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Introduction

1.1 Disperse multiphase flows

The majority of the equipment used in the chemical process industry employs multiphase flow. Bubble columns, fluidized beds, flame reactors, and equipment for liquid–liquid extraction, for solid drying, and size enlargement or reduction are common examples. In order to efficiently design, optimize, and scale up industrial systems, computational tools for simulating multiphase flows are very important. Polydisperse multiphase flows are also common in other areas, such as fuel sprays in auto and aircraft engines, brown-out conditions in aerospace vehicles and particulate flows occurring in the environment. Although at first glance the multifarious industrial and environmental multiphase flows appear to be very different from each other, they have a very important common element: it is possible to identify a continuous phase and a disperse phase (usually with a distribution of characteristic "particle sizes").

Historically the development of the theoretical framework and of computational models for disperse multiphase flows has focused on two different aspects: (i) the evolution of the disperse phase (e.g. breakage and coalescence of bubbles or droplets, particle–particle collisions, etc.) and (ii) multiphase fluid dynamics. The first class of models is mainly concerned with the description of the disperse phase, and is based on the solution of the *spatially homogeneous*[1] population balance equation (PBE). A PBE is a continuity statement written in terms of a *number density function* (NDF), which will be described in detail in Chapter 2. The NDF contains information about how the population constituted by the discrete elements of the disperse phase is distributed over certain characteristic properties that determine, for example, product quality. For example, in crystallization the final quality of the crystals very often depends on the crystal-size distribution (CSD). The CSD (or NDF) defines how the population of crystals is distributed over crystal size, and the PBE is a partial integro-differential equation that defines the evolution of the NDF, as described by Ramkrishna (2000) and Randolph & Larson (1971). Generally these models consist of a PBE coupled with *spatially homogeneous* mass and energy balances, and can be profitably used in modeling, design, and scale-up of process equipment, and in the development of

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[1] In the more sophisticated treatments, spatial inhomogeneities are modeled by connected "zones" or regions of space that are assumed to be homogeneous. The resulting population-balance equation (PBE) does not explicitly account for *local* variations in the flow field.

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control strategies for particulate systems (Chiu & Christofides, 1999; Crowley *et al.*, 2000; Nagy, 2009).

However, in many industrial and environmental applications the fluid-dynamic interactions between the disperse and continuous phases are also very important, and much research effort has focused on these aspects of the problem (e.g. Delnoij *et al.*, 1997; Fox, 2012; Gavi *et al.*, 2007; Gerber & Mousavi, 2007; Lain *et al.*, 2002; Laurent & Massot, 2001; Marchisio & Fox, 2007; Monahan & Fox, 2007; Petitti *et al.*, 2010; Prat & Ducoste, 2006; Rigopoulos, 2010; Sanyal *et al.*, 2005; Venneker *et al.*, 2002). For example, in gas–solid systems the application of the kinetic theory of gases to granular flows and the development of multiphase computational models have led to a deeper understanding of these issues (Gidaspow, 1994; Goldhirsch, 2003; Jenkins & Mancini, 1989). Generally these transport-phenomena-based models consist of *spatially inhomogeneous* mass, momentum, and energy (thermal and granular) balances between the disperse phase and the continuous phase, and spatial dependences are handled by using a finite-volume approach (Leveque, 2002) in the context of computational fluid dynamics (CFD). Important industrial examples of such flows include fluidized beds and riser flows, slurry-flow reactors, and bubble columns. In all of these examples, the coupling due to mass, momentum, and energy exchange between the disperse and continuous phases results in flow dynamics that are distinctly different than that observed in single-phase flows. Thus, the CFD models used for describing the fluid dynamics of disperse multiphase flows usually involve multiple continuity and momentum equations that are tightly coupled through phase-interaction terms (Drew & Passman, 1999; van der Hoef *et al.*, 2008; Ishii, 1975; Portela & Oliemans, 2006). For polydisperse multiphase flows, the situation becomes more complex because it is necessary to describe the "particle-size" distribution of the disperse phase (De Chaisemartin *et al.*, 2009; Fan *et al.*, 2004; Fox, 2007; Riber *et al.*, 2009), as well as the coupling with the continuous phase for particles of different sizes. One of the primary goals of the present work is to present a systematic modeling framework for accomplishing this task.

