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Computer Modeling of Sprays*

by

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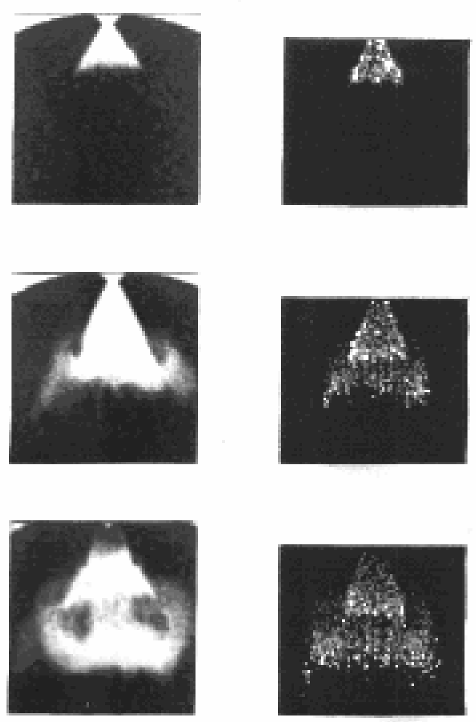
Pulsed hollow-cone spray simulations

Experiment **Model**



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PREFACE

Sprays are important in many industrial applications, and modeling of sprays can lead to significant improvements in the performance of spraying systems. The depth of analysis of sprays that is now possible with computer models is due, in part, to the fact that computer power has increased dramatically in the past few decades. This trend is likely to continue, and it is expected that CFD and spray modeling will become routinely used in engineering design and analysis.

The aim of these notes is to provide up-to-date and relevant information about computer modeling of sprays. The information should be useful as a review of the controlling phenomena in sprays not just to modelers, but also to researchers in spray technology in general.

The notes start by reviewing spray regimes and the governing equations for the two-phase (liquid-particle and gas) flows of interest in spray modeling, together with a discussion of, and motivation for, the use of submodels. Submodels for the atomization process are described next, followed by submodels for drop breakup and deformation, drop drag and turbulence effects on spray trajectories. This is followed by a discussion of drop collision and coalescence submodels, and drop vaporization and spray/wall impingement submodels. A brief review of spray combustion submodels then follows, together with an example of the application of computer modeling to the practical problem of predicting diesel engine emissions. The final section is devoted to a brief discussion of directions for future research needed to increase the accuracy of spray computations. The notes conclude with a (partial) listing of sources of available computer codes for spray modeling.

It should be noted that the literature on sprays is vast, and covers many disciplines. The perspective on spray modeling offered in these notes is the result of my own research which has been largely in the area of automotive applications. Modeling of automotive sprays is particularly challenging since the sprays perform in hostile, optically inaccessible environments. This makes it difficult to obtain experimental data for assessing the performance of models. The sprays are usually injected at high velocities and are dense, vaporizing and they often impinge on walls.

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NOMENCLATURE

a	Parent drop or jet radius
A	area
b	collision cross-section, impact parameter
B	mass transfer number
B_0	drop breakup model size constant
B_1	drop breakup model time constant
C_1, C_2	integration constants
C_D	discharge coefficient, drag coefficient
C_v, C_p	specific heats at constant volume and pressure, constants
C_μ, $C_{\varepsilon\iota}$,	turbulence model constants
d	drop diameter
d_L	ligament diameter
D	diffusion coefficient, turbulent diffusivity
D_{max}	drop spreading diameter
D, D_1, D_2	drop breakup time constants
E_{12}	collision efficiency
f	drop distribution function
F	Helmholtz free energy, rate of momentum transfer
F	drop acceleration
g	acceleration of gravity
h	convective heat transfer coefficient, enthalpy
H	sheet thickness
I	unit dyadic tensor
I	internal energy
I_0, I_1	modified Bessel functions of the first kind
J	heat flux vector
k	liquid thermal conductivity, turbulence kinetic energy, wave number
K_0, K_1	modified Bessel functions of the second kind
l/d	nozzle passage length-to-diameter ratio
ℓ	wave number, turbulence length scale
L	sheet or core breakup length, latent heat of vaporization
m	mass
n, N	drop number
Nu	Nusselt number
n	normal vector
p	random number uniform on the interval 0 to 1
P	pressure
Pr	Prandtl number
q	velocity magnitude (speed)
Q	heat transferred
r	drop radius
r_{32}	drop Sauter Mean Radius (SMR)

