{\partial \Lambda_r} T_{ab}(\boldsymbol{z}, t) k_b(\boldsymbol{z}, t) d\boldsymbol{\sigma}_z + \sum_{s=1}^{\nu} \sum_{\mathscr{S}_s} f_{rs,a}(t) + \rho_r V_r g_a \tag{4.19}$$

where ρ_r denotes the density of the particles of phase $\mathscr{S}_r$, $\dot{v}_{r,a}(t)$ the ath component of the acceleration of the particle center of mass, while $f_{rs,a}(t)$ the ath component of the force exerted on the r particle by the generic s particle of phase $\mathscr{S}_s$ when a collision takes place. This force does not vanish only if particles r and s are in direct contact (it is zero for most s particles). Notice also that $f_{rs,a}(t)$ vanishes when r and s refer to the same

particle, because particles r and s need, of course, to be different. The surface integral on the right-hand side of the equation is the overall force exerted by the fluid on the particle.

To average Eq. 4.19, we multiply both sides by $\psi(|\boldsymbol{x} - \boldsymbol{z}_r|)$ and sum over all the particles belonging to phase $\mathscr{S}_r$. Doing so gives:

$$\rho_r V_r \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \dot{v}_{r,a}(t) \right] = \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \int_{\partial \Lambda_r} T_{ab}(\boldsymbol{z}, t) k_b(\boldsymbol{z}, t) d\boldsymbol{\sigma}_z \right]$$

$$+ \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \sum_{s=1}^{\nu} \sum_{\mathscr{S}_s} f_{rs,a}(t) \right] + \rho_r V_r g_a \sum_{\mathscr{S}_r} \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \qquad (4.20)$$

We now employ Eqs. 3.19, 3.21, 4.11 and 4.17, with $\zeta_r \equiv \dot{v}_{r,a}$ in the second and $\zeta_r \equiv v_{r,a}$ in the forth, and the following relation, whose proof is left to the reader:

$$\sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \sum_{s=1}^{\nu} \sum_{\mathscr{S}_s} f_{rs,a}(t) \right] = \sum_{s=1}^{\nu} \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \sum_{\mathscr{S}_s} f_{rs,a}(t) \right] \qquad (4.21)$$

to obtain:

$$\rho_r V_r \left[\partial_t \left(n_r \langle v_a \rangle_p^r \right) + \partial_b \left(n_r \langle v_a v_b \rangle_p^r \right) \right]$$

$$= n_r \langle f_a \rangle_p^r + n_r \rho_r V_r g_a + \sum_{s=1}^{\nu} \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \sum_{\mathscr{S}_s} f_{rs,a}(t) \right] \qquad (4.22)$$

The first term on the right-hand side is the fluid-particle interaction force – which also features, with opposite sign, in Eq. 4.15. This force satisfies the action-and-reaction principle, as it should. The final term combines the resultant forces arising from the particle-particle contacts among particles that belong to the same phase ($s = r$) and to different phases ($s \neq r$). These contributions are conceptually different, insofar as the former is a self-interaction term that represents the stress internal to the phase under examination, while the latter is a contact force acting between the Eulerian solid phases. To let the collisional solid stress tensor associated with phase $\mathscr{S}_r$ appear explicitly in Eq. 4.22, we need to manipulate the equation further. We first consider the following double sum over the particles r and s of the rth phase:

$$\sum_{\mathscr{S}_r} \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_{rs}(t)|) f_{rs,a}(t) \right] \qquad (4.23)$$

in which $\boldsymbol{z}_{rs}(t)$ denotes the position vector of the point of mutual contact between the rigid particles r and s. This double sum vanishes, inasmuch as $\boldsymbol{z}_{rs} = \boldsymbol{z}_{sr}$ and, for the action-and-reaction principle, $f_{rs,a} = -f_{sr,a}$. If we then expand $\psi(|\boldsymbol{x} - \boldsymbol{z}_{rs}|)$ in a Taylor series around $\boldsymbol{z}_r$, letting $\boldsymbol{k}_{rs}$ denote the unit vector of the vector $\boldsymbol{z}_{rs} - \boldsymbol{z}_r$, we obtain from the equation above that:

$$\sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \sum_{\mathscr{S}_r} f_{rs,a}(t) \right] \approx \partial_b \left[n_r \langle M_{ab} \rangle_p^r - (1/2) \partial_c \left(n_r \langle N_{abc} \rangle_p^r \right) \right] \qquad (4.24)$$

where it is:

$$n_r(\boldsymbol{x}, t) \langle M_{ab} \rangle_p^r(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r} \left\{ \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) r_r \sum_{\mathscr{S}_r} \left[f_{rs,a}(t) k_{rs,b}(t) \right] \right\} \qquad (4.25)$$

$$n_r(\boldsymbol{x}, t) \langle N_{abc} \rangle_p^r(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r} \left\{ \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) r_r^2 \sum_{\mathscr{S}_r} \left[f_{rs,a}(t) k_{rs,b}(t) k_{rs,c}(t) \right] \right\} \qquad (4.26)$$

The second-order tensor so defined:

$$\langle C_{ab}\rangle_p^r \equiv n_r\langle M_{ab}\rangle_p^r - (1/2)\partial_c\Big(n_r\langle N_{abc}\rangle_p^r\Big) \tag{4.27}$$

is the collisional stress tensor of the rth particle phase which accounts for the transfer of linear momentum at collisions between alike particles over the distance $2r_r$ separating their centers. This physical phenomenon is important in dense fluidized suspensions, where the total volume occupied by the particles is not negligible compared with the volume of the vessel containing them. For rarefied granular gases, which one can model adopting the Boltzmann-Grad limit, defined as:

$$r_r \to 0 \quad ; \quad \nu_r \to \infty \quad ; \quad \nu_r r_r^2 \text{ bounded} \tag{4.28}$$

in which ν_r represents the overall number of particles belonging to solid phase $\mathscr{S}_r$, because $z_r \to z_{rs} \to z_s$, the collisional stress vanishes (this result is well known in kinetic theory of gases; see, for instance, Chapman & Cowling, 1970 or Gidaspow, 1994). This is consequence of the principle of action and reaction, insofar as in the Boltzmann-Grad limit it is:

$$\sum_{\mathscr{S}_r}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)\sum_{\mathscr{S}_r} f_{rs,a}(t)\right] \to \sum_{\mathscr{S}_r}\sum_{\mathscr{S}_r}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_{rs}(t)|)f_{rs,a}(t)\right] = 0 \tag{4.29}$$

Consider now the other contribution to the overall particle-particle contact force appearing on the right-hand side of Eq. 4.22. This term, which represents the contact forces acting between r particles of phase $\mathscr{S}_r$ and s particles of phase $\mathscr{S}_s$, can be expressed as:

$$\sum_{\mathscr{S}_r}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)\sum_{\mathscr{S}_s} f_{rs,a}(t)\right] \tag{4.30}$$

where $s \neq r$ and with particles r and s belonging to phases $\mathscr{S}_r$ and $\mathscr{S}_s$, respectively. Given its definition, this force should fulfill the principle of action and reaction, so that:

$$\sum_{\mathscr{S}_r}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)\sum_{\mathscr{S}_s} f_{rs,a}(t)\right] = -\sum_{\mathscr{S}_s}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_s(t)|)\sum_{\mathscr{S}_r} f_{sr,a}(t)\right] \tag{4.31}$$

Clearly, this condition is not satisfied, since even if $f_{rs,a} = -f_{sr,a}$, it is $\psi(|\boldsymbol{x} - \boldsymbol{z}_r|) \neq \psi(|\boldsymbol{x} - \boldsymbol{z}_s|)$. Only when $r_r \to 0$ and $r_s \to 0$ this equation holds. We conclude that the force in Eq. 4.30 cannot be regarded as the interaction force between phases $\mathscr{S}_r$ and $\mathscr{S}_s$, but must include an additional contribution which does not satisfy the action-and-reaction principle. To find this force, we expand $\psi(|\boldsymbol{x} - \boldsymbol{z}_{rs}|)$ in a Taylor series about the point $\boldsymbol{z}_r$. Doing so gives:

$$\sum_{\mathscr{S}_r}\left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)\sum_{\mathscr{S}_s} f_{rs,a}(t)\right] \approx n_r\langle f_a\rangle_p^{rs} + \partial_b\left[n_r\langle P_{ab}\rangle_p^{rs} - (1/2)\partial_c\Big(n_r\langle Q_{abc}\rangle_p^{rs}\Big)\right] \tag{4.32}$$

where it is:

$$n_r(\boldsymbol{x}, t)\langle f_a\rangle_p^{rs}(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r}\left\{\psi(|\boldsymbol{x} - \boldsymbol{z}_{rs}(t)|)\sum_{\mathscr{S}_s} f_{rs,a}(t)\right\} \tag{4.33}$$

$$n_r(\boldsymbol{x}, t)\langle P_{ab}\rangle_p^{rs}(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r}\left\{\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)r_r\sum_{\mathscr{S}_s}\left[f_{rs,a}(t)k_{rs,b}(t)\right]\right\} \tag{4.34}$$

$$n_r(\boldsymbol{x}, t)\langle Q_{abc}\rangle_p^{rs}(\boldsymbol{x}, t) \equiv \sum_{\mathscr{S}_r}\left\{\psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|)r_r^2\sum_{\mathscr{S}_s}\left[f_{rs,a}(t)k_{rs,b}(t)k_{rs,c}(t)\right]\right\} \tag{4.35}$$

Continuity equation – Fluid phase $$\partial_t \varepsilon + \partial_{\boldsymbol{x}} \cdot \left(\varepsilon \langle \boldsymbol{u} \rangle_e \right) = 0$$
Continuity equation – Particle phase r $$\partial_t \phi_r + \partial_{\boldsymbol{x}} \cdot \left(\phi_r \langle \boldsymbol{v} \rangle_p^r \right) = 0$$
Dynamical equation – Fluid phase $$\rho_e \left[\partial_t \left(\varepsilon \langle \boldsymbol{u} \rangle_e \right) + \partial_{\boldsymbol{x}} \cdot \left(\varepsilon \langle \boldsymbol{u} \rangle_e \langle \boldsymbol{u} \rangle_e \right) \right] = \partial_{\boldsymbol{x}} \cdot \langle \boldsymbol{S} \rangle_e - \sum_{r=1}^{\nu} n_r \langle \boldsymbol{f} \rangle_p^r + \varepsilon \rho_e \boldsymbol{g}$$
Dynamical equation – Particle phase r $$\rho_r \left[\partial_t \left(\phi_r \langle \boldsymbol{v} \rangle_p^r \right) + \partial_{\boldsymbol{x}} \cdot \left(\phi_r \langle \boldsymbol{v} \rangle_p^r \langle \boldsymbol{v} \rangle_p^r \right) \right] = \partial_{\boldsymbol{x}} \cdot \langle \boldsymbol{S} \rangle_p^r + n_r \langle \boldsymbol{f} \rangle_p^r + \sum_{s \neq r=1}^{\nu} n_r \langle \boldsymbol{f} \rangle_p^{rs} + \phi_r \rho_r \boldsymbol{g}$$

Table 1: Eulerian-Eulerian averaged equations of motion for a system of ν particle classes.

