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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 does 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 that is due to vaporization or condensation, flow modifications that are 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 a 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 2

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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 spatial 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 (μ m) 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 dropletvaporization 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 μ m so that, in recent years, more experimental information has been appearing. Nevertheless, theory and computation have led experiments 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

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because heat diffusion and mass diffusion in the surrounding gas film are the ratecontrolling (slowest) processes; this behavior is described as the d^2 law. These important phenomena are discussed in later chapters. Although 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 that are due to droplet motion or natural convection and subsequent internal liquid circulation are thoroughly studied. Transient heating (or cooling) and vaporization (or condensation) that are due to changing ambient conditions, unsteady liquid-phase diffusion, or unsteady gas-phase diffusion are analyzed. Multicomponent-liquid (including emulsions and slurries as well as blended liquids) droplet vaporization is studied. Near-critical and supercritical ambient conditions (and their effects on diffusion processes, phase change, solubility, and liquid-surface stripping that is due to shear) will be discussed. Interactions of droplets with other droplets and with turbulent or vortical structures are analyzed. Distortion of the spherical shape and secondary atomization of the droplets are also discussed. The effects of radiative heating of the liquid and of exothermic chemical reaction in the gas film are also 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 Chapters 2 and 3, we discuss the vaporization of individual droplets and study the phenomenon on the scale of the droplet diameter. Chapter 2 considers the case in which there is no relative motion between the droplet and the distant gas, and Chapter 3 covers the situation with a relative velocity. 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 4. Droplet behavior under near-critical or transcritical thermodynamic conditions is considered in Chapter 5. Secondary atomization and molecular-dynamic methods are also discussed there. Interactions among droplets and their effects on the modification of the theory are discussed in Chapter 6. The spray with its many droplets is examined first in Chapter 7. 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 specific computational issues are discussed in Chapter 8. Some of the theories and information in this book 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 just discussed.

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Applications of the spray theory to special laminar-flow configurations are discussed in Chapter 9. Turbulence–spray interactions are surveyed in Chapter 10. 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 11, we discuss exchanges of mass, momentum, and energy between the phases for a type of configuration other than droplets and sprays, i.e., liquid films. In Chapter 12, current research is discussed for the distortion and disintegration of liquid streams in processes leading to the formation of sprays. Important material on the underlying governing field equations, use of conserved scalars, and a summary of droplet models are given in the Appendices.

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,

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

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

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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. The Weber number (We) is 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 maximumentropy principle.

In the first approach, it is common practice to fit experimental data to a numberdistribution function for the droplet radius or diameter. With the current level of the theory, this is the most commonly used approach. 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

$$\frac{\int_{0}^{d} f(d')^{3} \,\mathrm{d}d'}{\int_{0}^{\infty} f(d)^{3} \,\mathrm{d}d} \equiv \Phi(d) = 1 - \exp\left(-\frac{d^{b}}{a}\right),\tag{1.3}$$

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

$$f(d) = \frac{b}{a^b} d^{b-4} \exp\left[-\left(\frac{d}{a}\right)^b\right].$$
 (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 $\int_0^{\infty} f(d) dd$ 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. The logarithm provides a geometric rather than an arithmetic averaging. Here, the log-normal number-distribution function for droplet side is

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

where d_{ng} 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 that is 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 spatial 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.

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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 Sirignano and Mehring (2000, 2005).

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. Although the concept remains controversial because 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. A discussion of the relevant research is presented in Chapter 12.

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Isolated Spherically Symmetric Droplet Vaporization and Heating

There is interest in the droplet-vaporization problem from two different aspects. First, we wish to understand the fluid-dynamic and -transport phenomena associated with the transient heating and vaporization of a droplet. Second, but just as important, we must develop models for droplet heating, vaporization, and acceleration that are sufficiently accurate and simple to use in a spray analysis involving so many droplets that each droplet's behavior cannot be distinguished; rather, an average behavior of droplets in a vicinity is described. We can meet the first goal by examining both approximate analyses and finite-difference analyses of the governing Navier-Stokes equations. The second goal can be addressed at this time with only approximate analyses because the Navier-Stokes resolution for the detailed flow field around each droplet is too costly in a practical spray problem. However, correlations from Navier-Stokes solutions provide useful inputs into approximate analyses. The models discussed herein apply to droplet vaporization, heating, and acceleration and to droplet condensation, cooling, and deceleration for a droplet isolated from other droplets. The governing partial differential equations reflecting the conservation laws are presented in Appendix A. Several coordinate systems are considered. Formulations with primitive velocity variables and formulations with stream functions are discussed. Appendix B discusses some conserved scalar variables whose analytical use can be very convenient and powerful under certain ideal conditions.

Introductory descriptions of vaporizing droplet behavior can be found in the works of Chigier (1981), Clift et al. (1978), Glassman (1987), Kanury (1975), Kuo (1986), Lefebvre (1989), and Williams (1985). Useful research reviews are given by Faeth (1983), Law (1982), and Sirignano (1983, 1993a, 1993b). The monographs by Sadhal et al. (1997) and Frohn and Roth (2000) are also noteworthy.

The vaporizing-droplet problem is a challenging, multidisciplinary issue. It can involve heat and mass transport, fluid dynamics, and chemical kinetics. In general, there is a relative motion between a droplet and its ambient gas. Here, the general aerodynamic characteristics of pressure gradients, viscous boundary layers, separated flows, and wakes can appear for the gas flow over the droplet. The Reynolds number based on the relative velocity, droplet diameter, and gas-phase properties

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is a very important descriptor of the gaseous-flow field. Internal liquid circulation, driven by surface-shear forces, is another important fluid-dynamic feature of the droplet problem.