In general, the first class of models mentioned above is able to describe the evolution of the NDF that characterizes the disperse phase. For example, if this approach is applied to crystallization problems, it is possible to describe the evolution of the CSD in a crystallizer working under certain operating conditions, taking into account all possible physical and chemical processes such as nucleation, molecular growth, aggregation, and breakage. However, these models are unable to take into account spatial gradients of properties and how they relate to the continuous or disperse phases, fluid-dynamic interactions between crystals and the continuous phase, and interactions among the crystals themselves. As a consequence, the first class of models is unable to predict the effect of local flow interactions on the evolution of the CSD. On the other hand, the second class of models is capable of describing detailed fluid-dynamic interactions, but for simplicity often assumes a constant (or even monodisperse) CSD. The principal aim of this book is to present the common underlying theory and, through the introduction of appropriate computational methods, to create a bridge between the two approaches. The resulting CFD-based computational models can then be used to solve a large variety of *polydisperse* particulate and multiphase flow problems.

A working definition of polydisperse multiphase flows

For the purposes of this book, it will be useful to have a clear definition of what is meant by *disperse* and *polydisperse* in the context of multiphase flows. By disperse, we mean that one or more of the phases is composed of clearly identifiable discrete entities such as solid particles, drops, or bubbles. By polydisperse, we mean that the properties of the disperse-phase entities can be different for each entity (e.g. particles with different mass, composition, or temperature). For example, fuel sprays have a region near the nozzle where the liquid jet is *not* disperse, followed by a region after breakup of the primary jet that is composed of individual droplets. The latter region would be considered a polydisperse multiphase flow and could be modeled using the methods described in this book. In contrast, bubble-column flows, for example, can be entirely monodisperse because all of the bubbles have (approximately) the same properties (e.g. bubble diameter). In practice, monodisperse multiphase flows are relatively rare and, hence, it will be important to have a modeling framework that naturally accounts for polydispersity.

Another important manifestation of “polydispersity” is the presence of disperse-phase entities (even those with identical physical properties) with different velocities. The reader familiar with the kinetic theory of molecular gases will recognize this type of polydispersity as leading to the *velocity-distribution function*, which plays an important role in the transport theory of polydisperse multiphase flows. As in the molecular kinetic theory, the *mesoscale* description of a monodisperse multiphase flow can be formulated in terms of a *kinetic equation* for the velocity-distribution function. However, unlike in molecular gases at standard temperatures and pressures, the disperse-phase entities often interact infrequently due to collisions, so the standard hydrodynamic approximations valid in the collision-dominated regime are no longer accurate. In analogy to molecular gases, such multiphase flows behave as *rarefied granular gases* wherein processes besides collisions (e.g. momentum exchange with the continuous phase) are dominant in determining the flow regime. For this reason, it is often necessary to retain the mesoscale description as the starting point for describing the disperse-phase flow dynamics.

In summary, a polydisperse multiphase flow consists of one (or more) disperse phases with entities of possibly different physical properties and velocities. The mesoscale modeling approach (described in more detail in Section 1.3) for describing such flows is the primary focus of this book. For multiphase flows that are not composed of a clearly distinct disperse phase, other modeling approaches must be followed (e.g. methods that resolve the dynamics of the interface separating the phases, or volume-averaging approaches and the concomitant *ad hoc* closures of the phase-interaction and transport terms). As will become clearer to the reader in subsequent chapters, the mesoscale modeling approach allows rigorous derivation of the macroscale transport equations, thereby ensuring that the resulting CFD models will be as accurate as possible when simulating real polydisperse multiphase flows.

1.2 Two example systems

In this section, we provide two examples of polydisperse multiphase systems. In the first example, the particles are assumed to be very small so that their inertia is small enough to be negligible relative to that of the fluid phase. Thus, the particle-size distribution (PSD) is governed by a PBE and undergoes changes due to aggregation and breakage. In the second example, the particles are assumed to be large enough to have finite inertia relative to the surrounding fluid, and we let all particles be identical and consider the distribution of the particle velocity, which is described by a kinetic equation (KE).

1.2.1 The population-balance equation for fine particles

As a first example, we consider a population of solid particles suspended in a liquid. We assume that the density and size of the particles are such that they move together with the fluid. Local velocity gradients in the fluid, which are generally quantified by the shear rate, induce particle aggregation and breakage, changing the PSD, as dictated by the corresponding PBE. In this context we will assume (as is often the case for colloidal systems) that aggregation and breakage are completely reversible, which means that, when particles aggregate, the aggregates formed can later be fragmented by breakage, and that the fragments formed by breakage can, in turn, aggregate together. In what follows we will analyze the PBE and introduce a set of dimensionless numbers and characteristic time scales that will turn out to be useful in the investigation of multiphase systems.