The second-order tensor so defined:

$$\langle D_{ab} \rangle_p^{rs} \equiv n_r \langle P_{ab} \rangle_p^{rs} - (1/2) \partial_c \left(n_r \langle Q_{abc} \rangle_p^{rs} \right) \tag{4.36}$$

is the collisional stress tensor related to the momentum transferred at collisions between phases $\mathscr{S}_r$ and $\mathscr{S}_s$. We find it natural now to introduce the following tensor:

$$\langle S_{ab} \rangle_p^r \equiv \langle C_{ab} \rangle_p^r + \sum_{s \neq r=1}^{\nu} \langle D_{ab} \rangle_p^{rs} - n_r \rho_r V_r \langle \hat{v}_a \hat{v}_b \rangle_p^r \tag{4.37}$$

This is the effective stress tensor of phase $\mathscr{S}_r$. The first two contributions, taken together, represent the (total) collisional stress tensor, while the last, which arises from the Reynolds decomposition of the convection term in the averaged dynamical equation, represents the kinetic stress tensor.

In light of the results obtained above, we can express the averaged linear momentum balance equation for phase $\mathscr{S}_r$ as follows:

$$\rho_r V_r \left[\partial_t \left(n_r \langle v_a \rangle_p^r \right) + \partial_b \left(n_r \langle v_a \rangle_p^r \langle v_b \rangle_p^r \right) \right] = \partial_b \langle S_{ab} \rangle_p^r + n_r \langle f_a \rangle_p^r + \sum_{s \neq r=1}^{\nu} n_r \langle f_a \rangle_p^{rs} + n_r \rho_r V_r g_a \tag{4.38}$$

In this equation, the interaction forces between the phases (represented by the second and third terms on the right-hand side) satisfy the action-and-reaction principle. Table 1 reports, in absolute notation, the multifluid equations of motion just derived.

5   The problem of closure

The averaged equations of motion for the fluid and solid phases just derived are mathematically unclosed, for they feature terms related to point (*i.e.*, microscopic) variables. In their current form, therefore, the equations cannot be solved. An example of such terms is given by the interaction force between the fluid phase and the generic solid phase $\mathscr{S}_r$. This force, as seen, is equal to:

$$\langle \boldsymbol{f} \rangle_p^r (\boldsymbol{x}, t) \equiv \frac{1}{n_r(\boldsymbol{x}, t)} \sum_{\mathscr{S}_r} \left[\psi(|\boldsymbol{x} - \boldsymbol{z}_r|) \int_{\partial \Lambda_r} \boldsymbol{T}(\boldsymbol{z}, t) \cdot \boldsymbol{k}(\boldsymbol{z}, t) d\boldsymbol{\sigma}_z \right] \tag{5.1}$$

To calculate it, one needs to know the point fluid stress distribution $\boldsymbol{T}(\boldsymbol{x}, t)$ over the surface of each particle as well as the position of each particle. This distribution is related to the point velocity field of the fluid, not to its volume average; because in a macroscopic description of the flow this field and the particle positions are unknown, Eq. 5.1 has no practical use (in a macroscopic modeling context).

We manipulated the averaged equations of motion in such a way that the closure problem is confined to a small number of well-defined terms. These are the effective stress tensor for each phase and the interaction forces between the fluid and each solid phase and between each pair of solid phases. Overcoming the closure problem means deriving expressions for them in terms of averaged variables only. Analytical closures based on purely theoretical arguments are prohibitively difficult to obtain; there is no guarantee that such equations even exist. Usually, the goal is far less ambitious and is finding equations that consent to analyze the systems of interest with the desired accuracy; such equations should be the simplest able to capture enough physics to describe the fluid dynamics of the suspension satisfactorily.

In what follows, we first present some strategies for modeling the effective fluid and solid stress tensors; we then analyze the mean fluid-particle interaction force, laying emphasis on the buoyancy and drag forces, and the mean particle-particle interaction force.

5.1   Effective stress

Owing to the many contributions, yielded by the averaging process, that make up the effective stress tensors, these are complex to model. Closing these quantities is further complicated by the absence of experimental measurements having a direct bearing on them. Notwithstanding, researchers usually suppose that both fluid and solid phases behave as Newtonian fluids, writing:

$$\boldsymbol{S}_e = -\left[p_e - \left(\kappa_e - \frac{2}{3}\mu_e\right)\text{tr}\boldsymbol{D}_e\right]\boldsymbol{I} + 2\mu_e\boldsymbol{D}_e \;\; ; \;\; \boldsymbol{S}_r = -\left[p_r - \left(\kappa_r - \frac{2}{3}\mu_r\right)\text{tr}\boldsymbol{D}_r\right]\boldsymbol{I} + 2\mu_r\boldsymbol{D}_r \quad (5.2)$$

where p_e, p_r, κ_e, κ_r, μ_e and μ_r are the averaged pressures, dilatational viscosities and shear viscosities of the fluid and rth solid phase, respectively; furthermore, $\boldsymbol{I}$ is the identity tensor, while $\boldsymbol{D}_e$ and $\boldsymbol{D}_r$ are the rate of deformation (or strain) tensors, defined as:

$$\boldsymbol{D}_e \equiv \frac{1}{2}\left(\partial_{\boldsymbol{x}}\boldsymbol{u}_e + \partial_{\boldsymbol{x}}\boldsymbol{u}_e^T\right) \quad ; \quad \boldsymbol{D}_r \equiv \frac{1}{2}\left(\partial_{\boldsymbol{x}}\boldsymbol{v}_r + \partial_{\boldsymbol{x}}\boldsymbol{v}_r^T\right) \quad (5.3)$$

From now on, as done in these last expressions, we simplify the notation by leaving out the angular brackets that imply averaging. Experimental evidence has shown that in several fluidization regimes the assumption of Newtonian behavior is satisfactory, especially for powders far from maximum packing.

If Eqs. 5.2 hold, the closure problem reduces to finding suitable constitutive expressions for the pressure, dilatational viscosity and shear viscosity of each phase. As done in Section 4, often one assumes that the fluid is incompressible, so that no constitutive equation is required for p_e, that κ_e is zero and that μ_e is proportional to ε, the proportionality constant being the shear viscosity of the pure fluid.

For the solid phases, constitutive expressions for these quantities have been derived from granular kinetic theory (Gidaspow, 1994; Brilliantov & Poschel, 2004), a generalization of the mathematical theory of dense non-uniform gases (Chapman & Cowling, 1970). The idea is that, because dense granular gases resemble in many ways dense molecular gases, the constitutive equations that govern the two should be derivable, at least in part, from the same theoretical framework. Similarly to a molecular gas, particle pressure and viscosities are functions of a granular temperature, which is governed by a balance equation for a pseudointernal energy related to the particle peculiar velocity. For solid phase $\mathscr{S}_r$, the balance equation is:

$$\rho_r\left[\partial_t\left(\phi_r U_r\right) + \partial_{\boldsymbol{x}} \cdot \left(\phi_r U_r \boldsymbol{v}_r\right)\right] = -\partial_{\boldsymbol{x}} \cdot \boldsymbol{q}_r + \boldsymbol{S}_r : \partial_{\boldsymbol{x}}\boldsymbol{v}_r + G_{d,r} - S_{v,r} - S_{c,r} \quad (5.4)$$

where $U_r \equiv 3/2\,\Theta_r$ is the pseudointernal energy per unit mass, Θ_r being the granular temperature, and $\boldsymbol{q}_r$ is the pseudothermal heat flux. The equation differs from the classical internal energy balance equation (Bird

et al., 1960) because of a sink term $S_{c,r}(\boldsymbol{x}, t)$ representing energy degradation caused by inelastic collisions, a source term $G_{d,r}(\boldsymbol{x}, t)$ representing generation of particle velocity fluctuations by fluctuating fluid-particle forces and a sink term $S_{v,r}(\boldsymbol{x}, t)$ representing their dampening by viscous resistance to particle motion. $\boldsymbol{q}_r$ is usually modeled using Fourier's law, writing:

$$\boldsymbol{q}_r = - k_r \partial_{\boldsymbol{x}} \Theta_r \tag{5.5}$$

where k_r is the granular thermal conductivity of the rth solid phase. Different closures have been developed for this parameter; Gidaspow et al. (1992), for instance, proposed:

$$k_r = \frac{150 \rho_r s_r (\pi \Theta_r)^{1/2}}{384 \alpha_r (1 + e_r)} \left[1 + (6/5) \phi_r \alpha_r (1 + e_r) \right]^2 + 2 \phi_r^2 \rho_r s_r \alpha_r (1 + e_r)(\Theta_r/\pi)^{1/2} \tag{5.6}$$

where s_r denotes the particle diameter, e_r the coefficient of restitution for particle collisions and α_r the radial distribution function for the rth solid phase. Various expressions are available for this function; for instance, that advanced by Iddir & Arastoopour (2005) reads:

$$\alpha_r = \left[1 - (\phi/\phi_{max}) \right]^{-1} + (3 s_r/2) \sum_{s=1}^{\nu} (\phi_s/s_s) \tag{5.7}$$

where ϕ is the overall solid volume fraction and ϕ_{max} is the maximum solid compaction (*i.e.*, the maximum value which ϕ can take). Here α_r diverges positively when ϕ approaches ϕ_{max}. An expression in which α_r is bounded is that of Lebowitz (1964), where ϕ_{max} does not feature:

$$\alpha_r = (1/\varepsilon) \left[1 + (3 s_r/2\varepsilon) \sum_{s=1}^{\nu} (\phi_s/s_s) \right] \tag{5.8}$$

To close Eq. 5.4, one needs constitutive equations also for the terms $G_{d,r}$, $S_{v,r}$ and $S_{c,r}$. For briefness, we do not report them; the interested reader may refer, for instance, to Gidaspow (1994), Syamlal et al. (1993), Fan & Zhu (1998) and Jackson (2000).