R	radius of curvature, rate of change of drop radius, gas constant, reference radius
Re	Reynolds number $U r / \nu$
s	sheet thickness
S	length
Sc	Schmidt number
Sh	Sherwood number
t	time, drop breakup time
t	tangent vector
T	temperature
u	gas velocity vector
u'	gas turbulence velocity vector
U	drop-gas relative velocity $\|\mathbf{u}+\mathbf{u}'-\mathbf{v}\|$, injection velocity
v	drop velocity vector
v	normal velocity component
V	velocity, volume
w	interface velocity vector
W	turbulence energy source, molecular weight
We	Weber number $\rho U^2 r / \sigma$
x	physical coordinate vector
X	penetration distance
y	physical coordinate, drop distortion parameter
Y	mass fraction
z	physical coordinate
Z	Ohnesorge number $\nu (\rho/\sigma r)^{1/2}$, mass transfer correction
α	impingement angle, thermal diffusivity
γ	drop radius ratio, r_1/r_2
δ	layer thickness, poppet diameter
Δ	length scale
ΔP	injection pressure
Δt	numerical timestep
ΔT	temperature change
ε	turbulence kinetic energy dissipation rate
η	wave amplitude
θ	void fraction, spray (half) angle
λ, Λ	wavelength, film thickness
μ	dynamic viscosity
ν	kinematic viscosity
ν_{12}	collision frequency
ρ	density
σ	surface tension coefficient
τ	drop vibration period, time scale, shear stress tensor breakup time, relaxation time
ϕ	drop deflection angle in plane of surface,

	potential function, equivalence ratio
Φ	extensive quantity
φ	intensive quantity
Ψ	stream function, azimuthal deflection angle
ω, Ω	wave growth rate

Subscripts

1	liquid, larger drop in collision
2	gas, smaller drop in collision
bu	breakup
coll	collision
d	drop
f	final
g	gas phase
i	incoming
l	liquid
m	species index, momentum
max	maximum value
n	normal component
o	initial, outgoing
res	residence
s	surface
x	based on x

Superscripts

.	time rate of change
-	mean quantity
c	combustion
s	spray

1. INTRODUCTION

Sprays are involved in many practical applications, including the process industries, coating applications (e.g., spray painting and crop spraying), spray combustion in rockets, gas turbines and diesel engines, and port fuel injection in spark-ignited engines. To be able to describe sprays it is necessary to obtain a detailed understanding of spray subprocesses. The atomization process has a strong influence on spray vaporization rates because it increases the total surface area of liquid fuel greatly. Fast vaporization may be desirable in certain applications, but undesirable in others, where the liquid is required to penetrate and impinge on a target. The trajectories of the spray drops are governed by the drop's injected momentum, drag forces and interactions between the drops and the surrounding gas. Detailed modeling of these and other spray processes can lead to significant improvements in performance, quality of product, and reduction of emission of pollutants (Chigier, 1993). The status of current models is reviewed in these notes.

1.1 Computer Models

Current computer models solve the conservation equations for the transient dynamics of vaporizing fuel sprays interacting with flowing multi-component gases which are undergoing mixing, ignition, chemical reactions, and heat transfer in arbitrary shaped (moving) geometries (e.g., reciprocating engine piston cylinders), including the effects of turbulence and wall heat transfer. The depth of analysis of sprays now possible using computer modeling is due, in part, to the fact that computer power has increased dramatically in the past few decades. This trend is likely to continue. In fact, the stated goal of supercomputer manufacturers is to produce teraflop computers (10^{12} floating-point operations per second) by the second half of this decade. It has been estimated that a medium size scientific computation that now takes 5 hours on a Cray YMP running at 200 megaflops (i.e., 28 years on a Macintosh at 0.004 megaflops) would require less than 4 seconds on a teraflop computer (Karniadakis and Orszag, 1993).

