Fluid Dynamics and Transport of Droplets and Sprays

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Introduction

1.1 OVERVIEW

A spray is one type of two-phase flow. It involves a liquid as the dispersed or discrete phase in the form of droplets or ligaments and a gas as the continuous phase. A dusty flow is very similar to a spray except that the discrete phase is solid rather than liquid. Bubbly flow is the opposite kind of two-phase flow wherein the gas forms the discrete phase and the liquid is the continuous phase. Generally, the liquid density is considerably larger than the gas density, so bubble motion involves lower kinematic inertia, higher drag force (for a given size and relative velocity), and different behavior under gravity force than droplet motion.

Important and intellectually challenging fluid-dynamic and -transport phenomena can occur in many different ways with sprays. On the scale of an individual droplet size in a spray, boundary layers and wakes develop because of relative motion between the droplet center and the ambient gas. Other complicated and coupled fluid-dynamic factors are abundant: shear-driven internal circulation of the liquid in the droplet, Stefan flow due to vaporization or condensation, flow modifications due to closely neighboring droplets in the spray, hydrodynamic interfacial instabilities leading to droplet-shape distortion and perhaps droplet shattering, and droplet interactions with vortical structures in the gas flow (e.g., turbulence).

On a much larger and coarser scale, we have the complexities of the integrated exchanges of mass, momentum, and energy of many droplets in some subvolume of interest with the gas flow in the same subvolume. The problem is further complicated by the strong coupling of the phenomena on the different scales; one cannot describe the mass, momentum, and energy exchanges on the large scale without detailed knowledge of the fine-scale phenomena. Note that in some practical applications, these scales can differ by several orders of magnitude so that a challenging subgrid modelling problem results.

Detailed consideration will be given to applications in which the mass vaporization rate is so large that the physical behavior is modified. This is the most complex situation and therefore its coverage leads to the most general formulation of the theory. In particular, as the vaporization rate increases, the coupling between the two phases becomes stronger and, as the droplet lifetime becomes as short as some of the other characteristic times, the transient or dynamic character of the problem emerges in a dominant manner.

The fast vaporization rate is especially prominent in situations in which the ambient gas is at very high temperatures (of the order of 1000 K or higher). Combustion with liquid fuels is the most notable example here. The spray combustion regime is a most interesting limiting case of the more general field of thermal and dynamic behavior of sprays. In the high-temperature domain, rapid vaporization causes droplet lifetimes to be as short as the time for a droplet to heat throughout its interior. It can be shorter than the time for liquid-phase mass diffusion to result in the mixing of various components in a multicomponent liquid. The combustion limit is inherently transient from the perspective of the droplet, richer in terms of scientific issues, and more challenging analytically and numerically than low-temperature spray problems. Vaporization might still be longer than other combustion processes such as mixing or chemical reaction; therefore it could be the rate-controlling process for energy conversion.

The spray problem can be complicated by the presence of spacial temperature and concentration gradients and internal circulation in the liquid. Interaction among droplets is another complication to be treated.

There is a great disparity in the magnitudes of the scales. Liquid-phase mass diffusion is slower than liquid-phase heat diffusion, which, in turn, is much slower than the diffusion of vorticity in the liquid. Transport in the gas is faster than transport in the liquid. Droplet diameters are typically of the order of a few tens of micrometers (μm) to a few hundreds of micrometers in diameter. Resolution of internal droplet gradients can imply resolution on the scale of micrometers or even on a submicrometer scale. Combustor or flow chamber dimensions can be 5 to 6 orders of magnitude greater than the required minimum resolution. Clearly, subgrid droplet-vaporization models are required for making progress on this problem.