Various closures for the solid pressure are available in the literature, all derived from the granular kinetic theory. As an example, we report the expression advanced by Lun et al. (1984), suitably extended to cater for polydisperse suspensions:

$$p_r = \left[1 + 2 \sum_{s=1}^{\nu} (s_{rs}/s_r)^3 \phi_s \alpha_{rs} (1 + e_{rs}) \right] \phi_r \rho_r \Theta_r \tag{5.9}$$

where s_r and s_s are the particle diameters for phases r and s, respectively, e_{rs} is the coefficient of restitution for collisions between particles of phases r and s, while:

$$s_{rs} \equiv (s_r + s_s)/2 \quad ; \quad \alpha_{rs} \equiv (s_r \alpha_s + s_s \alpha_r)/(s_r + s_s) \tag{5.10}$$

As an example of constitutive equations for the solid-phase dilatational and shear viscosities, we report those given in Gidaspow (1994), even if several are available in the literature:

$$\kappa_r = (4/3) \phi_r^2 \rho_r s_r \alpha_r (1 + e_r)(\Theta_r/\pi)^{1/2} \tag{5.11}$$

$$\mu_r = \frac{10 \rho_r s_r (\pi \Theta_r)^{1/2}}{96 \alpha_r (1 + e_r)} \left[1 + (4/5) \phi_r \alpha_r (1 + e_r) \right]^2 + (4/5) \phi_r^2 \rho_r s_r \alpha_r (1 + e_r)(\Theta_r/\pi)^{1/2} \tag{5.12}$$

These expressions are those originally developed for monodisperse suspensions and do not directly account for the presence of the other solid phases.

The expressions given above, as said, are based on the kinetic theory of granular flows. This assumes that particles are smooth and spherical, that collisions are binary and instantaneous, and that the suspension is far

from the frictional packing limit, which marks the transition from the viscous to the frictional flow regime. In the first regime, particles undergo transient contacts, momentum transfer is translational and collisional, and the granular kinetic theory holds; in the second, particles undergo enduring contacts and momentum transfer is mainly frictional. Granular kinetic theory does not account for these interactions and thus in the frictional flow regime the closures reported above are inadequate.

In regions of high solid volume fraction, particles interact with multiple neighbors and the mechanism for stress generation is not merely due to kinetic and (particularly) collisional contributions, but also to sustained contacts among particles. Such contacts make particles dissipate considerable energy, letting them form very dense regions in the bed. This increases the ability of the granular assembly to resist shearing, for tangential frictional forces at contact points are now present. Hence, the solid viscosity is larger than that predicted by the granular kinetic theory.

To describe the frictional stress other models, empirical, phenomenological or based on the theory of soil mechanics, are needed. Usually, one assumes that it is:

$$\boldsymbol{S}_r^\star = -\,p_r^\star \boldsymbol{I} + 2\mu_r^\star \boldsymbol{D}_r \tag{5.13}$$

where the star indicates that the quantity refers to the frictional flow regime. Syamlal et al. (1993) proposed this equation for the frictional pressure:

$$p_r^\star = \phi_r p^\star \quad , \quad p^\star \equiv 10^A (\phi - \phi_f)^B \tag{5.14}$$

where ϕ_f denotes the frictional solid packing (the solid volume fraction threshold value at which the powder enters the frictional flow regime). The coefficients A and B are very high, with typical values of 25 and 10, respectively. For other constitutive equations the reader is referred to the literature. An expression often used for the frictional shear viscosity is that of Schaeffer (1987), which reads:

$$\mu_r^\star = \frac{p_r^\star \sin \vartheta_r}{2\sqrt{I_2(\boldsymbol{D}_r)}} \left(\sum_{s=1}^{\nu} \phi_s \right)^{-1} \quad , \quad I_2(\boldsymbol{D}_r) \equiv \frac{1}{2}\left[(\mathrm{tr}\boldsymbol{D}_r)^2 - \mathrm{tr}\boldsymbol{D}_r^2 \right] \tag{5.15}$$

where ϑ_r is the angle of internal friction of the rth granular material, while $I_2(\boldsymbol{D}_r)$ is the second invariant of the rate of deformation tensor. Other expressions are available in the literature. In the frictional flow regime, one usually accounts also for the kinetic and collisional contributions to the solid stress; the easiest way to do this is adding the viscous stress tensor to the frictional one.

5.2   Fluid-particle interaction force

There are five main contributors to the fluid-particle interaction force. The first is the buoyancy force, whose definition in the context of multiphase flows is not unique and needs to be discussed. The second acts in the direction of the fluid-particle slip velocity – that is, the fluid velocity relative to an observer moving with the same local mean velocity as the particles. The third is normal to the slip velocity, the fourth is parallel to the relative acceleration between the phases and the fifth is proportional to the local mean acceleration of the fluid. The last four terms are commonly referred to as drag force, lift force, virtual mass force and local fluid acceleration force, respectively. As we shall see, *the local fluid acceleration force is not always present, but features only when one definition of buoyancy force is used* – in particular, the classical definition presented later on. Among these five terms, often the buoyancy and drag forces are dominant.

5.2.1   Buoyancy force

A first definition sets this force equal to the weight of the fluid displaced by the solid; accordingly, if we refer the force to the unit volume of suspension, it is:

$$n_r \boldsymbol{f}_{B,r}^\star \equiv -\,\phi_r \rho_e \boldsymbol{g} \tag{5.16}$$

Since it is consistent with the Archimedes's principle original formulation, we call this *classical definition*. For a given value of ϕ_r, this force is constant, being unrelated to the flow.

The second definition relates the force to the effective fluid stress tensor, as reported by Jackson (2000); per unit volume of suspension, it is:

$$n_r \boldsymbol{f}_{B,r}^{\bullet} \equiv \phi_r \partial_{\boldsymbol{x}} \cdot \boldsymbol{S}_e \qquad (5.17)$$

Another definition often encountered in the literature considers solely the isotropic part of the effective stress tensor of the fluid; the closure therefore takes the form:

$$n_r \boldsymbol{f}_{B,r}^{\circ} \equiv -\phi_r \partial_{\boldsymbol{x}} p_e \qquad (5.18)$$

These definitions lead to different values of the buoyancy force. There is nothing wrong with this, for we are free to define this force as we like: what is crucial is that the *total* fluid-particle interaction force $n_r \boldsymbol{f}_r$, which has an objective physical meaning, be correctly calculated. Thus, modelers who adopt different definitions of buoyancy force will also need to employ different expressions for the complementary force that makes up the total fluid-particle interaction force. The value of the latter must be the same in all models. So, for instance, if one opts to use Eq. 5.18, the contribution of the deviatoric part of $\boldsymbol{S}_e$ must be included in the complementary force: it will still be present, the only difference being that it is not regarded as part of the buoyancy force, but as part of the complementary force.

To better understand the meaning of these definitions, consider a monodisperse suspension of motionless particles equally distributed in space (*i.e.*, an ideal homogeneous bed). The second and third definitions here coincide, because $\boldsymbol{D}_e$ vanishes and $\boldsymbol{S}_e$ is therefore isotropic:

$$\boldsymbol{S}_e = -p_e \boldsymbol{I} \quad \Rightarrow \quad n \boldsymbol{f}_B^{\bullet} = n \boldsymbol{f}_B^{\circ} \qquad (5.19)$$

where n is the particle number density. We can derive an expression for this force using the mean dynamical equations reported in Table 1; these reduce to:

$$n \boldsymbol{f} = -\partial_{\boldsymbol{x}} p_e + \varepsilon \rho_e \boldsymbol{g} \quad ; \quad n \boldsymbol{f} = -\phi \rho_s \boldsymbol{g} \qquad (5.20)$$

where ϕ denotes the solid volume fraction, ρ_s the particle density and $n \boldsymbol{f}$ the fluid-particle interaction force. Subtracting the two equations and using Eq. 5.18 gives:

$$\partial_{\boldsymbol{x}} p_e = (\varepsilon \rho_e + \phi \rho_s) \boldsymbol{g} \quad ; \quad n \boldsymbol{f}_B^{\bullet} = n \boldsymbol{f}_B^{\circ} = -\phi(\varepsilon \rho_e + \phi \rho_s) \boldsymbol{g} \qquad (5.21)$$

Thus, for ideal uniform fluidized beds the difference between the first and the other two definitions reduces to the density choice in the force expression: the first requires the fluid density, while the second the suspension bulk density. For further details about this topic, we refer to Jackson (2000).

5.2.2 Local fluid acceleration force

If the classical definition of buoyancy force is employed, the complementary force to the total fluid-particle interaction force must include a term known as local fluid acceleration force (*this term is absent otherwise*). Per unit volume of suspension, this force is given by:

$$n_r \boldsymbol{f}_{A,r}^{\star} \equiv \phi_r \rho_e D_t^e \boldsymbol{u}_e \quad , \quad D_t^e \boldsymbol{u}_e \equiv \partial_t \boldsymbol{u}_e + \boldsymbol{u}_e \cdot \partial_{\boldsymbol{x}} \boldsymbol{u}_e \qquad (5.22)$$

where the derivative on the right-hand side is a material derivative relative to a Lagrangian observer moving with the locally averaged velocity of the fluid.

