Fluid Dynamics and Transport of Droplets and Sprays

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To Lynn Sirignano
and
To My Parents, Anthony and Lucy Sirignano

Fluid Dynamics and Transport of Droplets and Sprays

The study of droplets and sprays has developed rapidly over the past two decades because of their many important applications, from automobile engine combustion to drug aerosols.

This book addresses the complex subject of the interactions of droplets and sprays. It describes the behavior of an individual droplet in a spray, the behavior of a spray, and the criticial relationships between the two. In particular, it discusses the fluid mechanics and transport phenomena that govern the behavior of droplets and sprays in many important applications.

Along with a strong theoretical foundation, the book presents results in a way that will be useful for engineering practice, with summaries of key formulas and examples of various spray computations. Among topics covered are transient heating (or cooling) and vaporization (or condensation), multicomponent liquid droplet vaporization, near-critical and supercritical ambient conditions, interaction of droplets with turbulent or vortical structures, distortion of the spherical shape and secondary atomization of the droplets, and computational issues.

As an authoritative review of the science and technology of droplets and sprays, this book will be useful for graduate students, researchers, and practicing engineers.

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Preface

The fluid dynamics and transport of sprays is a rapidly developing field of broad importance. There are many interesting applications of spray theory related to power, propulsion, heat exchange, and materials processing. Spray phenomena also have natural occurrences. Spray and droplet behaviors have a strong impact on vital economic and military issues. Examples include the diesel engine and gas-turbine engine for automotive, power-generation, and aerospace applications. Manufacturing technologies including droplet-based net form processing, coating, and painting are important applications. Applications involving medication, pesticides and insecticides, and other consumer uses add to the impressive list of important industries that use spray and droplet technologies. These industries involve annual production certainly measured in tens of billions of dollars and possibly higher. The potentials for improved performance, improved market shares, reduced costs, and new products and applications are immense. An effort is needed to optimize the designs of spray and droplet applications and to develop strategies and technologies for active control of sprays in order to achieve the huge potential in this answer.

In this book, I have attempted to provide some scientific foundation for movement toward the goals of optimal design and effective application of active controls. The book, however, will not focus on design and controls. Rather, I discuss the fluid mechanics and transport phenomena that govern the behavior of sprays and droplets in the many important applications. Various theoretical and computational aspects of the fluid dynamics and transport of sprays and droplets are reviewed in detail. I undertook this writing because no previous treatise exists that broadly addresses theoretical and computational issues related to both spray and droplet behavior. There are other books that address either sprays on a global scale or individual isolated droplets on the fine scale. However, no other book has attempted a true integration of these two critically related topics. My research interests have focused on the theoretical and computational aspects of the spray problem. Therefore this monograph will emphasize those aspects. Major but not total attention will be given to the works of my research team since we have many research publications and review papers on this subject. On the basis of these research studies over the years, a decent comprehensive portrayal of the field is achievable. I have given emphasis to liquid-fuel droplets and to combustion applications since my experience is centered in that domain and, more importantly, since the high temperatures and rapid vaporization makes the dynamics of the phenomenon much more interesting and general. Rapidly vaporizing sprays have a richness of the scientific phenomena and several, often disparate, time scales. The discussions are

often also relevant to other important applications including materials processing, heat exchange, and coatings. Since the field of droplet and spray studies is still developing in terms of both science and technology, a critical review is undertaken here.

This monograph was developed largely on the basis of my lecture notes generated during several offerings of a graduate course. This treatise can serve both as a graduate-level text and as a reference book for scientists and engineers.

Attention is given to the behavior of individual droplets including the effects of forced convection due to relative droplet–gas motion, Stefan convection due to the vaporization or condensation of the liquid, multicomponent liquids (and slurries), and internal circulation of the liquid. Flow-field details in the gas boundary layer and wake and in the liquid-droplet interior are examined. Also, the determinations of droplet lift and drag coefficients and Nusselt and Sherwood numbers and their relationships with Reynolds number, transfer number, Prandtl and Schmidt numbers, and spacing between neighboring droplets are extensively discussed. Results from droplet analyses are presented in a manner that makes them useful as subgrid models in spray computations. Several examples of spray computations for which these models are used are presented. The two-phase flow equations governing spray behavior are presented in various forms and thoroughly discussed. Attention is given to issues of computational accuracy and efficiency. Various configurations for spray flows are studied. Droplet interactions with vortical and turbulent fields are analyzed. Droplet behavior at near-critical and supercritical conditions is discussed.

