1.1 PARTICLE/SPRAY BASIC PROPERTIES

To characterize gas-particle or gas-spray flows, it is necessary first to describe the particle/spray basic properties [1–4] as follows.

1.1.1 Particle/Droplet Size and Its Distribution

The particle/droplet size distribution is frequently expressed by the semiempirical Rosin–Rammler formula as:

\[ R(d_k) = \exp\left[-\left(\frac{d_k}{\bar{d}}\right)^n\right] \]  

where \( R(d_k) \) is the weight fraction of particles with sizes larger than \( d_k \), \( n \) is the index of nonuniformness, and \( \bar{d} \) is a characteristic size. Both \( n \) and \( \bar{d} \) are determined by experiments. The derivative of \( R(d_k) \) is

\[ \frac{dR}{d(d_k)} = n(d_k)^{n-1}(\bar{d})^{-n}\exp\left[-\left(\frac{d_k}{\bar{d}}\right)^n\right] \]

which expresses the differential particle size distribution, and \( R(d_k) \) is the integral size distribution. The mean particle sizes can be defined as:

\[ d_{10} = \frac{\sum n_k d_k}{\sum n_k} \]
\[ d_{20} = \left(\frac{\sum n_k d_k^2}{\sum n_k}\right)^{1/2} \]
\[ d_{30} = \left(\frac{\sum n_k d_k^3}{\sum n_k}\right)^{1/3} \]
\[ d_{32} = \frac{\sum n_k d_k^3}{\left(\sum n_k d_k^2\right)} \]

where \( d_{10}, d_{20}, d_{30}, \) and \( d_{32} \) are diameter-averaged, surface-averaged, volume-averaged, and Sauter mean sizes, respectively. The Sauter diameter is most widely used in engineering. The typical particle sizes are:

- Coal particles in fluidized beds: 1–10 mm
- Liquid spray: 10–200 μm
- Pulverized coal: 1–100 μm
- Soot particles: 1–5 μm
1.1.2 Apparent Density and Volume Fraction

For gas-particle/droplet flows there are differently defined densities. The relationships among them are:

\[
\rho_m = \rho + \rho_p = \rho + \sum \rho_k = \rho + \left( \sum n_k \pi d_k^3 / 6 \right) \bar{\rho}_p
\]  

(1.4)

where \( \rho_m, \rho, \rho_p, \rho_k, \) and \( \bar{\rho}_p \) are mixture density, fluid apparent density, particle total apparent density, \( k \)-th size particle apparent density and particle material density, respectively. The particle volume fraction and fluid volume fraction are defined as:

\[
\alpha_p = \frac{\rho_p}{\bar{\rho}_p}; \quad \alpha_f = 1 - \alpha_p = 1 - \frac{\rho_p}{\bar{\rho}_p}
\]

(1.5)

For dilute gas-particle flows we have:

\[
\rho = \bar{\rho}(1 - \rho_p/\bar{\rho}_p) \approx \bar{\rho}
\]

where \( \bar{\rho} \) is the fluid material density. Obviously, the fluid apparent density in dilute gas-particle flows is almost equal to the fluid material density. The so-called mass loading, which is the ratio of particle mass flux to fluid mass flux, is defined as \( \rho_{p0}u_{p0}/(\rho_0u_0) \). When the fluid initial velocity is equal to the particle initial velocity, the mass loading is equal to the ratio of apparent densities. For example, in spray or pulverized-coal flames the typical value of the mass loading is:

\[
\frac{\rho_p}{\rho} = 1/15 = \frac{\bar{\rho}_p}{\rho} \frac{\alpha_p}{1 - \alpha_p} \approx 1000 \frac{\alpha_p}{1 - \alpha_p}
\]

namely, \( \alpha_p < 0.01\% \), hence the spray flame and pulverized-coal flame are dilute gas-particle flows. Other examples are: pneumatic transport \( \alpha_p \approx 0.1\% \) (mass loading \( \approx 1 \)), fluidized beds and flows in gun barrels \( \alpha_p \approx 0.8-1 \). It can be seen that when \( \alpha_p = 0.1\% \), due to \( 1 = 1000\pi d_p^3/6 \), the average inter-particle size will be:

\[
\Delta \approx n^{-1/3} = (1000\pi/6)^{1/3} d_p = 8.1 d_p. \quad \Delta > 20 d_p
\]