If the fluid acceleration is far less than the gravitational acceleration, the local fluid acceleration force is far less than the buoyancy force and so its contribution is negligible. This force, nonetheless, is conceptually important, as the following thought experiment reveals. Consider a uniform assembly of particles at rest in a

body of fluid. The fluid is also at rest in a vertical container placed on a horizontal plane. The system resides in a uniform gravitational field. If the plane supporting the container and the constraints keeping the particles at rest are suddenly removed, the entire system falls freely with an acceleration equal to $\boldsymbol{g}$. Since the mean velocity fields of both phases are uniform and no pressure gradients are present, the effective stress tensors of both phases vanish, and the dynamical equations in Table 1 reduce to:

$$\varepsilon \rho_e D_t^e \boldsymbol{u}_e = - n\boldsymbol{f} + \varepsilon \rho_e \boldsymbol{g} \quad ; \quad \phi \rho_s D_t^s \boldsymbol{v}_s = n\boldsymbol{f} + \phi \rho_s \boldsymbol{g} \tag{5.23}$$

For convenience, we have used the non-conservative formulation of the equations; to obtain them, one must combine the dynamical and continuity equations (see, for instance, Bird et al., 1960). The material derivative for the solid phase is defined similarly to that for the fluid phase. In the case at hand, both material derivatives are equal to the gravitational acceleration, and Eqs. 5.23 lead to the same result: the fluid-particle interaction force must vanish. This condition can be met only if the local fluid acceleration force is accounted for. As the two phases move identically, no slip velocity and acceleration are present between them; consequently, the drag, virtual mass and lift forces are all zero (see the sections below dedicated to these forces). Conversely, if its classical definition is adopted, the buoyancy force is nonzero. So, the total fluid-particle interaction force can vanish only if the local fluid acceleration force is considered:

$$n\boldsymbol{f} = n\boldsymbol{f}_B^\star + n\boldsymbol{f}_A^\star = - \phi \rho_e \boldsymbol{g} + \phi \rho_e \boldsymbol{g} = \boldsymbol{0} \tag{5.24}$$

If the other definitions of buoyancy force are adopted, the local fluid acceleration force must not be included, because in both cases, being the effective fluid stress tensor zero, the buoyancy force vanishes. Note that this is not only true for solid suspensions but also for single bodies moving in pure fluids.

5.2.3   A consideration on the complementary force

As stated, all models need to agree on the value ascribed to the total fluid-particle interaction force, but they can use different repartitions for such force. A model may use the classical definition for the buoyancy force and include the local fluid acceleration force, while another may adopt one of the buoyancy force definitions given in Eqs. 5.17 and 5.18 without including the local fluid acceleration force. Both choices are acceptable, but the models will have to adopt different expressions for the complementary force to the total fluid-particle interaction force. Let us write:

$$n_r \boldsymbol{f}_r = \phi_r \rho_e (D_t^e \boldsymbol{u}_e - \boldsymbol{g}) + n_r \boldsymbol{f}_r^\star \quad ; \quad n_r \boldsymbol{f}_r = \phi_r \partial_{\boldsymbol{x}} \cdot \boldsymbol{S}_e + n_r \boldsymbol{f}_r^\bullet \tag{5.25}$$

We wonder how the complementary forces $n_r \boldsymbol{f}_r^\star$ and $n_r \boldsymbol{f}_r^\bullet$ are related. To answer this question, we consider the following relation, obtained by combining the equations above:

$$n_r \boldsymbol{f}_r^\bullet = n_r \boldsymbol{f}_r^\star + \phi_r (\rho_e D_t^e \boldsymbol{u}_e - \rho_e \boldsymbol{g} - \partial_{\boldsymbol{x}} \cdot \boldsymbol{S}_e) \tag{5.26}$$

Then, using the dynamical equation for the fluid phase reported in Table 1, with a few mathematical passages not reported for briefness, one can prove that:

$$\phi_r (\rho_e D_t^e \boldsymbol{u}_e - \rho_e \boldsymbol{g} - \partial_{\boldsymbol{x}} \cdot \boldsymbol{S}_e) = - (\phi_r / \varepsilon) \sum_{s=1}^{\nu} n_s \boldsymbol{f}_s^\bullet \tag{5.27}$$

We now use this relation in Eq. 5.26 and then sum both sides of the resulting equation over the phase index r. Doing so gives:

$$\sum_{r=1}^{\nu} \left[n_r \boldsymbol{f}_r^\star - (1/\varepsilon) n_r \boldsymbol{f}_r^\bullet \right] = \boldsymbol{0} \tag{5.28}$$

This is the condition that needs to be satisfied to render the two models consistent. This condition can be met by imposing the following restriction:

$$n_r \boldsymbol{f}_r^{\bullet} = \varepsilon \left(n_r \boldsymbol{f}_r^{\star} \right) \tag{5.29}$$

If we denote as $\boldsymbol{\tau}_e$ the deviatoric part of the effective stress tensor of the fluid, then, using the equation above, we immediately obtain:

$$n_r \boldsymbol{f}_r^{\circ} = \varepsilon \left(n_r \boldsymbol{f}_r^{\star} \right) + \phi_r \partial_{\boldsymbol{x}} \cdot \boldsymbol{\tau}_e \tag{5.30}$$

where $n_r \boldsymbol{f}_r^{\circ}$ represents the complementary force to the total fluid-particle interaction force that arises when Eq. 5.18 is employed for defining the buoyancy force.

The main constituents of the complementary forces defined above are the drag force, the lift force and the virtual mass force. We will now discuss how these forces are expressed constitutively.

5.2.4 Drag force

By definition, the drag force is parallel to the fluid-particle slip velocity (a vector that fulfills the principle of material frame-indifference); hence, it is:

$$n_r \boldsymbol{f}_{D,r} \equiv \beta_r \left(\boldsymbol{u}_e - \boldsymbol{v}_r \right) \tag{5.31}$$

where β_r denotes the drag coefficient for the rth particle phase. Finding a closure for the drag force amounts to finding a constitutive expression for β_r. We now report some of these expressions, *written in a way that is consistent with the classical definition of buoyancy force*.

Ergun & Orning (1949) developed an empirical correlation for assessing the unrecoverable pressure drop through packed beds. Extending its range of validity to homogeneous fluidized suspensions, one obtains the following constitutive equation:

$$\beta_r = 150 \frac{\mu_e \phi_r (1 - \varepsilon)}{(\varepsilon s_r)^2} + 1.75 \frac{\rho_e \phi_r |\boldsymbol{u}_e - \boldsymbol{v}_r|}{\varepsilon s_r} \tag{5.32}$$

Gidaspow (1994) recommends using this closure for values of the void fraction up to 0.80, even if the Ergun equation was developed (and has been extensively verified) for fixed beds in which the void fraction is small, with values close to 0.40. For void fraction values larger than 0.80, Gidaspow (1994) recommends using the expression of Wen & Yu (1966), which is one of the most popular correlations for the calculation of the drag coefficient in dense fluidized suspensions:

$$\beta_r = \frac{3}{4} C_D(\mathrm{Re}_r) \frac{\rho_e \phi_r |\boldsymbol{u}_e - \boldsymbol{v}_r|}{s_r} \varepsilon^{-2.70} \tag{5.33}$$

where:

$$\mathrm{Re}_r \equiv \frac{\rho_e \varepsilon |\boldsymbol{u}_e - \boldsymbol{v}_r| s_r}{\mu_e} \quad ; \quad C_D(\mathrm{Re}_r) = \begin{cases} \left(24/\mathrm{Re}_r \right) \left(1 + 0.15 \mathrm{Re}_r^{0.687} \right) & \text{for } \mathrm{Re}_r < 1000 \\ 0.44 & \text{for } \mathrm{Re}_r \geq 1000 \end{cases} \tag{5.34}$$

The expression above has been proposed by Schiller & Naumann (1935). In Eq. 5.33, as we see, the exponent in the voidage function $\varepsilon^{-\alpha}$ is constant and equal to 2.70.

Di Felice (1994) suggested that the exponent α should be a function of the particle Reynolds number; the expression that he proposed is:

$$\alpha(\mathrm{Re}_r) = 2.70 - 0.65 \exp \left[-(1/2)(1.50 - \log_{10} \mathrm{Re}_r)^2 \right] \tag{5.35}$$

The value of the exponent reduces to that employed in the expression of Wen & Yu (1966) for very small and very large values of the Reynolds number. In the intermediate region, nevertheless, the deviation from 2.70 is significant, the exponent reaching a minimum value of 2.05 when $\mathrm{Re}_r \approx 32$.

The closures reported above are extensively used; nevertheless, they are not consistent with the empirical equation developed by Richardson & Zaki (1954) to describe the expansion of homogeneous fluidized beds of non-cohesive particles. Since this equation is very accurate, the inconsistency is a shortcoming of the drag force closures. To overcome this limitation, Mazzei & Lettieri (2007) derived an expression that is consistent with the Richardson and Zaki correlation over the entire range of fluid-dynamic regimes and for any value of the suspension void fraction. It has the following formulation:

$$\alpha(\varepsilon, \mathrm{Re}_r) = -\,(1/\ln\varepsilon)\ln\left\{\frac{\left[0.63 + 4.80(\mathrm{Re}_r/\varepsilon^\gamma)^{-1/2}\right]^2}{\left(0.63 + 4.80\mathrm{Re}_r^{-1/2}\right)^2}\,\varepsilon^{2(1-\gamma)}\right\} \tag{5.36}$$

where:

$$\gamma(\varepsilon, \mathrm{Re}_r) = \frac{4.80 + 2.40 \cdot 0.175(\mathrm{Re}_r/\varepsilon^\gamma)^{3/4}}{1 + 0.175(\mathrm{Re}_r/\varepsilon^\gamma)^{3/4}} \tag{5.37}$$

To calculate γ one needs to solve a nonlinear equation. Since γ has a very narrow range of variation, finding the solution requires few iterations. For a detailed discussion on how this closure was derived and on how it compares with the other expressions reported above, we refer to Mazzei & Lettieri (2007).