Experiments have been successful primarily in resolving the global characteristics of sprays. The submillimeter scales associated with the spray problem have made detailed experimental measurements very difficult. If an attempt is made to increase droplet size, similarity is lost; the droplet Reynolds number can be kept constant by decreasing velocity but the Grashof number grows, implying that buoyancy becomes relatively more important. Also, the Weber number increases as droplet size increases; surface tension becomes relatively less important and the droplet is more likely to acquire a nonspherical shape. Modern nonintrusive laser diagnostics have made resolution possible on a scale of less than 100 μm so that, in recent years, more experimental information has been appearing. Nevertheless, theory and computation have led experiment in terms of resolving the fluid-dynamical characteristics of spray flows.

Classical texts on droplets, including burning-fuel droplets, tend to consider an isolated spherical droplet vaporizing in a stagnant environment. In the simplified representation, the liquid has one chemical component, ambient-gas conditions are subcritical, and vaporization occurs in a quasi-steady fashion. The classical result is that the square of the droplet radius or diameter decreases linearly with time since heat diffusion and mass diffusion in the surrounding gas film are the rate-controlling (slowest) processes; this behavior is described as the d^2 law. These important phenomena will be discussed in later chapters. While most researchers are now addressing these relevant and interesting factors that cause major deviations from classical behavior, there are still some researchers who persist in the study of the classical configuration. Here we will relax these simplifications, one at a time, to gain a more accurate and more relevant understanding. Convective effects due to droplet motion or natural convection and subsequent internal liquid circulation will be thoroughly studied. Transient heating (or cooling) and vaporization (or condensation) due to changing ambient conditions, unsteady liquid-phase diffusion, or unsteady gas-phase diffusion will be analyzed. Multicomponent liquid (including emulsions and slurries as well as blended liquids) droplet vaporization will be studied. Near-critical and supercritical ambient conditions (and their effects on diffusion processes, phase change, solubility, and liquid-surface stripping due to shear) will be discussed. Interactions of droplets with other droplets and with turbulent or vortical structures will be analyzed. Distortion of the spherical shape and secondary atomization of the droplets will also be discussed. The effects of radiative heating of the liquid and of exothermic chemical reaction in the gas film will also be studied.

Current texts do not explain in a unified fashion the various approaches to calculation of the behaviors of the many droplets present in a spray. Efficient and accurate methods for predicting the trajectories, temperatures, and vaporization rates of a large number of droplets in a spray are discussed here. Sprays in both laminar and turbulent environments are discussed.

Some comments about primary atomization and droplet-size determination are given in Section 1.2. In Chapter 2, we shall discuss the vaporization of individual droplets and study the phenomenon on the scale of the droplet diameter. The theoretical models and correlations of computational results for individual droplets can be used to describe exchanges of mass, momentum, and energy between the phases in a spray flow. The vaporization of multicomponent droplets, including slurry droplets, is discussed in Chapter 3. Interactions among a few droplets and their effects on the modification of the theory are discussed in Chapter 4. The spray with its many droplets is examined in Chapter 5. The spray equations are examined from several aspects; in particular, two-continua, multicontinua, discrete-particle, and probabilistic formulations are given. The choice of Eulerian or Lagrangian representation of the liquid-phase equations within these formulations is discussed, including important computational issues and the relationship between the Lagrangian method and the method of characteristics. Some of the theories and information in this monograph have already had an impact on computational codes; modification of the codes to address more recent advances should not be difficult. One shortcoming, of course, is the limited experimental verification, as discussed above. Applications of the spray theory to special configurations are discussed in Chapter 7. Turbulence–droplet interactions are surveyed in Chapter 8. The spray discussions of Chapters 5 and 7 precede the topics of Chapter 8 because vorticity–droplet interactions and turbulence–droplet interactions have not yet been fully integrated into a comprehensive spray theory. These interaction studies are still active research domains, and, so far, little application to engineering practice has occurred. In Chapter 9 droplet behavior in near-critical and supercritical thermodynamic environments is discussed; secondary atomization and molecular dynamic methods are also discussed.