Relevant dimensionless numbers and time scales

As described in Chapter 4, the following PBE governs the evolution of the PSD, representing the state of the solid aggregates:

$$\frac{\partial n}{\partial t} + \frac{\partial v_{\mathrm{f}} n}{\partial x} = \Gamma \frac{\partial^2 n}{\partial x^2} + \mathbb{C}, \tag{1.1}$$

where v_{f} is the known fluid velocity with which the particles are advected and Γ is a diffusion coefficient. For simplicity, in this example, only one spatial coordinate x is considered and the diffusion coefficient Γ is constant. The PSD, denoted by n, is a number-density function (NDF) representing the number concentration of particles with volumes between V and $V + \mathrm{d}V$. The PSD is a function of time t, of the spatial coordinate x, and of the volume of the aggregates V. The aggregates are composed of spherical primary particles with fixed diameter d_{p}. If just one primary particle is included in the aggregate then $V = \pi d_{\mathrm{p}}^3/6$, whereas for an aggregate composed of two primary particles $V = \pi d_{\mathrm{p}}^3/3$, and so on for larger aggregates. As described in Chapter 5, the source term due to aggregation and breakage is

$$\begin{aligned}\mathbb{C} = {} & \frac{1}{2}\int_0^V a(V - V', V')n(V - V')n(V')\mathrm{d}V' - \int_0^\infty a(V, V')n(V)n(V')\mathrm{d}V' \\ & + \int_V^\infty b(V')N(V|V')n(V')\mathrm{d}V' - b(V)n(V),\end{aligned} \tag{1.2}$$

where $a(V, V')$ and $b(V)$ are the aggregation and breakage kernels, $N(V|V')$ is the daughter distribution function, and the time and space dependences are omitted for clarity. As will be described in more detail in later chapters, the aggregation and breakage kernels express the tendency of the particles to aggregate and break. Generally speaking, these kernels depend strongly on the spatial coordinate x, since real multiphase systems are characterized by regions where aggregation and breakage occur at very different rates. For example, particles suspended in a stirred tank might experience intense breakage near the impeller and strong aggregation in other regions. The daughter distribution function gives instead the size distribution of particles generated by the breakup of a single aggregate.

In order to highlight the different regimes exhibited by Eq. (1.1) and the different treatments that are more suitable for its solution in each regime, the PBE has to be normalized and made dimensionless. Different quantities can be used to this end, such as the moments of order zero and one of the PSD:

$$\begin{aligned} m_0(t, x) &= \int_0^\infty n(t, x, V)\mathrm{d}V, \\ m_1(t, x) &= \int_0^\infty V n(t, x, V)\mathrm{d}V. \end{aligned} \tag{1.3}$$

The zeroth-order moment identifies the total aggregate number density (i.e. the total number of aggregates per unit volume), whereas the first-order moment is the disperse-phase volume fraction, more frequently denoted by α_p. For this simple two-phase system, if α_f is used to indicate the fluid-phase volume fraction, by definition $\alpha_\mathrm{p} + \alpha_\mathrm{f} = 1$. By using these moments, one can define a mean particle volume corresponding to the ratio between the moments of order one and zero and, in addition, one can define the dimensionless PSD $\psi(\xi) = n(t, x, V)\, m_1(t, x)/m_0^2(t, x)$ with $\xi = V m_0/m_1$. The dimensionless PSD has first- and second-order moments equal to unity, and is useful when searching for the self-similar solution that characterizes pure aggregation, pure breakage and simultaneous aggregation and breakage problems (Ramkrishna, 2000). The moment of order two of the PSD,

$$m_2(t, x) = \int_0^\infty V^2 n(t, x, V)\mathrm{d}V, \tag{1.4}$$

is instead useful in the definition of the standard deviation of the PSD, which is equal to $m_2 - m_1^2/m_0$. Here the PSD and Eq. (1.1) are made dimensionless by introducing the characteristic length L, velocity U, aggregate volume ζ, and total aggregate number density N_t. For example, for particles suspended in a stirred tank, L could be the tank diameter and U the impeller-tip velocity, whereas ζ and N_t could be extracted by the volume-average PSD in the vessel at steady state. The last two quantities can in turn be used to define the characteristic disperse-phase volume fraction: $\phi_\mathrm{p} = \zeta N_\mathrm{t}$.