5.2.5 Virtual mass and lift forces

If a body immersed in a fluid accelerates, some of the surrounding medium must also accelerate; this results in a force, named virtual mass force, equal to:

$$n_r \boldsymbol{f}_{V,r} \equiv \phi_r \rho_e C_V(\phi_r)(D_t^e \boldsymbol{u}_e - D_t^r \boldsymbol{v}_r) \tag{5.38}$$

where $D_t^e(\cdot)$ and $D_t^r(\cdot)$ are the material derivatives associated with the fluid and rth solid phase, respectively. The virtual mass coefficient, denoted as $C_V(\phi_r)$, depends on the particle shape and on the volume fraction of the solid phase considered. For very dilute mixtures of spherical particles, $C_V(\phi_r)$ is taken to be $1/2$, since this is the calculated value for a single sphere in an infinite fluid (Maxey & Riley, 1983). The same result was found by Zhang & Prosperetti (1994) for an inviscid fluid and low particle concentration. For larger values of the solid volume fraction the coefficient is expected to increase. Using lattice-Boltzmann simulations (but for bubbly suspensions), Sankaranarayanan et al. (2002) showed that $C_V(\phi_r)$ is nearly linear; at moderate values of the solid volume fraction, Zuber (1964) suggested that:

$$C_V(\phi_r) = (1 + 3\phi_r)/2 \tag{5.39}$$

The virtual mass force is important when the density of the fluid is higher than that of the disperse phase; so, in fluidized beds, especially when the fluidization medium is a gas, this force usually plays a secondary role. In bubble columns, conversely, it strongly affects the dynamics of the system.

If an object moves in a fluid which is in shearing flow, it experiences a force transverse to the direction of relative motion. This lift force is equal to:

$$n_r \boldsymbol{f}_{L,r} \equiv \phi_r \rho_e C_L(\phi_r)(\partial_{\boldsymbol{x}} \times \boldsymbol{u}_e) \times (\boldsymbol{u}_e - \boldsymbol{v}_r) \tag{5.40}$$

The lift coefficient, denoted as $C_L(\phi_r)$, depends on the particle shape and on the volume fraction of the solid phase considered. For very dilute mixtures of spherical particles, $C_L(\phi_r)$ is also taken to be $1/2$. One reason for this is that Eqs. 5.38 and 5.40 are not frame-independent when taken separately, but their sum satisfies the principle of material objectivity if the coefficients of the two forces are equal. Hence, to satisfy this principle, one should set $C_L(\phi_r) = C_V(\phi_r)$. In fluid-solid systems the lift force is often (slightly) more important than the virtual mass force, but both forces are outweighed by the drag force. For more details about these forces, we refer to Marchisio & Fox (2013) and the references therein provided.

5.2.6 Other forces

Other contributions to the fluid-particle force could be considered. A comprehensive overview can be found in Drew & Passman (1998). Here we cite only the Faxen force and a history-dependent term analogous to the Basset force for the motion of isolated particles (Basset, 1888). For the latter, we can reasonably believe that for fluidized suspensions the averaging of history-dependent forces should result in a vanishing contribution, since averaging would most probably erase any historical effects of the motion of the particles on the fluid in their immediate neighborhood. We thus expect this force to be negligible.

5.3 Particle-particle interaction force

In fluidized mixtures of several monodisperse particle classes, each class exchanges linear momentum with all the others; this momentum transfer arises from particle collisions and results into a particle-particle drag force. Soo (1967) was among the first to quantify it, deriving a theoretical expression for the force acting on a single particle of species r in a cloud of particles of species s. Nakamura & Capes (1976) and Arastoopour et al. (1982) made similar efforts. Many authors have since then put forward other correlations, most of them being variations of earlier works. The force is expressed as the product of a drag coefficient by the velocity of slip between the particle classes:

$$n_r \boldsymbol{f}_{rs} \equiv \zeta_{rs} (\boldsymbol{v}_s - \boldsymbol{v}_r) \tag{5.41}$$

where $n_r \boldsymbol{f}_{rs}$ is the force exerted by phase s on phase r per unit volume of suspension (see Table 1) and ζ_{rs} is the particle-particle drag coefficient for the two particle classes involved. The closure problem reduces to finding a constitutive expression for ζ_{rs}. Gidaspow et al. (1985) advanced the relation:

$$\zeta_{rs} = C_{rs}(1 + e_{rs}) \left[\frac{\phi_r \phi_s \rho_r \rho_s (s_r + s_s)^2}{\rho_r s_r^3 + \rho_s s_s^3} \right] |\boldsymbol{v}_s - \boldsymbol{v}_r| \tag{5.42}$$

where ρ_r, ρ_s, s_r and s_s are the densities and diameters of the particles of classes r and s, respectively, e_{rs} is their coefficient of restitution and C_{rs} is given by:

$$C_{rs} \equiv \frac{3\Phi_{rs}^{1/3} + (\phi_r + \phi_s)^{1/3}}{4\left[\Phi_{rs}^{1/3} - (\phi_r + \phi_s)^{1/3} \right]} \tag{5.43}$$

where:

$$\Phi_{rs} \equiv (1 - s_{rs})\left[\Phi_r + (1 - \Phi_r)\Phi_s \right](1 - X_{rs}) + \Phi_r \quad \text{for} \quad X_{rs} \geq \frac{\Phi_r}{\Phi_r + (1 - \Phi_r)\Phi_s}$$

$$\Phi_{rs} \equiv \left[(\Phi_r - \Phi_s) + (1 - s_{rs})(1 - \Phi_r)\Phi_s \right]\left[\Phi_r + (1 - \Phi_r)\Phi_s \right]\frac{X_{rs}}{\Phi_r} + \Phi_s \quad \text{otherwise} \tag{5.44}$$

In the relations above, Φ_r and Φ_s are the particle volume fractions at maximum packing for phases r and s, respectively; moreover, it is:

$$X_{rs} \equiv \frac{\phi_r}{\phi_r + \phi_s} \quad ; \quad s_{rs} \equiv \left(\frac{s_s}{s_r} \right)^{1/2} \text{ if } s_r \geq s_s \text{ and } s_{rs} \equiv \left(\frac{s_r}{s_s} \right)^{1/2} \text{ otherwise} \tag{5.45}$$

Another popular closure if that of Syamlal (1987), which reads:

$$\zeta_{rs} = \frac{3}{4}(1 + e_{rs})\left(1 + \frac{\pi}{4}F_{rs} \right)\left[\frac{\phi_r \phi_s \rho_r \rho_s g_{rs}(s_r + s_s)^2}{\rho_r s_r^3 + \rho_s s_s^3} \right]|\boldsymbol{v}_s - \boldsymbol{v}_r| \tag{5.46}$$

in which F_{rs} denotes a coefficient of friction for phases r and s, while g_{rs} the radial distribution function of Lebowitz (1964), given by Eq. 5.8. Gera et al. (2004) suggested that the equations above should include an

additional term that is necessary to prevent the particle phases from segregating when they are fully packed. Without it, Eqs. 5.42 and 5.46 permit packed particles of different size to segregate, a phenomenon which is not observed experimentally. To prevent this, they recommended adding to the coefficient ζ_{rs} the term $\Psi p^\star$, where $p^\star$ is given by Eq. 5.14 and Ψ is a coefficient that must be adjusted to match the actual segregation rate of the powder considered. The value that Gera et al. (2004) used was 0.30, but they stressed that this is not of general validity. $\Psi p^\star$ is added so that when the powder approaches maximum packing the particle-particle drag increases sufficiently to make the solid phases r and s move together as if they were one phase, thereby hindering segregation. This additional term is included only for $\phi > \phi_f$.

6 Population balance modeling

In the previous sections, we have presented the Eulerian equations of motion for dense fluidized suspensions constituted of ν particle classes, the rth class being characterized by a density ρ_r and a diameter s_r. A serious limitation of this modeling approach is that changes in particle size are not permitted: particles can segregate or mix, and so the particle size distribution (PSD) in every real-space point can change in time, but the size of the particles for each class is fixed. In general, nevertheless, particles can grow, shrink, aggregate and break, and new particles, of vanishing small size, may nucleate; these size changes reflect the physical and chemical processes taking place in the system and strongly affect the evolution of the PSD. Predicting this evolution is essential for a realistic description of the system behavior. We now introduce a modeling approach, referred to as *population balance modeling*, which has this capability.

Population balance modeling is statistical in nature; it can be regarded as a generalization of the statistical modeling approach presented in Section 3.1. There, the state of a particle was identified by two coordinates: position in real space $\boldsymbol{x}$ and velocity $\boldsymbol{v}$; this number can be increased, if additional properties are required to fully characterize the particle state. Here we will add only the particle size s. The complete description (in a statistical sense) of the system is given by the master joint PDF, which we introduced in Section 3.1; now, this function depends on 7ν internal coordinates plus the time coordinate (the phase space of the entire particulate system has 7ν dimensions). To calculate many of the macroscopic properties of practical interest, however, the one-particle marginal PDF, or equivalently the number density function, suffices; this is because many of the microscopic functions of interest take the following form:

$$b(\boldsymbol{r}) = \sum_{s=1}^{\nu} b_1(\boldsymbol{x}_s, \boldsymbol{v}_s, s_s) = \sum_{s=1}^{\nu} b_1(\boldsymbol{r}_s) \tag{6.1}$$

where b_1 is an arbitrary function of the phase-space state *of one particle*, and where $\boldsymbol{r}$ and $\boldsymbol{r}_s$ are the position points of the entire particulate system and of particle s in their phase spaces, respectively. For a function of this kind, one can prove that:

$$\langle b \rangle_s(t) = \int_{\Omega_x} \int_{\Omega_v} \int_{\Omega_s} b_1(\boldsymbol{x}_1, \boldsymbol{v}_1, s_1) f_1(\boldsymbol{x}_1, \boldsymbol{v}_1, s_1, t) d\boldsymbol{x}_1 d\boldsymbol{v}_1 ds_1 \tag{6.2}$$

where Ω_s is the range of variation of s, while f_1 is the NDF. By definition, $f_1(\boldsymbol{x}, \boldsymbol{v}, s, t) d\boldsymbol{x} d\boldsymbol{v} ds$ represents the expected number of particles located at time t in the volume $d\boldsymbol{x}$ around the point $\boldsymbol{x}$ with velocity in the range $d\boldsymbol{v}$ around the velocity $\boldsymbol{v}$ with size in the range ds around the size s. $f_1(\boldsymbol{x}, \boldsymbol{v}, s, t) d\boldsymbol{x} d\boldsymbol{v} ds$, therefore, is an observable representing the mean particle number density in the seven-dimensional phase space made up by the union of the real space Ω_x, velocity space Ω_v and size space Ω_s. Knowing the NDF is equivalent to knowing the particle size and velocity distributions in any real-space point at any time. In Eq. 6.2, $\langle b \rangle_s$ is only a function of time, since b does not depend on real-space, velocity-space and size-space coordinates.