1.2 PARTICLE DRAG, HEAT, AND MASS TRANSFER

For different ranges of particle Reynolds number the particle drag is given as:

- Newton drag formula: \( c_d = 0.44 \) (\( \text{Re}_p > 1000 \))
- Wallis–Kliachko drag formula: \( c_d = (1 + \text{Re}_p^{2/3}/6)24/\text{Re}_p (1 < \text{Re}_p < 1000) \)
- Stokes drag formula: \( c_d = 24/\text{Re}_p (\text{Re}_p < 1) \)  

(1.6)

where \( \text{Re}_p \) is the particle Reynolds number of particle motion relative to fluid. When the particle temperature is higher than the gas temperature, the
particle drag will increase according to the so-called 1/3 law. The gas viscosity in the particle Reynolds number will be:

\[ \nu = \nu_p/3 + 2\nu_g/3 \]  

(1.7)

where the subscripts \( p \) and \( g \) denote the gas viscosity under the particle temperature and gas temperature, respectively. The particle mass loss due to evaporation, devolatilization, or heterogeneous combustion will reduce the particle drag to:

\[ c_d = c_{d0}\ln(1 + B)/B \]  

(1.8)

where \( B \) is a dimensionless parameter given by

\[ \ln(1 + B) = m/\left(\pi d_p \rho D\right) \]  

(1.9)

The particle heat and mass transfer are given by the Ranz–Marshall formula:

\[ \text{Nu} = 2 + 0.6\text{Re}_p^{0.5}\text{Pr}_t^{0.33} \]  

\[ \text{Sh} = 2 + 0.6\text{Re}_p^{0.5}\text{Sc}^{0.33} \]  

(1.10)

where \( \text{Nu} \), \( \text{Sh} \), \( \text{Re} \), \( \text{Pr} \), and \( \text{Sc} \) are the Nusselt number, Shewald number, Reynolds number, Prandtl number, and Schmidt number, respectively. The droplet mass, diameter, and temperature change during evaporation and solid-fuel particle mass and temperature change during moisture evaporation, devolatilization, and char combustion are given in the combustion theory, see Chapter 3, Fundamentals of Combustion.

1.3 SINGLE-PARTICLE DYNAMICS

Consider the single-particle motion in a known simple flow field and neglect the effect of particles on the fluid flow; this is single-particle dynamics [6]. For turbulent gas-particle flows single-particle dynamics is a basic phenomenon observed in practical cases.

1.3.1 Single-Particle Motion Equation

Taking into consideration only the drag and gravitational forces, the simplest single-particle motion equation can be given as:

\[ \frac{dv_{pi}}{dt_p} = \left(v_i - v_{pi}\right)/\tau_r + g_i \]  

(1.11)

where \( \tau_r \) is the particle relaxation time, expressing the ratio of particle inertia to particle drag, determined by the drag law.
1.3.2 Motion of a Single Particle in a Uniform Flow Field

Assuming a particle with initial velocity \( v_{p0} \) and Stokes’ drag law, moving in a uniform flow field (Fig. 1.1), when neglecting the gravitational force, the particle momentum equation in the \( x \) direction is

\[
\frac{du_p}{dt} = (u_\infty - u_p) / \tau_r
\]  
(1.12)

where \( \tau_r = \frac{d_p^2 \rho_p}{(18 \mu)} \). Integration of Eq. (1.12) with an initial condition of \( u_p = u_{p0} \) at \( t = 0 \) gives the particle longitudinal velocity

\[
u_p = u_\infty - (u_\infty - u_{p0}) \exp(-t/\tau_r)
\]  
(1.13)

The particle lateral velocity can be obtained in a similar way as

\[
u_p = v_{p0} \exp(-t/\tau_r)
\]  
(1.14)

Integration of Eqs. (1.13) and (1.14) with respect to \( t \) gives the particle trajectory equations as

\[
x_p = u_\infty t - (u_\infty - u_{p0}) \tau_r (1 - e^{-t/\tau_r})
\]  
(1.15)

\[
y_p = v_{p0} \tau_r (1 - e^{-t/\tau_r})
\]  
(1.15)

Similar equations can also be derived for non-Stokes’ particle drag. Eqs. (1.13, 1.14, 1.15) point out that as the time approaches \( \infty \), the particle longitudinal velocity approaches the fluid velocity, the particle lateral velocity approaches zero and the particle lateral displacement approaches \( y = v_{p0} \tau_r \). When \( t = \tau_r \), we have \( v_p = v_{p0} / \tau_r \). Hence the physical meaning of the particle relaxation time is the time needed for the fluid-particle velocity slip to decrease to \( 1/e \) of its initial value. It expresses the easiness with which particles follow the fluid.