Knowledge of these characteristic quantities suffices for the calculation of the characteristic time scales for aggregation $\tau_\mathrm{a} = [a(\zeta, \zeta)N_\mathrm{t}]^{-1}$ and breakage $\tau_\mathrm{b} = [b(\zeta)]^{-1}$. These two time scales represent the average time interval between two subsequent aggregation or breakage events. When these time scales are very short, aggregation and breakage events are very frequent, resulting in rapid evolution of the PSD. In fact, as particles move and diffuse in the domain, many aggregation and breakage events occur, resulting in a quick adaptation of the PSD to its local “equilibrium” value $n_\mathrm{eq}(t, x, V)$, which is dictated by the local values of the aggregation and breakage kernels. Here the term equilibrium refers to the steady state reached when aggregation and breakage counterbalance each other.[2] Because of the hypothesis of reversible aggregation and breakage, this equilibrium will be different from point to point, since it depends on the local values of the aggregation and breakage kernels. The equilibrium solution corresponds to the resulting PSD, in the case of particles unable to move away from point x, but evolving in time according to the local aggregation and breakage kernels at point x. In contrast, when the characteristic time scales are very long, aggregation and breakage events are not very frequent, and the evolution of the PSD becomes quite slow. Therefore as particles move and diffuse in the domain, due to the low aggregation and breakage frequencies and the slow changes in the PSD, only the averaged rates are perceived. The evolution of the PSD is then determined by the volume-average kernels, rather than by their local values.

Closer observation of the aggregation time scale shows that it is inversely proportional to the characteristic total aggregate number density N_t, which is related to the characteristic disperse-phase volume fraction ϕ_p. When the system is dilute (i.e. $\phi_\mathrm{p} \ll 1$), N_t is

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[2] Depending on the functional form of the aggregation and breakage kernels, different scenarios are possible. When aggregation prevails, the system can undergo extensive aggregation. Since when particles aggregate their number is reduced, the *gelling limit*, where the total number of particles tends to zero, can be reached. In contrast, when breakage prevails, the total number of particles can go to infinity, giving the opposite limit known as *shattering*. When aggregation and breakage counterbalance each other, a population of particles can evolve to a steady state. This steady state can be calculated by setting the collision source term in Eq. (1.2) equal to zero. We refer to this steady-state solution as the *equilibrium PSD*.

small and as a consequence the aggregation time scale is large. Under these conditions aggregation events are separated by long time intervals. In fact, for dilute systems with very few particles, longer time intervals are necessary to observe a collision between two particles. In contrast, as the system becomes more concentrated (i.e. as N_t and ϕ_p increase) the time interval between two aggregation events becomes very short, since as more particles are suspended in the fluid more collisions (and aggregation events) will occur. The characteristic disperse-phase volume fraction also affects the breakage time scales; in fact, as aggregation events become more frequent the resulting characteristic aggregate volume ζ increases. Since generally the breakage kernel increases with increasing particle size (i.e. larger aggregates are more likely to break than smaller ones), the breakage time scale also becomes shorter. In summary, dilute systems are characterized by large aggregation and breakage time scales, whereas for dense systems these time scales are very short.

A more quantitative definition of dilute and dense systems is possible only by analyzing the normalized and dimensionless PBE. By letting $\xi = V/\zeta$, $n^* = n\zeta/N_\mathrm{t}$, $x^* = x/L$, $v_\mathrm{f}^* = v_\mathrm{f}/U$, and $t^* = t\Gamma/L^2$ the following dimensionless PBE is obtained:

$$\begin{aligned}\frac{\partial n^*}{\partial t^*} + \mathrm{Pe}\frac{\partial v_\mathrm{f}^* n^*}{\partial x^*} - \frac{\partial^2 n^*}{\partial x^{*2}} = \mathrm{Da_a}\Bigg[&\frac{1}{2}\int_0^{\xi} a^*(\xi-\xi',\xi')n^*(\xi-\xi')n^*(\xi')\mathrm{d}\xi' \\ &- \int_0^{+\infty} a^*(\xi,\xi')n^*(\xi)n^*(\xi')\mathrm{d}\xi'\Bigg] \\ + \mathrm{Da_b}\Bigg[&\int_{\xi}^{+\infty} b^*(\xi')N(\xi|\xi')n^*(\xi')\mathrm{d}\xi' - b^*(\xi)n^*(\xi)\Bigg], \end{aligned} \tag{1.5}$$

where the normalized aggregation and breakage kernels are given by $a^*(\xi,\xi') = a(V,V')/a(\zeta,\zeta)$ and $b^*(\xi) = b(V)/b(\zeta)$. The Péclet number, defined by

$$\mathrm{Pe} = \frac{UL}{\Gamma} = \frac{L^2/\Gamma}{L/U}, \tag{1.6}$$

is the ratio between the particle-diffusion and particle-advection time scales. The aggregation Damköhler number, defined by

$$\mathrm{Da_a} = \frac{a(\zeta,\zeta)L^2N_\mathrm{t}}{\Gamma} = \frac{L^2/\Gamma}{1/(a(\zeta,\zeta)N_\mathrm{t})}, \tag{1.7}$$