1.2 DROPLET-SIZE DETERMINATION

The droplet size is an important factor in its behavior. Droplet shape is another factor with profound implications. Surface tension will tend to minimize the droplet surface area, given its volume, resulting in a spherical shape for sufficiently small droplets. The size of a spherical droplet will be represented most commonly by its diameter d or radius R. In most sprays, droplets of many different sizes will exist. Vaporization, condensation, droplet coalescence, and droplet shattering will cause a temporal variation in droplet sizes. For a spray, a distribution function of the instantaneous diameter $f(d)$ is typically used to describe a spray. This function gives the number of droplets possessing a certain diameter. Often an average droplet diameter d_{mn} is taken to represent a spray. In particular,

$$d_{mn} = \frac{\int_0^\infty f(d) d^m \, \mathrm{d}d}{\int_0^\infty f(d) d^n \, \mathrm{d}d}. \tag{1.1}$$

In practice, $f(d)$ will not be a continuous function. However, for a spray with many droplets (millions can be common) the function is well approximated as a continuously varying function. One example of an average droplet is the Sauter mean diameter d_{32}, which is proportional to the ratio of the total liquid volume in a spray to the total droplet surface area in a spray.

The aerodynamic forces on a droplet will depend on its size in a functional manner different from the dependence of droplet mass on the size. As a result, smaller droplets undergo more rapid acceleration or deceleration than larger droplets. Heating times and vaporization times will be shorter for smaller droplets. Accuracy in the initial droplet-size distribution is mandatory therefore if we wish to predict droplet behavior. Unfortunately, we must currently rely mostly on empirical methods to represent droplet distribution; it cannot be predicted from a first-principles approach for most liquid injection systems.

Liquid streams injected into a gaseous environment tend to be unstable under a wide range of conditions. An important parameter is the Weber number,

$$\mathrm{We} = \frac{\rho \Delta U^2 L}{\sigma}, \tag{1.2}$$

where ρ is the gas density, ΔU is the relative gas–liquid velocity, L is the characteristic dimension of the stream, and σ is the surface-tension coefficient. We represent the ratio of the aerodynamic force related to dynamic pressure to the force of surface tension. Depending on the stream shape, oscillation of the stream and breakup occur above some critical value of the Weber number. These interface oscillations can occur at any wavelength, but some wavelengths will have larger rates of amplitude growth. Below the critical value of the Weber number, the surface-tension forces are large enough to overcome the aerodynamic force that tends to distort the stream. So here the basic shape of the stream is maintained without disintegration. At higher Weber numbers, the aerodynamic force dominates, leading to distortion and disintegration. This process is called atomization.

Disintegration or atomization typically results in liquid ligaments or droplets with a characteristic dimension that is smaller than the original length scale associated with the stream. Disintegration will continue in a cascade fashion until the decreased length scale brings the Weber number for the resulting droplets below the critical value for the droplets. Other parameters will affect the critical value of the Weber number; they include the ratio of liquid density to gas density and a nondimensional representation of viscosity (e.g., Reynolds number).

Practical atomization systems use a variety of mechanisms to achieve the critical Weber numbers that are necessary. Jet atomizers use a sufficiently large pressure drop across an orifice to obtain the necessary liquid velocity. Air-assist and air-blast atomizers force air flow as well as liquid flow. The critical Weber number depends on the relative air–liquid velocity here. Some atomizers use swirl vanes for the liquid or air to create a tangential component of velocity; this can increase the relative velocity. Rotary atomizers involve spinning cups or disks upon which the liquid is flowed; the centrifugal effect creates the relative velocity. Sometimes other means are used for atomization including acoustic or ultrasonic oscillations, electrostatic forces, and the injection of a bubbly liquid. An excellent review of practical atomization systems is given by Lefebvre (1989).

There are three general approaches to the prediction of the droplet sizes that result from atomization of a liquid stream. The most widely used approach involves the use of empirical correlations. Another approach requires the solution of the Navier–Stokes equations or of their inviscid limiting form, the Euler equations, to predict disintegration of the liquid stream. Often the linearized form of the equations is taken. The third approach assumes that, in addition to conservation of mass momentum and energy, the droplet-size distribution function satisfies a maximum entropy principle.