1.3.3 Particle Gravitational Deposition

For an initially stagnant particle acting only by Stokes’ drag and gravity, the motion equation is:

\[
\frac{dv_p}{dt} + \frac{v_p}{\tau_r} - g = 0
\]  
(1.16)
For the initial condition of $v_p(0) = 0$ at $t = 0$, its solution is:

$$v_p = \tau_r g \left( 1 - e^{-t/\tau} \right)$$ (1.17)

As the time approaches infinity, $v_p$ approaches $\tau_r g = v_{pr}$, the particle acceleration becomes zero and the gravity and drag force will be in equilibrium. In this case the particle velocity is called the terminal velocity.

### 1.3.4 Forces Acting on Particles in Nonuniform Flow Field

#### 1.3.4.1 Magnus Force

As a nonspherical particle moves in the flow field with velocity gradient, in particular after its impact on the wall, it may rotate, causing a lifting force perpendicular to the direction of relative velocity, called the Magnus force. Its magnitude is:

$$F_M = \pi d_p^3 \rho \omega_p - \Omega$$ (1.18)

where $\omega_p$ is the angular velocity of particle rotation, and $\Omega$ is the half of fluid vorticity. It has been estimated that the ratio of Magnus force to the drag force is 0.04 for a 1-μm particle and 3 for a 10-μm particle. However, experimental studies have shown that in most regions of the flow field, particles do not rotate due to fluid viscosity. Therefore, except in the region adjacent to the wall, the Magnus force is not important.

#### 1.3.4.2 Saffman Force

If the particle is sufficiently large and there is a large velocity gradient in the flow field (for example, near the wall), there will be a particle-lifting force called the Saffman force. Its magnitude is

$$F_s = 1.6(\mu C_1)^{1/2} d_p^{1/2} \left| v - v_p \right| \frac{\partial v}{\partial y}^{1/2}$$ (1.19)

The ratio of the Saffman force to the Magnus force is much greater than unity; hence the Saffman force may play an important role, in particular in the region of a large velocity gradient, such as in the recirculation region and the near-wall region.

#### 1.3.4.3 Particle Thermophoresis, Electrophoresis, and Photophoresis

Tiny particles smaller than 1 μm may move under the effects of so-called “thermophoresis,” “electrophoresis,” and “photophoresis,” caused by a large
temperature gradient, electric field gradient, and nonuniform light radiation, respectively. The forces of thermophoresis and electrophoresis can be estimated by

$$ F_{ij} = -4.5 \nu^2 (\rho / T) d_p \left[ \lambda (2 \lambda + \lambda_p) \right] \frac{\partial T}{\partial x_j} $$

$$ F_E = (\pi / 6) \rho d_p^3 qE $$

where $\lambda$ and $\lambda_p$ are the gas and particle thermoconductivities, respectively, and $E$ and $q$ are electric field strength and particle electric charge, respectively. All of these forces are significant merely for submicron or ultrafine particles.

### 1.3.5 Generalized Particle Motion Equation

Eq. (1.11) is a very simple particle motion equation. C.M. Tchen [7], using a method of intuitive superposition of various possible forces, proposed a generalized particle motion equation, with Stoke drag and accounting for the Magnus force, Saffman force, thermophoresis, and electrophoresis forces, as

$$ m_p \frac{dv_p}{dt} = F_{di} + F_{vmi} + F_{pi} + F_{ai} + F_{Mi} + F_{si} + F_{Ti} + F_{EI} + $$

$$ \ldots = 3 \pi d_p \mu (v_i - v_{pi}) + 0.5 (\pi d_p^3 / 6) \rho \frac{d}{dt} (v_i - v_{pi}) + $$

$$ (\pi d_p^3 / 6) \rho \frac{dv_i}{dt} + 1.5 (\pi \rho \mu)^{1/2} d_p^2 \int_0^t \frac{d}{d\tau} (v_i - v_{pi})(\tau - t) d\tau + $$

$$ F_{Mi} + F_{si} + F_{Ti} + F_{EI} + \ldots $$

where the first, second, third, and fourth terms on the right-hand side of Eq. (1.21) denote the drag force, virtual-mass force, pressure-gradient force, and Basset force (due to unsteady flow), respectively. It should be noted that in most cases the forces other than the drag force are of minor importance, so the approximation made in Eq. (1.11) is still valid.