is the ratio between the particle-diffusion and particle-aggregation time scales. The breakage Damköhler number, defined by

$$\mathrm{Da_b} = \frac{b(\zeta)L^2}{\Gamma} = \frac{L^2/\Gamma}{1/b(\zeta)}, \tag{1.8}$$

is the ratio between the particle-diffusion and breakage time scales. Depending on the values of Pe, $\mathrm{Da_a}$, and $\mathrm{Da_b}$ different regimes can be identified. For example, when Pe becomes much smaller than unity, diffusive particle transport becomes more important than advective transport. Under this condition, different scenarios are still possible, depending on the values of $\mathrm{Da_a}$ and $\mathrm{Da_b}$. When both numbers are much smaller than unity, diffusion is much faster than aggregation and breakage, whereas when both are much greater than unity aggregation and breakage are faster than particle diffusion. It is important to recall here that particle diffusion tends to homogenize the PSD in the spatial domain, whereas, since kernels generally contain some form of spatial dependence, aggregation and breakage tend to create gradients in the PSD.

Major operating regimes

From the discussion above, three major operating regimes can be identified from Eq. (1.5).

(i) Under **dilute** conditions such that $\phi_\text{p} \ll 1$, aggregation and breakage are slower than particle diffusion, or, in other words, $\text{Da}_\text{a} \ll 1$ and $\text{Da}_\text{b} \ll 1$. The evolution of the PSD is not controlled by the local values of the aggregation and breakage kernels, but rather by their volume-average values. Under dilute conditions, since diffusion mixes particles faster than the kernels let them aggregate and break, the two-phase system is generally considered as spatially homogeneous or well mixed (i.e. the PSDs at different points of the domain are identical). The evolution of the PSD for a well-mixed system $\hat{n}(t, V)$ is governed by a volume-average PBE:

$$\begin{aligned}\frac{\partial \hat{n}}{\partial t} = {} & \frac{1}{2}\int_0^V \hat{a}(V - V', V')\hat{n}(V - V')\hat{n}(V')\,\text{d}V' - \int_0^\infty \hat{a}(V, V')\hat{n}(V)\hat{n}(V')\,\text{d}V' \\ & + \int_V^\infty \hat{b}(V')N(V|V')\hat{n}(V')\,\text{d}V' - \hat{b}(V)\hat{n}(V),\end{aligned} \tag{1.9}$$

where $\hat{a}$ and $\hat{b}$ are the volume-average aggregation and breakage kernels, which, due to their non-linear dependence on the spatial coordinates, are generally quite different from the local kernels a and b. A system is generally considered dilute (and therefore well mixed) when Da_a and Da_b are smaller than 10^{-2}. Depending on the type of problem and the functional form of the aggregation and breakage kernels, these conditions result in different constraints for the characteristic disperse-phase volume fraction. For most applications, it is reasonable to consider the operating regime as dilute when $\phi_\text{p} < 10^{-3}$.

(ii) Under **moderately dense** conditions, Da_a and Da_b are greater than 10^{-2} but smaller than 10^2. The characteristic time scales for aggregation and breakage are then comparable to that of particle diffusion. Under these conditions the system cannot be considered to be well mixed, and the PSD is subjected to large variations across the spatial domain. As a consequence, the movement of particles in physical space and their aggregation and breakage cannot be decoupled, and the evolution of the two-phase system is found by solving Eq. (1.5).

(iii) Under **dense** conditions Da_a and Da_b are both greater than 10^2, and hence aggregation and breakage are very fast (or almost instantaneous) compared with particle diffusion. Thanks to the hypothesis of reversibility of aggregation and breakage, as particles diffuse in the domain, they instantaneously adapt to the local equilibrium solution, i.e. n_eq. In this case the evolution of the PSD is completely determined by the local aggregation and breakage kernels and the resulting local steady state.

In summary, for fine particles undergoing aggregation and breakage different modeling approaches should be used for each of the regimes described above. Under dilute conditions, the system can be approximated as a well-mixed system, since spatial gradients in the PSD are not relevant. The evolution of the system is governed by Eq. (1.9) using the volume-average aggregation and breakage kernels. Under moderately dense conditions, spatial gradients of the PSD are not negligible and therefore the evolution of the system is governed by Eq. (1.5). Under dense conditions the system evolves according to the equilibrium solution found by setting the right-hand side of Eq. (1.2) equal to zero.

1.2.2 The kinetic equation for gas–particle flow

As a second example, we consider the kinetic equation (KE) for monodisperse, isothermal solid particles suspended in a constant-density gas phase. For clarity, we assume that the particle material density is significantly larger than that of the gas so that only the fluid drag and buoyancy terms are needed to account for momentum exchange between the two phases (Maxey & Riley, 1983). In this example, the particles are large enough to have finite inertia and thus they evolve with a velocity that can be quite different than that of the gas phase.