So, knowing the NDF permits calculating observables associated with microscopic functions of the class defined by Eq. 6.1. To calculate observables of this kind, one has to know how the NDF evolves in the phase space of one particle. An evolution equation for it is hence necessary. This is called *(generalized) population balance equation* (PBE). One may derive this equation rigorously starting from the microscopic description

of the particulate system, given by the transport equation of the master joint PDF, which is a generalization of the Liouville equation (Marchisio & Fox, 2013). Here we follow a less rigorous, and therefore easier, method that regards the population balance equation as a simple continuity statement written in terms of the number density function in the phase space of one particle (this space in our case has seven dimensions: three in real space, three in velocity space and one in size space). This is the most popular derivation method used in the literature on polydisperse fluid-particle systems.

Consider an arbitrary, fixed control volume $\Lambda_r \equiv \Lambda_x \cup \Lambda_v \cup \Lambda_s$ in the phase space of a single particle. The number of particles that accumulate in it per unit time is:

$$ACC = \partial_t \int_{\Lambda_r} f_1 d\boldsymbol{r} = \int_{\Lambda_r} \partial_t f_1 d\boldsymbol{r} \tag{6.3}$$

where, to simplify the notation, we have denoted as $\boldsymbol{r}$ the position point of the particle in its phase space. The operations of time differentiation and space integration can be interchanged insofar as the control volume is not time-dependent. The net number of particles entering Λ_r per unit time is:

$$IN - OUT = - \int_{\partial \Lambda_r} f_1 \dot{\boldsymbol{r}} \cdot \boldsymbol{n}_r d\boldsymbol{\sigma}_r = - \int_{\Lambda_r} \partial_{\boldsymbol{r}} \cdot f_1 \dot{\boldsymbol{r}} d\boldsymbol{r} \tag{6.4}$$

where $\dot{\boldsymbol{r}}$ and $\partial_{\boldsymbol{r}}$ are the particle velocity and the nabla operator in phase space, respectively, and where $\boldsymbol{n}_r$ is the unit vector normal to the hypersurface bounding Λ_r directed outwards. To turn the surface integral into a volume integral, we have used the Gauss theorem.

The difference between the two terms above has to balance the net number of particles generated per unit time within Λ_r. Particle generation is caused by collisions, breakage, aggregation and similar *instantaneous processes* (no process, of course, is instantaneous; however, these processes have characteristic times that are so smaller than those characterizing the evolution of the NDF that we can regard them as instantaneous). For instance, if two particles located outside Λ_v collide, their velocities vary abruptly, and after the collision one particle (or even both) might be located within Λ_v, having thus entered Λ_r without crossing its boundaries. If we denote as $\mathbb{G}_r$ the net number of particles generated per unit volume of phase space and unit time owing to instantaneous phenomena, it is:

$$GEN = \int_{\Lambda_r} \mathbb{G}_r d\boldsymbol{r} \tag{6.5}$$

If we equate the accumulation term to the sum of the convection and generation terms, we obtain, after a few minor rearrangements, the following integral equation:

$$\int_{\Lambda_r} (\partial_t f_1 + \partial_{\boldsymbol{r}} \cdot f_1 \dot{\boldsymbol{r}} - \mathbb{G}_r) d\boldsymbol{r} = 0 \tag{6.6}$$

Because the integration volume Λ_r is arbitrary and the integrand is (assumed to be) continuous, we conclude that the integrand must vanish:

$$\partial_t f_1 = - \partial_{\boldsymbol{r}} \cdot f_1 \dot{\boldsymbol{r}} + \mathbb{G}_r \tag{6.7}$$

This is the PBE. We find it convenient to rewrite it in terms of the velocities which the particles possess in the real, velocity and size spaces. Letting $\partial_{\boldsymbol{v}}$ and ∂_s represent the nabla operators in the velocity and size spaces, respectively, and $\dot{\boldsymbol{v}}$ and $\dot{s}$ be the particle velocities in the velocity and size spaces, respectively, ($\dot{\boldsymbol{v}}$ represents the particle acceleration in real space and $\dot{s}$ the particle growth rate), we can write:

$$\partial_t f_1 = - \partial_{\boldsymbol{x}} \cdot f_1 \boldsymbol{v} - \partial_{\boldsymbol{v}} \cdot f_1 \dot{\boldsymbol{v}} - \partial_s (f_1 \dot{s}) + \mathbb{G}_r \tag{6.8}$$

or equivalently:

$$\partial_t f_1 = - \boldsymbol{v} \cdot \partial_{\boldsymbol{x}} f_1 - \partial_{\boldsymbol{v}} \cdot f_1 \dot{\boldsymbol{v}} - \partial_s (f_1 \dot{s}) + \mathbb{G}_r \tag{6.9}$$

The two expressions are equivalent insofar as the real-space particle velocity $\boldsymbol{v}$ is an independent coordinate and not a function of $\boldsymbol{x}$; the same is not true for $\dot{\boldsymbol{v}}$ and $\dot{s}$, which in general may depend on the coordinates $\boldsymbol{v}$ and s, respectively. For instance, since $\dot{\boldsymbol{v}}$ is the real-space particle acceleration, and since this is equal to the total force per unit mass acting on the particle, if the latter depends on the particle velocity also $\dot{\boldsymbol{v}}$ will. This is surely the case in fluidized beds, where a component of the force is the drag.

The PBE, as said, is the transport equation of the NDF. Solving it allows determining the NDF evolution. The equation, nevertheless, can be solved only if it is closed. Here by *closed* we mean that all the terms in the equation can be computed from knowledge of the number density function (of course, these functionals need to be known). This is not the case for the generation term, because, as we know from statistical mechanics, it involves correlations between two particles (involving therefore the two-particle marginal PDF). A closure, consequently, will have to be introduced to express $\mathbb{G}_r$ in terms on the NDF. This is a significant challenge, because these closures are in general complex to derive (Balescu, 1975). Once this has been done, the PBE is closed, but its solution will be extremely difficult to obtain. This is because in general the PBE results to be a nonlinear, integral, partial differential, functional equation in a seven-dimensional space. As a consequence, one does not usually attempt to solve it, using the equation to extract solely the information about the system behavior that is of interest in the application at hand.

The topics of how to close the PBE and how to solve it are vast. We thus refer to the specialized literature (we strongly recommend Chapman & Cowling, 1970, Gidaspow, 1994, Ramkrishna, 2000 and Marchisio & Fox, 2013). Here we just briefly mention a powerful solution method that allows tuning the PBE into a set of four-dimensional equations that can be solved with normal computational fluid dynamics numerical codes. This is called quadrature-based moment method (several variants exist, but all of them are based on the same idea, which we will now present).

Often engineers are only interested in few integral properties of the NDF. Called moments, these may be important because they control the product quality or because they are simple to measure and monitor. The idea behind the *method of moments* is to derive transport equations for the moments of interest by integrating out the coordinates $\boldsymbol{v}$ and s from the PBE. For any given function $\varphi(\boldsymbol{v}, s)$, we can write:

$$\partial_t \int_{\Omega_v}\int_{\Omega_s} \varphi(\boldsymbol{v}, s) f_1 \, d\boldsymbol{v} \, ds = -\int_{\Omega_v}\int_{\Omega_s} \varphi(\boldsymbol{v}, s) \partial_{\boldsymbol{r}} \cdot f_1 \dot{\boldsymbol{r}} \, d\boldsymbol{v} \, ds + \int_{\Omega_v}\int_{\Omega_s} \varphi(\boldsymbol{v}, s) \mathbb{G}_r \, d\boldsymbol{v} \, ds \qquad (6.10)$$

The integral on the left-hand side is the moment of f_1 associated with the function $\varphi(\boldsymbol{v}, s)$, and depends only on $\boldsymbol{x}$ and t. As a consequence, the equation above, which governs the evolution in time and real space of the moment of the NDF associated with $\varphi(\boldsymbol{v}, s)$, can be solved by any CFD numerical code. We have therefore overcome the dimensionality issue. The problem with the equation above is that it is usually unclosed, since for any set of moments which the modeler wishes to track, obtained with a finite set of functions $\varphi_1, \ldots, \varphi_n$, the equations involve also moments external to the set.

To overcome the closure problem, we can operate as follows. As mentioned, the moment method aims to solve the dimensionality issue by turning a problem involving one higher-dimensional differential equation into a problem involving a set of four-dimensional differential equations solvable by a CFD code. To capture all the information contained in the PBE, one would have to consider an infinite set of equations. But since we neither want nor can solve an infinite number of equations, the idea behind the method of moments is to satisfy only a finite number of them. This leaves the NDF largely undetermined, because only the infinite set would yield the correct NDF. This means that we can choose – to a certain extent – the NDF arbitrarily and then let the moment equations determine the details which we have left unspecified. Moment methods differ in the choice of the function φ and in the arbitrary input for the NDF. Their common feature is to choose the latter so that f_1 is a given function of $\boldsymbol{v}$ and s containing 3α undetermined parameters (two scalars and one vector) depending on $\boldsymbol{x}$ and t. So, if we take 5α scalar moment transport equations, we obtain 5α differential equations for the unknown parameters. One hopes that, for α sufficiently large, the result is accurate enough and independent of the form chosen for the NDF.