These flow features have a critical impact on the exchanges of mass, momentum, and energy between the gas and the liquid phases. They are important for both vaporizing and nonvaporizing situations. The vaporizing case is complicated by regressing interfaces and boundary-layer blowing.

We will see six types of droplet-vaporization models. In order of increasing complexity, they are (i) constant-droplet-temperature model (which yields the famous d^2 law whereby the square of the droplet diameter or radius decreases linearly with time), (ii) infinite-liquid-conductivity model (uniform but time-varying droplet temperature), (iii) spherically symmetric transient droplet-heating (or conduction-limit) model, (iv) effective-conductivity model, (v) vortex model of droplet heating, and (vi) Navier–Stokes solution. There are various differences among these models, but the essential issue is the treatment of the heating of the liquid phase that is usually the rate-controlling phenomenon in droplet vaporization, especially in high-temperature gases. Some of the models will be shown to be limits of another model. These models are explained in this chapter and in the next chapter, summarized in a user-friendly manner in Appendix C, and used in spray calculations discussed in other chapters.

In the first five models a quasi-steady gas phase is often considered but that feature is not necessary; the models can be constructed to include unsteady gas phases. The first three models can be directly applied to the situation in which there is no relative motion between the droplet and the ambient gas or in which a correction based on the Reynolds number can be applied to account for convective heat transfer from the gas to the liquid. However, internal circulation is not considered in those three models. (Actually, the internal circulation has no impact on heating when liquid temperature is uniform or constant.) The effective-conductivity models account for internal circulation and internal convective heating in an ad hoc manner whereas the vortex model more directly describes the physical situation. Obviously the Navier–Stokes solutions are, in principle, exact in the continuum regime.

Generally, the thermal diffusivity in the gas phase is much larger than the liquidphase thermal diffusivity. So transient liquid heating generally takes longer than the gas-phase transient. Often, then, a quasi-steady gas-phase behavior can be assumed, neglecting time derivatives there while keeping them for the liquid phase. An exception can occur near the thermodynamic critical point where differences between gas and liquid properties, including diffusivities, are diminished. Of course, if ambientgas properties are undergoing a transient behavior, then the characteristic time for gas-phase diffusion (the square of characteristic length divided by gas diffusivity) must be compared with the characteristic time for the change of the ambient conditions. As gas-phase ambient conditions change more rapidly and as droplet size increases, transient behavior becomes more important; consequently, the quasi-steady gas-phase assumption is weakened. However, gas-phase quasi-steadiness is broadly applicable in practice. We will generally consider quasi-steadiness in this book but will consider exceptions. For example, we have sections that deal with situations in

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which the gas film surrounding the droplet has a behavior such that time derivatives become important: e.g., a droplet in a near-critical gas, the interaction of a droplet with an acoustical wave, or the interaction of a droplet with a vortical structure.

In a gas, mass diffusivity and heat diffusivity are comparable in magnitude, yielding comparable characteristic times. For a common liquid, mass diffusivity is much smaller than thermal diffusivity. So, for multicomponent liquid droplets, we shall see in Chapter 4 that mass mixing in the droplet is slower than thermal mixing.

The combustion of liquid fuels is an application in which droplet vaporization can be critical because the vaporization can be the slowest process determining the overall burning rate. Classical droplet-vaporization and -burning theory describes a fuel droplet in a spherically symmetric gas field. There, the only relative motion between liquid and gas involves radial convection that is due to vaporization. This model implies that droplets would travel through a combustion chamber at the gas velocity. Such an implication could be true, however, for only very small droplets (often much less than 30 μ m in diameter). Because droplet mass is proportional to the cube of diameter and droplet drag is proportional to diameter to a power no greater than squared, we can expect acceleration to be inversely proportional to some positive power of diameter. Acceleration that is due to drag will always tend to decrease the relative velocity between gas and liquid. Of course, this tendency could be overcome in certain situations in which the gas itself is accelerating because of pressure gradients or viscous stresses in such a manner so as to increase the relative velocity. In any event, the larger droplets will have a greater kinematic inertia.

In developing the study of the gas-flow field surrounding the droplet and of the liquid flow in the droplet, certain assumptions are made. A small Mach number is considered so that kinetic energy and viscous dissipation are negligible. Gravity effects, droplet deformation, Dufour energy flux, and mass diffusion that is due to pressure and temperature gradients are all neglected. (Note, however, that thermophoresis can affect the transport rates for submicrometer particles: e.g., soot.) Radiation is commonly neglected, but it is briefly discussed. The multicomponent gas-phase mixture is assumed to behave as an ideal gas. Phase equilibrium is stated at the droplet–gas interface. Gas-phase density and thermophysical parameters are generally considered variable, unless otherwise stated.

In the limiting case in which there is no relative motion between the droplet and the gas, a spherically symmetric field exists for the gas field surrounding the droplet and for the liquid field. If a small relative velocity occurs, the droplet acceleration becomes so large that the relative velocity between the droplet and the surrounding gas immediately goes to zero. Therefore, in this limit, relative velocity remains zero even as the gas velocity varies. Here, the fluid motion is reduced to a Stefan convection in the radial direction. Many of the important issues discussed in this case also appear in the more general case with droplet motion discussed in the next chapter.

The approach here is the presentation of the zero Reynolds number (spherically symmetric) analysis in this chapter, whereas, in the next chapter, we discuss low Reynolds number analysis and analyses for intermediate to high Reynolds numbers. When these several theories are patched together, a respectable engineering model