Relevant dimensionless numbers

As in all mathematical descriptions of transport phenomena, the theory of polydisperse multiphase flows introduces a set of dimensionless numbers that are pertinent in describing the behavior of the flow. Depending on the complexity of the flow (e.g. variations in physical properties due to chemical reactions, collisions, etc.), the set of dimensionless numbers can be quite large. (Details on the physical models for momentum exchange are given in Chapter 5.) As will be described in detail in Chapter 4, a kinetic equation can be derived for the number-density function (NDF) of the velocity of the disperse phase $n(t, x, v)$. Also in this example, for clarity, we will assume that the problem has only one particle velocity component v and is one-dimensional in physical space with coordinate x at time t. Furthermore, we will assume that the NDF has been normalized (by multiplying it by the volume of a particle) such that the first three velocity moments are

$$\begin{aligned} \alpha_{\mathrm{p}} &\equiv \int_{-\infty}^{+\infty} n \, \mathrm{d}v, \\ \alpha_{\mathrm{p}} U_{\mathrm{p}} &\equiv \int_{-\infty}^{+\infty} v n \, \mathrm{d}v, \\ \alpha_{\mathrm{p}} \Theta_{\mathrm{p}} + \alpha_{\mathrm{p}} U_{\mathrm{p}}^2 &\equiv \int_{-\infty}^{+\infty} v^2 n \, \mathrm{d}v, \end{aligned} \tag{1.10}$$

where α_{p}, U_{p}, and Θ_{p} are the volume fraction, mean velocity, and granular temperature of the disperse phase, respectively. The example kinetic equation is then given by

$$\frac{\partial n}{\partial t} + \frac{\partial v n}{\partial x} + \frac{\partial \mathbb{A} n}{\partial v} = \mathbb{C}, \tag{1.11}$$

where the acceleration (due to buoyancy, gravity, and drag) and collision terms are defined, respectively, by

$$\begin{aligned} \mathbb{A} &\equiv -\frac{1}{\rho_{\mathrm{p}}} \frac{\partial p_{\mathrm{g}}}{\partial x} + g_x + \frac{1}{\tau_{\mathrm{p}}} (U_{\mathrm{g}} - v), \\ \mathbb{C} &\equiv \frac{1}{\tau_{\mathrm{c}}} (n_{\mathrm{eq}} - n). \end{aligned} \tag{1.12}$$

In these expressions, g_x is the x-component of the gravity force, ρ_{p} is the particle density, and p_{g} is the gas-phase pressure. τ_{p} and τ_{c} are characteristic time scales for drag and collisions, respectively. U_{g} is the velocity of the gas phase, and n_{eq} is the equilibrium distribution. For simplicity, we have used a linear collision model[3] in which the first two moments of n_{eq} are the same as those of n, and the third is

$$\frac{1+e^2}{2}\alpha_{\mathrm{p}}\Theta_{\mathrm{p}} + \alpha_{\mathrm{p}}U_{\mathrm{p}}^2 = \int_{-\infty}^{+\infty} v^2 n_{\mathrm{eq}}\,\mathrm{d}v, \tag{1.13}$$

and $0 \le e \le 1$ is the coefficient of restitution for particle–particle collisions. For elastic collisions, $e = 1$, whereas $e < 1$ corresponds to inelastic collisions.

The disperse-phase kinetic equation is coupled to the continuity and momentum equations for the continuous phase, which are given, respectively, by

$$\begin{gathered}\frac{\partial \alpha_{\mathrm{g}}}{\partial t} + \frac{\partial(\alpha_{\mathrm{g}}U_{\mathrm{g}})}{\partial x} = 0,\\ \frac{\partial(\alpha_{\mathrm{g}}U_{\mathrm{g}})}{\partial t} + \frac{\partial(\alpha_{\mathrm{g}}U_{\mathrm{g}}U_{\mathrm{g}})}{\partial x} = \alpha_{\mathrm{g}}\nu_{\mathrm{g}}\frac{\partial^2 U_{\mathrm{g}}}{\partial x^2} - \frac{\alpha_{\mathrm{g}}}{\rho_{\mathrm{g}}}\frac{\partial p_{\mathrm{g}}}{\partial x} + \alpha_{\mathrm{g}}g_x + \frac{\rho_{\mathrm{p}}\alpha_{\mathrm{p}}}{\rho_{\mathrm{g}}\tau_{\mathrm{p}}}(U_{\mathrm{p}} - U_{\mathrm{g}}),\end{gathered} \tag{1.14}$$