The quadrature methods of moments are examples of this approach; they overcome the closure problem by assuming that the NDF has the following functional expression:

$$f_1(\boldsymbol{x}, \boldsymbol{v}, s, t) = \sum_{r=1}^{\alpha} n_r(\boldsymbol{x}, t) \boldsymbol{\delta}\Big[\boldsymbol{v} - \boldsymbol{v}_r(\boldsymbol{x}, t)\Big]\delta\Big[s - s_r(\boldsymbol{x}, t)\Big] \tag{6.11}$$

This is a quadrature formula, in which α is the number of nodes, $\boldsymbol{v}_r(\boldsymbol{x}, t)$ and $s_r(\boldsymbol{x}, t)$ are the rth quadrature nodes and $n_r(\boldsymbol{x}, t)$ is the rth quadrature weight. This formula represents the particle population by means of α solid phases, the rth having number density $n_r(\boldsymbol{x}, t)$ and being made up of particles with velocity $\boldsymbol{v}_r(\boldsymbol{x}, t)$ and size $s_r(\boldsymbol{x}, t)$. The difference between this representation and that used in Section 4 is that here the size of each particle class is not fixed, but evolves in time and space. Here the 3α parameters which one must obtain via the moment transport equations are $n_r(\boldsymbol{x}, t)$, $\boldsymbol{v}_r(\boldsymbol{x}, t)$ and $s_r(\boldsymbol{x}, t)$. For details about how this is done, we refer the reader to the literature previously cited.

7 Conclusions

We presented three strategies for modeling fluidized beds: Eulerian-Lagrangian Modeling, Discrete Particle Modeling and Eulerian-Eulerian Modeling. Tracking the motion of each particle, the first two give a detailed description of the system dynamics; these methods, however, are too expensive computationally to be of any use for describing systems of industrial interest. We thus focused on Eulerian-Eulerian modeling, describing the averaging techniques that turn granular systems into continuous media and deriving the volume-averaged equations of mass and linear momentum balance for fluidized suspensions made up of ν particle classes. We then addressed the closure problem, describing the main constitutive equations used by modelers to express the fluid-particle and particle-particle interaction forces and the effective fluid dynamic stress. We concluded the chapter by introducing the population balance modeling, which permits describing systems in which the particles are continuously distributed over the size, and in which the size is free to vary owing to continuous and discontinuous processes, such as chemical reaction, growth, aggregation and breakage.

8 Appendix

8.1 Fluid-phase volume average of point variable spatial derivatives

We intend to derive an expression for the fluid-phase volume average of point variable spatial derivatives; to this end, we start by considering the derivative:

$$\partial_a \Big[\varepsilon(\boldsymbol{x}, t)\langle\zeta\rangle_e(\boldsymbol{x}, t)\Big] \tag{8.1}$$

Now, using the definition of fluid-phase volume average given in Eqs. 3.17 and the derivation chain rule, we write the quantity above as:

$$\partial_{x_a}\int_{\Lambda_e}\zeta(\boldsymbol{z}, t)\psi(|\boldsymbol{x} - \boldsymbol{z}|)d\boldsymbol{z} = \int_{\Lambda_e}\zeta(\boldsymbol{z}, t)\partial_{x_a}\psi(|\boldsymbol{x} - \boldsymbol{z}|)d\boldsymbol{z} = -\int_{\Lambda_e}\zeta(\boldsymbol{z}, t)\partial_{z_a}\psi(|\boldsymbol{x} - \boldsymbol{z}|)d\boldsymbol{z}$$

$$= \int_{\Lambda_e}\Big[\partial_{z_a}\zeta(\boldsymbol{z}, t)\Big]\psi(|\boldsymbol{x} - \boldsymbol{z}|)d\boldsymbol{z} - \int_{\Lambda_e}\partial_{z_a}\Big[\zeta(\boldsymbol{z}, t)\psi(|\boldsymbol{x} - \boldsymbol{z}|)\Big]d\boldsymbol{z} \tag{8.2}$$

For the first integral, we can write:

$$\int_{\Lambda_e}\Big[\partial_{z_a}\zeta(\boldsymbol{z}, t)\Big]\psi(|\boldsymbol{x} - \boldsymbol{z}|)d\boldsymbol{z} = \varepsilon(\boldsymbol{x}, t)\langle\partial_a\zeta\rangle_e(\boldsymbol{x}, t) \tag{8.3}$$

For the second, the Gauss theorem allows writing:

$$\int_{\Lambda_e}\partial_{z_a}\Big[\zeta(\boldsymbol{z}, t)\psi(|\boldsymbol{x} - \boldsymbol{z}|)\Big]d\boldsymbol{z}$$

$$= \int_{\partial \Lambda_x} \zeta(\boldsymbol{z}, t) n_a(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z - \sum_{r=1}^{\nu} \sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} \zeta(\boldsymbol{z}, t) k_a(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z \quad (8.4)$$

where $\partial \Lambda_x$ is the surface bounding the domain containing the mixture and $n_a(\boldsymbol{x}, t)$ is the ath component of the unit vector normal to $\partial \Lambda_x$ pointing away from the mixture. If the shortest distance from the generic point $\boldsymbol{x} \in \partial \Lambda_x$ is considerably larger than the weighting function radius, the first term of the right-hand side of the equation above is much smaller than the second. Neglecting it, we obtain Eq. 4.3.

8.2 Fluid-phase volume average of point variable time derivatives

Similarly, to derive an expression for the fluid-phase volume average of point variable time derivatives, we start by considering the derivative:

$$\partial_t \Big[\varepsilon(\boldsymbol{x}, t) \langle \xi \rangle_e(\boldsymbol{x}, t) \Big] \tag{8.5}$$

Using the definition of fluid-phase volume average given in Eqs. 3.17 and then applying the Leibnitz theorem allows writing this as:

$$\partial_t \int_{\Lambda_e} \zeta(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{z} = \int_{\Lambda_e} \Big[\partial_t \zeta(\boldsymbol{z}, t) \Big] \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{z}$$

$$- \sum_{r=1}^{\nu} \sum_{\mathscr{S}_r} \int_{\partial \Lambda_r} \zeta(\boldsymbol{z}, t) \boldsymbol{u}(\boldsymbol{z}, t) \cdot \boldsymbol{k}(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z$$

$$+ \int_{\partial \Lambda_x} \zeta(\boldsymbol{z}, t) \boldsymbol{u}(\boldsymbol{z}, t) \cdot \boldsymbol{n}(\boldsymbol{z}, t) \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{\sigma}_z \quad (8.6)$$

The integral on $\partial \Lambda_x$ can be neglected for the same reasons given in Section 8.1. Now, using the definition of fluid-phase volume average given in Eqs. 3.17, we have:

$$\int_{\Lambda_e} \Big[\partial_t \zeta(\boldsymbol{z}, t) \Big] \psi(|\boldsymbol{x} - \boldsymbol{z}|) d\boldsymbol{z} = \varepsilon(\boldsymbol{x}, t) \langle \partial_t \zeta \rangle_e(\boldsymbol{x}, t) \tag{8.7}$$

Obtaining Eq. 4.4 is then immediate. Note that if Λ_x is time independent, $\boldsymbol{u}(\boldsymbol{z}, t) = \boldsymbol{0}$ on $\partial \Lambda_x$, and therefore the last integral on the right-hand size of Eq. 8.6 rigorously vanishes.

8.3 Particle-phase volume average of point variable time derivatives

We intend to derive an expression for the particle-phase volume average of point variable time derivatives; in this case, we consider the derivative:

$$\partial_t \Big[n_r(\boldsymbol{x}, t) \langle \zeta \rangle_p^r(\boldsymbol{x}, t) \Big] \tag{8.8}$$

Now, employing the definition of particle-phase volume average given in Eq. 3.21, we can express the partial derivative above as:

$$\sum_{\mathscr{S}_r} \partial_t \Big[\zeta_r(t) \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \Big] = \sum_{\mathscr{S}_r} \Big[\dot{\zeta}_r(t) \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \Big] + \sum_{\mathscr{S}_r} \Big[\zeta_r(t) \partial_t \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \Big] \quad (8.9)$$

From the definition of particle-phase volume average, it is:

$$\sum_{\mathscr{S}_r} \Big[\dot{\zeta}_r(t) \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \Big] = n_r(\boldsymbol{x}, t) \langle \dot{\zeta} \rangle_p^r(\boldsymbol{x}, t) \tag{8.10}$$

Applying the derivation chain rule yields:

$$\sum_{\mathscr{S}_r} \left[\zeta_r(t) \partial_t \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \right] = - \sum_{\mathscr{S}_r} \left[\zeta_r(t) v_{r,a}(t) \partial_{x_a} \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \right]$$

$$= - \partial_{x_a} \sum_{\mathscr{S}_r} \left[\zeta_r(t) v_{r,a}(t) \psi(|\boldsymbol{x} - \boldsymbol{z}_r(t)|) \right] = - \partial_{x_a} \left[n_r(\boldsymbol{x}, t) \langle \zeta v_a \rangle_p^r(\boldsymbol{x}, t) \right] \quad (8.11)$$

having used again the partial derivatives commutative property and the definition of particle-phase average. Replacing these last two results in Eq. 8.9 yields Eq. 4.17.

References

Allen MP, Tildesley DJ (1990) Computer Simulations of Liquids. Oxford Science Publications, New York.

Anderson TB, Jackson R (1967) A fluid mechanical description of fluidized beds. Equations of motion. Ind. Eng. Chem. Fundam. 6:527-539.

Arastoopour H, Wang CH, Weil SA (1982) Particle-particle interaction force in a dilute gas-solid system. Chem. Eng. Sci. 37:1379-1386.

Balescu R (1975) Equilibrium and Nonequilibrium Statistical Mechanics. Wiley, New York.

Basset AB (1888) Treatise on Hydrodynamics. Deighton Bell, London.