The Rosin–Rammler distribution equation governs the volume of liquid contained in all droplets below a given diameter d. In particular, the fractional volume of liquid $\Phi(d)$ is described as

$$\frac{\int_0^d f(d')^3 \, \mathrm{d}d'}{\int_0^\infty f(d)^3 \, \mathrm{d}d} \equiv \Phi(d) = 1 - \exp\left(-\frac{d^b}{a}\right), \tag{1.3}$$

where a and b are constants to be chosen to fit the relevant experimental data. It follows that

$$f(d) = \frac{b}{a^b} d^{b-4} \exp\left[-\left(\frac{d}{a}\right)^b\right]. \tag{1.4}$$

Another correlating equation commonly chosen is the Nukiyama–Tanasawa equation, which states that

$$f(d) = ad^2 \exp(-bd^c). \tag{1.5}$$

The constant a is related to a gamma function by the condition that the integral $\int_0^\infty f(d) \, \mathrm{d}d$ equals the total number of droplets. So two parameters remain to be adjusted to fit the experimental data.

Sometimes a Gaussian or normal distribution with the natural logarithm of the droplet diameter as the variable gives a good correlation for the experimental data. Here

$$f(d) = \frac{1}{\sqrt{2\pi}} \frac{1}{sd} \exp\left[-\frac{(\log d - \log d_{mn})^2}{2s^2} \right], \tag{1.6}$$

where d_{nm} is the number geometric mean droplet diameter and s is the corresponding standard deviation. See Lefebvre (1989) and Bayvel and Orzechowski (1993) for further details on droplet-size distributions.

The second major approach to the prediction of droplet-size and -velocity distributions in a spray involves analysis guided by the first principles of hydrodynamics with an account of surface-tension forces. This approach dates back to Rayleigh (1878) but yet is still in its infancy. The theory addresses the distortion of the liquid stream due to hydrodynamic instability, often of the Kelvin–Helmholtz variety. The theory is limited mostly to linearized treatments, although, with modern computational capabilities, more nonlinear analysis has been occurring recently. The analyses sometimes predict the first step of disintegration of a liquid stream but generally are not able, except in the simplest configurations, to predict droplet-size distribution.

Rayleigh (1878) analyzed the temporal instability of a round liquid jet and predicted that the greatest growth rate of the instability occurs for a disturbance wavelength that is 4.508 times larger than the diameter of the undisturbed jet. With one droplet forming every wavelength, conservation of mass leads to the prediction of a droplet diameter to jet diameter ratio of approximately 1.9. Weber (1931) extended the analysis to account for spacial instability with a mean jet velocity. Hence a dependence on the now-famous Weber number was demonstrated. A useful review of the theory of instability of the round jet is given by Bogy (1979). As the Weber number of the liquid stream increases, aerodynamic effects become increasingly important and droplets of decreasing diameter result from the disintegration process. A good review of these effects with a classification of the various regimes is given by Reitz and Bracco (1982).

In many applications, the liquid stream is injected as a thin sheet to maximize the surface area and to enhance the ratio of disintegration into small droplets. Examples of this sheet configuration are hollow cone sprays and fan sheets. The theory on this configuration is more limited than that for the round jet. Some overview discussions are given by Lefebvre (1989), Bayvel and Orzechowski (1993), and Mehring and Sirignano (1998).

The third approach in which a maximum entropy approach is used is the youngest and least developed of the approaches to predicting droplet-size distribution. While the concept remains controversial since all the constraints on the maximization process might not have yet been identified, it is a worthy development to follow. See for example Chin et al. (1995) and Archambault et al. (1998).

In summary, the current ability to predict initial droplet-size distribution in a spray is based on empirical means, but interesting and challenging theoretical developments offer promise for the future.