where α_{g}, ρ_{g}, and ν_{g} are the gas-phase volume fraction, density, and kinematic viscosity,[4] respectively. By definition, $\alpha_{\mathrm{p}} + \alpha_{\mathrm{g}} = 1$. In order to make Eqs. (1.14) dimensionless, we introduce a characteristic gas-phase velocity U and characteristic length L. The dimensionless time is then $t^* = tU/L$. On noting that α_{g} is dimensionless and letting $x^* = x/L$, $U_{\mathrm{g}}^* = U_{\mathrm{g}}/U$, and $U_{\mathrm{p}}^* = U_{\mathrm{p}}/U$, we then have

$$\begin{gathered}\frac{\partial \alpha_{\mathrm{g}}}{\partial t^*} + \frac{\partial \alpha_{\mathrm{g}}U_{\mathrm{g}}^*}{\partial x^*} = 0,\\ \frac{\partial(\alpha_{\mathrm{g}}U_{\mathrm{g}}^*)}{\partial t^*} + \frac{\partial(\alpha_{\mathrm{g}}U_{\mathrm{g}}^*U_{\mathrm{g}}^*)}{\partial x^*} = \frac{\alpha_{\mathrm{g}}}{\mathrm{Re}_{\mathrm{g}}}\frac{\partial^2 U_{\mathrm{g}}^*}{(\partial x^*)^2} - \alpha_{\mathrm{g}}\frac{\partial p_{\mathrm{g}}^*}{\partial x^*} + \frac{\alpha_{\mathrm{g}}}{\mathrm{Fr}_{\mathrm{g}}^2}g_x^* + \frac{\alpha_{\mathrm{g}}\phi_2}{\mathrm{St}}(U_{\mathrm{p}}^* - U_{\mathrm{g}}^*),\end{gathered} \tag{1.15}$$

where $p_{\mathrm{g}}^* = p/(\rho_{\mathrm{g}}U^2)$ and $g_x^* = g_x/g$. The gas-phase Reynolds and Froude numbers are defined, respectively, by $\mathrm{Re}_{\mathrm{g}} = UL/\nu_{\mathrm{g}}$ and $\mathrm{Fr}_{\mathrm{g}} = U/(Lg)^{1/2}$, where g is the gravitational acceleration constant. The Stokes number is defined by $\mathrm{St} = U\tau_{\mathrm{p}}/L$, and the phase-mass ratio by $\phi_2 = \alpha_{\mathrm{p}}\rho_{\mathrm{p}}/(\alpha_{\mathrm{g}}\rho_{\mathrm{g}})$. The latter is an important parameter insofar as it determines whether the gas phase "sees" the disperse phase (i.e. momentum coupling is negligible when $\phi_2 \ll 1$).

The kinetic equation given by Eq. (1.11) is made dimensionless by defining $v^* = v/U$ and $n^* = Un$:

$$\frac{\partial n^*}{\partial t^*} + \frac{\partial(v^*n^*)}{\partial x^*} + \frac{\partial(\mathbb{A}^*n^*)}{\partial v^*} = \mathbb{C}^*, \tag{1.16}$$

where $n^*(t^*, x^*, v^*)$ is the dimensionless velocity distribution function,[5] and

$$\begin{aligned}\mathbb{A}^* &\equiv -\frac{1}{\phi_1}\frac{\partial p_{\mathrm{g}}^*}{\partial x^*} + \frac{g_x^*}{\mathrm{Fr}_{\mathrm{g}}^2} + \frac{1}{\mathrm{St}}(U_{\mathrm{g}}^* - v^*),\\ \mathbb{C}^* &\equiv \frac{\phi_3}{\mathrm{Kn}_{\mathrm{p}}}(n^* - n).\end{aligned} \tag{1.17}$$

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[3] See Chapter 6 for more details on collision models.

[4] For a 1D flow the viscosity term would normally be zero. However, we include the viscosity term as a placeholder for the fully 3D case in order to show the Reynolds-number dependence.

[5] Note that n and n_{eq} are made dimensionless in a manner such that $\alpha_{\mathrm{p}} = \int n^*\,\mathrm{d}v^*$. Because the kinetic equation is linear in n, no new dimensionless numbers are generated by this process.