My interactions over the past two decades with twelve postdoctoral associates and sixteen graduate students on the subject of sprays have been very productive, stimulating, and instructive. These junior (at the time) collaborators are well represented in the references. They are Boris Abramzon, Suresh K. Aggarwal, Nasser Ashgriz, Rakesh Bhatia, C.H. "Jeff" Chiang, Gaetano Continillo, Jean-Pierre Delplanque, Amar Duvvur, Eva Gutheil, Howard Homan, Inchul Kim, Pedro Lara-Urbaneja, C.K. "Ed" Law, D.N. Lee, Steven Lerner, Jun Li, Mansour Masoudi, Constantine Megaridis, Carsten Mehring, Kamyar Molavi, Gopal Patnaik, Satya Prakash, M.S. Raju, Roger Rangel, David Schiller, Bartendu Seth, Douglas Talley, and Albert Tong. Exciting interactions with senior collaborators are also recognized: H.A. Dwyer, S.E. Elghobashi, G.J. Fix, B.R. Sanders, E. Suuberg, and S.C. Yao are identified here. Several federal funding agencies and industrial organizations have been supportive of my spray research; special recognition for continuing support goes to Julian Tishkoff of AFOSR, David Mann of ARO, and Gabriel Roy of ONR. Jennifer Chien, Brandi Hicks, Sue Kanda, and Lisa Rehbaum are acknowledged for their outstanding word-processing efforts. Special appreciation is extended to Sue Kanda for her role in proofreading and indexing.

Nomenclature

a	droplet acceleration; constant of curvature in stagnation point flow
a, b	constants in Eq. (1.3); variable parameters in Section 2.3, Eq. (2.70); also constant parameters in equation of state (9.3)
A	constant in Section 2.3; area
$\tilde{A}$	liquid-vortex strength
b_T, b_M	corrections to transfer number
B	Spalding transfer number
$\mathrm{Bo} = \rho_l a R^2/\sigma$	Bond number
c_l	liquid specific heat
c_p	specific heat at constant pressure
C_D, C_L	drag and lift coefficients
C_F	friction coefficient
d	droplet diameter; distance of vortex from droplet path
D	mass diffusivity; droplet center-to-center spacing; drag force
e	thermal energy; error; unit vector
E	activation energy
E_i	externally imposed electric field
f	Blasius function; droplet distribution function (probability density function)
f_H	defined by Eq. (8.10e)
f_i	fugacity of species i
F	drag force per unit mass on droplet; friction force
F_{Di}	aerodynamic forces per unit volume on droplets
F, G	functions defined in Section 2.3, Eqs. (2.67)
G	response factor for combustion instability; also Chiu group combustion number
g	acceleration due to gravity
g_1, g_2	functions defined in Section 2.3 by Eq. (2.66)