Bird RB, Stewart WE, Lightfoot EN (1960) Transport Phenomena. Wiley, New York.

Brilliantov NV, Poschel T (2004) Kinetic Theory of Granular Gases. Oxford University Press, Oxford.

Buyevich YA (1971) Statistical hydrodynamics of disperse systems. Part 1. Physical background and general equations. J. Fluid Mech. 49:489-507.

Chapman S, Cowling TG (1970) The Mathematical Theory of Non-Uniform Gases. Cambridge University Press, Cambridge.

Cundall PA, Strack OD (1979) A discrete numerical model for granular assemblies. Géotechnique 29:47-65.

Deen NG, Peters EAJF, Padding JT, Kuipers JAM (2014) Review of direct numerical simulation of fluid-particle mass, momentum and heat transfer in dense gas-solid flows. Chem. Eng. Sci. 116:710-724.

Di Felice R (1994) The voidage function for fluid-particle interaction systems. Int. J. Multiphase Flow 20:153-159.

Di Renzo A, Cello F, Di Maio FP (2011) Simulation of the layer inversion phenomenon in binary liquid-fluidized beds by DEM-CFD with a drag law for polydisperse systems. Chem. Eng. Sci. 66:2945-2958.

Drew DA (1971) Averaged field equations for two-phase media. Stud. Appl. Math. 50:133-166.

Drew DA, Lahey RT (1993) Analytical modelling of multiphase flow. In Particulate Two-Phase Flow. Butterworth-Heinemann, Boston.

Drew DA, Passman SL (1998) Theory of Multicomponent Fluids. Applied Mathematical Sciences. Springer, New York.

Drew DA, Segel LA (1971) Averaged equations for two-phase flows. Stud. Appl. Math. 50:205-231.

Drew DA (1983) Mathematical modelling of two-phase flow. Annu. Rev. Fluid Mech. 15:261-291.

Enwald H, Peirano E, Almstedt AE (1996) Eulerian two-phase flow theory applied to fluidization. Int. J. Multiphase Flow 22:21-66.

Ergun S, Orning AA (1949) Fluid flow through randomly packed columns and fluidized beds. Ind. Eng. Chem. 41:1179-1184.

Fan LS, Zhu C (1998) Principles of Gas-Solid Flows. Cambridge University Press, Cambridge.

Gera D, Syamlal M, O'Brien TJ (2004) Hydrodynamics of particle segregation in fluidized beds. Int. J. Multiphase Flow. 30:419-428.

Gidaspow D (1994) Multiphase Flow and Fluidization. Academic Press, London.

Gidaspow D, Ettehadieh B (1983) Fluidization in two-dimensional beds with a jet. Part II: hydrodynamic modeling. Ind. Eng. Chem. Fundam. 22:193-201.

Gidaspow D, Bezburuah R, Ding J (1992) Hydrodynamics of circulating fluidized beds. Kinetic theory apparoach. In proc. of the 7th International Conference on Fluidization. Brisbane, Australia.

Gidaspow D, Syamlal M, Seo YC (1985) Hydrodynamics of fluidization of single and binary particles: supercomputer modeling. In proc. of the 5th International Conference on Fluidization. Elsinore, Denmark.

Gidaspow D, Syamlal M, Seo YC (1986) Hydrodynamics of fluidization: supercomputer generated vs. experimental bubbles. J. Powder & Bulk Solids Tech. 10:19-23.

He Y, Wang T, Deen N, van Sint Annaland M, Kuipers JAM, Wen D (2012) Discrete particle modeling of granular temperature distribution in a bubbling fluidized bed. Particuology 10:428Ű437.

Hinch EJ (1977) An averaged equation approach to particle interactions in a fluid suspension. J. Fluid Mech. 83:695-720.

Hoomans BPB, Kuipers JAM, Briels WJ, van Swaaij WPM (1996) Discrete particle simulation of a two-dimensional gas-fluidized bed: a hard sphere approach. Chem. Eng. Sci. 51:99-118.

Iddir H, Arastoopour H (2005) Modeling of multitype particle flow using the kinetic theory approach. AIChE J. 51:1620-1632.

Jackson R (1997) Locally averaged equations of motion for a mixture of identical spherical particles and a Newtonian fluid. Chem. Eng. Sci. 52:2457-2469.

Jackson R (1998) Erratum. Chem. Eng. Sci. 53:1955.

Jackson R (2000) The Dynamics of Fluidized Particles. Cambridge Monographs on Mechanics. Cambridge University Press, Cambridge.

Jenkins JT, Savage SB (1983) A theory for the rapid flow of identical, smooth, nearly elastic, spherical particles. J. Fluid Mech. 130:187-202.

Kafui KD, Thornton C, Adams MJ (2002) Discrete particle-continuum fluid modelling of gas-solid fluidised beds. Chem. Eng. Sci. 57:2395-2410.

Lebowitz JL (1964) Exact solution of generalised Percus-Yevick equation for a mixture of hard spheres. Phys. Rev. 133:895-899.

Leva M (1959). Fluidization. McGraw-Hill, New York.

Lu H, Wang S, Zhao Y, Yang L, Gidaspow D, Ding J (2005) Prediction of particle motion in a two-dimensional bubbling fluidized bed using hard-sphere model. Chem. Eng. Sci. 60:3217-3231.

Lun CKK, Savage SB, Jeffrey DJ, Chepurniy N (1984) Kinetic theories for granular flow: Inelastic particles in Couette flow and slightly inelastic particles in a general flow field. J. Fluid Mech. 140:223-256.

Marchisio DL, Fox RO (2013) Computational Models for Polydisperse Particulate and Multiphase Systems. Cambridge University Press, Cambridge.

Maxey MR, Riley JJ (1983) Equation of motion for a small rigid sphere in a nonuniform flow. Phys. Fluids 26:883-889.

Mazzei L, Lettieri P (2007) A drag force closure for uniformly-dispersed fluidized suspensions. Chem. Eng. Sci. 62:6129-6142.

Nakamura K, Capes CE (1976) Vertical pneumatic conveying of binary particle mixtures. In: Keairns DL (ed) Fluidization Technology. Hemisphere Publishing Corporation, Washington DC, pp 159-184.

Nigmatulin RI (1979) Spatial averaging in the mechanics of heterogeneous and dispersed systems. Int. J. Multiphase Flow. 5:353-385.

Ouyang J, Li J (1999) Particle-motion-resolved discrete model for simulating gas-solid fluidization. Chem. Eng. Sci. 54:2077-2083.

Owoyemi O, Mazzei L, Lettieri P (2007) CFD modeling of binary-fluidized suspensions and investigation of role of particle-particle drag on mixing and segregation. AIChE J. 53:1924-1940.

Pan TW, Joseph DD, Bai R, Glowinski R, Sarin V (2002) Fluidization of 1204 spheres: simulation and experiments. J. Fluid Mech. 451:169-191.

Pandit JK, Wang XS, Rhodes MJ (2005) Study of Geldart's Group A behaviour using the discrete element method simulation. Powder Technol. 160:7-14.

Pritchett JW, Blake TR, Garg SK (1978) A numerical model of gas fluidized beds. AIChE Symp. Ser. 176:134-148.

Ramkrishna D (2000) Population Balances. Academic Press, London.

Richardson JF, Zaki WN (1954) Sedimentation and fluidization: Part I. Trans. Inst. Chem. Eng. 32:35-53.

Sankaranarayanan K, Shan X, Kevrekidis IG, Sundaresan S (2002) Analysis of drag and virtual mass forces in bubbly suspensions using an implicit formulation of the lattice Boltzmann method. J. Fluid Mech. 452:61Ű96.

Schaeffer DG (1987) Instability in the evolution equations describing incompressible granular flow. J. Diff. Eq. 66:19-50.

Schiller L, Naumann Z (1935) A drag coefficient correlation. Z. Ver. Deutsch. Ing. 77:318-320.

Soo SL (1967) Fluid Dynamics of Multiphase Systems. Waltham, Mass, Blaisdell Publishing Company.

Syamlal M (1987) The particle-particle drag term in a multiparticle model of fluidization. National Technical Information Service. DOE/MC/21353-2373, NTIS/DE87006500.

Syamlal M, Rogers WA, O'Brien TJ (1993) MFIX Documentation and Theory Guide. DOE/METC94/1004, NTIS/DE94000087. Electronically available from: http://www.mfix.org.

Tsuji Y, Kawaguchi T, Tanaka T (1993) Discrete particle simulation of two-dimensional fluidized bed. Powder Technol. 77:79-87.

van der Hoef MA, Beetstra R, Kuipers JAM (2005) Lattice Boltzmann simulations of low Reynolds number flow past mono- and bidisperse arrays of spheres: results for the permeability and drag force. J. Fluid. Mech. 528:233-254.

Wang J, van der Hoef MA, Kuipers JAM (2013) Particle granular temperature of Geldart A, A/B and B particles in dense gas-fluidized beds. Chem. Eng. Sci. 97:264-271.

Wen CY, Yu YH (1966) Mechanics of Fluidization. Chem. Eng. Prog. Symp. Ser. 62:100-111.

Whitaker S (1969) Advances in the theory of fluid motion in porous media. Ind. Eng. Chem. 61:14-28.

Xu BH, Yu AB (1997) Numerical simulation of the gas-solid flow in a fluidized bed by combining discrete and particle method with computational fluid dynamics. Chem. Eng. Sci. 52:2785-2809.

Ye M, van der Hoef MA, Kuipers JAM (2005) The effects of particle and gas properties on the fluidization of Geldart A particles. Chem. Eng. Sci. 60:4567-4580.

Zhang DZ, Prosperetti A (1994) Averaged equations for inviscid disperse two-phase flow. J. Fluid. Mech. 267:185-219.

Zhu HP, Zhou ZY, Yang RY, Yu AB (2008) Discrete particle simulation of particulate systems: a review of major applications and findings. Chem. Eng. Sci. 63:5728-5770.

Zuber N (1964) On dispersed two-phase flow in the laminar flow regime. Chem. Eng. Sci. 19:897-903.