The phase-density ratio is defined by $\phi_1 = \rho_\mathrm{p}/\rho_\mathrm{g}$ and, since $\phi_1 \gg 1$, the buoyancy term is negligible. The two new dimensionless numbers generated in this process are the phase-velocity ratio $\phi_3 = U_\mathrm{p}^\dagger/U$,[6] and the disperse-phase Knudsen number $\mathrm{Kn}_\mathrm{p} = U_\mathrm{p}^\dagger\tau_\mathrm{c}/L$. In addition, the dimensionless form of Eqs. (1.10),

$$\begin{aligned} \alpha_\mathrm{p} &= \int_{-\infty}^{+\infty} n^*\,\mathrm{d}v^*, \\ \alpha_\mathrm{p}U_\mathrm{p}^* &= \int_{-\infty}^{+\infty} v^*n^*\,\mathrm{d}v^*, \\ \alpha_\mathrm{p}\frac{\phi_3^2}{\mathrm{Ma}_\mathrm{p}^2} + \alpha_\mathrm{p}(U_\mathrm{p}^*)^2 &= \int_{-\infty}^{+\infty} (v^*)^2 n^*\,\mathrm{d}v^*, \end{aligned} \tag{1.18}$$

introduces the disperse-phase Mach number $\mathrm{Ma}_\mathrm{p} = U_\mathrm{p}^\dagger/\Theta_\mathrm{p}^{1/2}$. By analogy to compressible gas flows, Ma_p is the ratio of the characteristic mean particle velocity $U_\mathrm{p}^\dagger$ and the speed of "sound" ($\Theta_\mathrm{p}^{1/2}$) in the disperse phase. Thus for $\mathrm{Ma}_\mathrm{p} \ll 1$ transport in the disperse phase is predominantely due to velocity fluctuations, whereas for $\mathrm{Ma}_\mathrm{p} \gg 1$ it is due to mean advection.

Following the convention used in gas dynamics, we will define the velocity ratio and disperse-phase Knudsen number differently according to whether the disperse phase is subsonic or supersonic:

$$\begin{aligned} &\text{for } \mathrm{Ma}_\mathrm{p} \le 1, \quad \phi_3 = \frac{\Theta_\mathrm{p}^{1/2}}{U}, \quad \mathrm{Kn}_\mathrm{p} = \frac{\Theta_\mathrm{p}^{1/2}\tau_\mathrm{c}}{L} = \frac{\pi^{1/2}d_\mathrm{p}}{12\alpha_\mathrm{p}g_0L}; \\ &\text{for } \mathrm{Ma}_\mathrm{p} \ge 1, \quad \phi_3 = \frac{U_\mathrm{p}^\dagger}{U}, \quad \mathrm{Kn}_\mathrm{p} = \frac{U_\mathrm{p}^\dagger\tau_\mathrm{c}}{L} = \frac{\pi^{1/2}d_\mathrm{p}}{12\alpha_\mathrm{p}g_0L}\mathrm{Ma}_\mathrm{p}. \end{aligned} \tag{1.19}$$

Here d_p is the particle diameter,[7] $g_0(\alpha_\mathrm{p}/\alpha_\mathrm{p}^*)$ is the radial distribution function, and $\alpha_\mathrm{p}^* \approx 0.63$ is the maximum volume fraction at close packing. For $\alpha_\mathrm{p} \ll \alpha_\mathrm{p}^*$, $g_0 \approx 1$. However, as α_p approaches α_p^*, g_0 diverges to infinity.

Note that the ratio ϕ_3 will depend strongly on the Stokes number,

$$\mathrm{St} = \frac{U\tau_\mathrm{p}}{L} = \frac{\rho_\mathrm{p}d_\mathrm{p}^2U}{18\rho_\mathrm{g}\nu_\mathrm{g}L}, \tag{1.20}$$

where this expression for τ_p is valid for small particle Reynolds numbers, defined by

$$\mathrm{Re}_\mathrm{p} \equiv \frac{d_\mathrm{p}|U_\mathrm{p} - U_\mathrm{g}|}{\nu_\mathrm{g}}. \tag{1.21}$$

When $\mathrm{St} \gg 1$ the kinetic equation will be uncoupled from the gas phase and the disperse phase will behave as a granular gas. In the opposite limit where $\mathrm{St} \ll 1$, $\Theta_\mathrm{p} \approx 0$ and $U_\mathrm{p}^\dagger \approx U$, so that the disperse-phase Mach number will be very large and $\phi_3 \approx 1$. At intermediate values of the Stokes number, a rich variety of flow phenomena depending on all the values of the dimensionless parameters can be observed.

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[6] Because ϕ_3 and Kn_p appear together in Eq. (1.17), they could be combined into one dimensionless number. We keep them separate so that Kn_p and Ma_p depend only on disperse-phase variables.

[7] At fixed volume fraction α_p, reducing d_p increases the collision rate because the total number concentration of particles N increases significantly.