$\mathrm{Gr} = gR^3/\nu^2$	Grashof number
h	enthalpy; heat transfer coefficient; scale factors
k	nondimensional constant in Section 2.3; also turbulence wave number
k_E	generalized Einstein coefficient
K	constant in vaporization-rate law; constants in model equations; strain rate
$K(t, t-\tau)$	kernel in history integral, Chapter 8
L	latent heat of vaporization; differential operator
Le	Lewis number
m	droplet mass
$\dot{m}$	droplet mass vaporization rate
m_f	mass of fluid displaced by droplet or particle
m_p	mass of particle or droplet
$\dot{M}$	mass source term (rate per unit volume); vaporization rate per unit volume for spray
M_{A1}, M_{A2}	acceleration numbers defined by Eqs. (8.3) and (8.6)
n	droplet number density; direction normal to interface; fuel mass flux
n_i	number of moles of species i
N	number of droplets; ratio of droplet heating time to droplet lifetime
Nu	Nusselt number
p	pressure
Pe	Peclet number
Pr	Prandtl number
q_α	electric charge on droplet
$\dot{q}$	heat flux
Q	energy per unit mass of fuel
r	spherical radial coordinate
$\tilde{r}$	cylindrical radial coordinate
r_f	flame radius
R	droplet radius
R_2	droplet radii ratio
R	gas constant
$\mathrm{Re} = R\Delta U/\nu$	droplet Reynolds number (In discussions in which a Reynolds number based on diameter or some special properties is used, it will be specified in the text.)
s	nondimensional radius; transformed variable defined by Eq. (7.14b)
S	weighted area in numerical interpolation schemes; distribution function for radiative heat transfer

Sc	Schmidt number
Sh	Sherwood number
Sl	Strouhal number
t	time
T	temperature
u, v	velocity
U	free-stream velocity; particle or droplet velocity
v	velocity in the argument of distribution function; specific volume
V	volume in eight-dimensional phase space; liquid volume
$\dot{w}$	chemical reaction rate, fractional change per unit time
W	molecular weight
$\mathrm{We} = \rho_l R(\Delta U)^2/\sigma$	Weber number
x	spacial coordinate
X	mole fraction; position
y	normal coordinate in boundary layer
Y	mass fraction
z	spacial coordinate
Z	nondimensional temperature

Greek Symbols

α	thermal diffusivity
β	Shvab variables
ΔU	relative droplet velocity
γ	reciprocal of Lewis number; fraction of radiation absorbed at surface and in interior; ratio of specific heats
Γ	circulation
δ	distance ratio in Section 6.3; thickness of oxide layer; fraction of radiation absorbed at droplet surface; Dirac delta function
$\tilde{\delta}$	upstream distance for application of boundary condition
δ_{99}	the point, measured from the stagnation point, where 99% of the mass fraction variation has occurred
ε	species flux fraction; correction in Section 6.3 for application of ambient conditions; radiative emissivity
ε_0	electrical permittivity of a vacuum
η	Blasius coordinate; nondimensional radius
θ	void volume fraction; porosity
κ	reciprocal of characteristic length of temperature variation
λ	thermal conductivity; eigenvalues

μ	dynamic viscosity; chemical potential
ν	stoichiometric coefficient (mass of fuel per mass of oxygen); kinematic viscosity
ρ	density
ρ_r	ratio of particle (or droplet) density to gas density
$\bar{\rho}$	bulk density
σ	surface-tension coefficient; Stefan–Boltzmann constant, nondimensional vortex core size
τ	nondimensional time; viscous stress
τ_H	droplet-heating time
τ_L	droplet lifetime
τ^*	droplet-heating time with uniform temperature
ϕ	normalized stream function; entropy variable defined by Eq. (7.18)
ϕ_m	metal volume fraction
ϕ_r	ratio of acceleration numbers defined by Eq. (8.6)
φ	generic variable
Φ	fractional volume of fluid
χ	ratio of effective thermal diffusivity to thermal diffusivity; ratio of thermal diffusivities for slurry droplets
ψ	liquid volume fraction; stream function
ω	vorticity

Subscripts

0	initial condition
∞	condition at infinity
Al	aluminum property
b	boiling point Al (aluminum property); bubble
c	critical conditions
eff	effective value
F	fuel vapor
g	gas phase
H	related to thermal transfer
i	index for vectorial component; index for initial value
j	index for vectorial component
e	edge of boundary layer
L	lift
l	liquid
M	related to mass transfer

max	maximum
m	index for species; index for metal
mix	mixture
n, p	integers for numerical mesh points
N	nitrogen
ox	oxide
O	oxygen
p	particle
P	product
s	droplet-surface condition
T	related to thermal transfer
wb	wet bulb

Superscripts

k	index for droplet group
.	rate or time derivative
$'$	derivative

Contents

1

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.