### 1.3.6 Recent Studies on Particle Dynamics

particles using a Lattice–Boltzmann simulation. From these simulation results the exact forces acting on the particles can be obtained. For example, it is found that the virtual mass force can be neglected, if the ratio of the fluid material density to the particle material density is small. The effect of small-scale turbulence on the forces acting on particles is also studied. Michaelides [12,13] systematically summarized the research results of forces and heat and mass transfer acting on particles and proposed a more comprehensive particle motion equation. A comparison was made between the classical analytic solutions and the recent results of DNS and Lattice–Boltzmann simulation results. For example, the effect of particle concentration on particle drag force was discussed.

Alternatively, in some cases the electric forces and van der Waals forces are also considered when particles are located in the electric field and are very near to each other. The contact force and collision forces between particles should be considered for dense gas-particle flows. For further details the reader should refer to Refs [14,15].

REFERENCES

Theory and Modeling of Dispersed Multiphase Turbulent Reacting Flows


FURTHER READING

Chapter 2

Basic Concepts and Description of Turbulence

2.1 INTRODUCTION

As this book is related to multiphase turbulent reacting flows, some knowledge of the fundamental concepts and description of turbulence are introduced. More than 100 years ago, Osborn Reynolds (1883–94) first indicated that flows can be either laminar or turbulent by observing injected dyed water flow in a tube. A parameter called the Reynolds number Re = \( \frac{vd}{\nu} \) (where \( v \) is the velocity, \( d \) is the size, and \( \nu \) is the kinematic viscosity) is used to identify these two flow regimes. He first suggested the decomposition of the flow variables into time-averaged and fluctuation quantities for mathematically analyzing turbulent flows.

Turbulent flows widely occur in nature and engineering, particularly in astronomy and natural water bodies. In engineering facilities, turbulent flows are encountered in fluid machines, heat exchangers, and combustors, because frequently in these facilities the fluid velocity is higher, and the geometrical sizes are large, in other words, the Reynolds number is large. However, in some cases, even if the Re number is not large, but there are rough walls and flow separation by obstacles, turbulence may also be produced.

Examples of turbulent flows are the discharge of smoke from a stack, as shown in Fig. 2.1, and a turbulent gas jet flame, as shown in Fig. 2.2. The flows of small soot particles and combustion products show on one hand the irregular behavior of instantaneous gas flows, but on the other hand, some organized structures—the so-called “coherent structures.” Therefore, turbulent flows have both random and organized structures. Fig. 2.3 shows the vorticity map of a sudden-expansion flow by large-eddy simulation (LES). It gives the detailed turbulence structures. It can be seen that there are different length scales of eddies in turbulent flows.

2.2 TIME AVERAGING

Let us consider a variable \( \tilde{a}(x; t) \) changing with time at a given spatial location of the turbulent flow field. O. Reynolds first introduced the concept of time averaging of a variable \( \phi \) [1] as:

\[
\overline{\phi}(x, y, z) = \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} \phi(x, y, z; t) dt
\]  

(2.1)
Here $\phi$ may be any variable in the turbulent flow field, such as the velocity component $v_i$, or temperature $T$ (enthalpy $h$), or species concentration $Y_s$. The time-averaging period $\tau$ must be much larger in comparison with the integral time scale of turbulent fluctuation, but should be smaller than the macroscopic time period of unsteady flows, such as the wavy flows. The so-called Reynolds’ expansion is defined as:

$$\phi = \overline{\phi} + \phi'$$

$$\overline{\phi} = \overline{\phi}; \quad \overline{\phi'} = 0; \quad \overline{\phi'\phi'} \neq 0 \quad (2.2)$$

For compressible flows, the so-called Favre averaging or density-weighed averaging usually is used, and is defined as:

$$\phi = \bar{\phi} + \phi''$$

$$\bar{\phi} = \overline{\rho\phi / \rho}; \quad \overline{\phi''} \neq 0 \quad \overline{\rho\phi''} = 0 \quad (2.3)$$

### 2.3 PROBABILITY DENSITY FUNCTION

A different description of the fluctuation of a variable is the so-called probability density function (PDF). The PDF- $p(f)$ is defined as follows: the