However, even with the expected advances in computer power over the next decades, computer models are still unlikely to be entirely predictive. This is due to the wide range of length and time scales that characterize sprays. For example, in a 3-dimensional finite-difference computation, to begin to resolve the flow-field around 10 μm diameter drops (typical of the drop Sauter mean diameter in combustion applications) in a 10 cm diameter combustion chamber requires about 10^{12} grid points (see Fig. 1.1). Due to limitations of computer storage and run times, a practical upper-limit for current super-computers is about 10^5 grid points. The missing 7 orders of magnitude will not be realized in the next decade, even with the most optimistic projections about computer power increases.

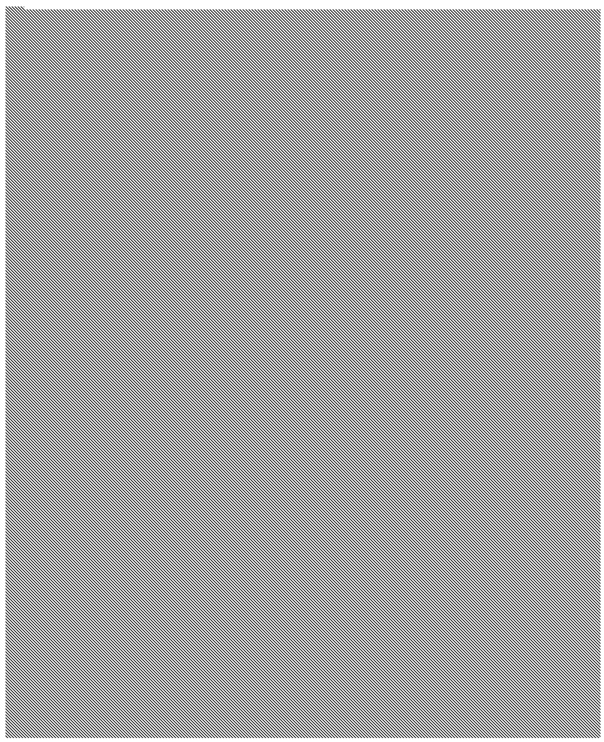

Fig. 1.1 Accurate submodels are needed for detailed spray processes since drop sizes are much smaller than practical computer numerical grids.

1.2 Submodels

To be able to describe sub-grid scale physics it is necessary to introduce submodels into spray computations for processes that occur on time and length scales that are too short to be resolved. The use of submodels to describe unresolved physical processes necessarily introduces empiricism into computations. However, the compromise between accuracy and feasibility of computation is justified by the insight that model calculations offer. Confidence in the model predictions and knowledge of their limitations is gained by comparison with experiments.

Sub-processes that need to be modeled in practical sprays include atomization, drop distortion and drag, drop breakup and collision/coalescence, drop turbulence dispersion and turbulence modulation effects, drop vaporization, and spray/wall interaction. In addition, submodels need to be developed or refined to describe other important physical processes, such as the effect of nozzle cavitation and turbulence on the atomization process, multi-component fuel drop vaporization, drop micro-explosion, spray ignition and combustion, soot and pollutant formation, and others. Realistic physical models are required to describe each of these processes, and current progress in the development of these models is discussed below.

Analytic models and controlled experiments that isolate the relevant processes have been used to generate correlations to form the basis of submodels. Individual models have been developed starting from simplified theoretical models or experiments that isolate that particular process. However, the accuracy of computer code predictions, made using combinations of submodels to describe the performance of the overall system, must still be assessed by comparisons with detailed and informative experiments (Reitz, 1991a). Once verified, the computer models can be used as design tools by the industry to reduce product development time and costs. An important benefit of the use of computer models is that they can give insights about key processes that would be difficult to obtain in any other way, since direct measurement is often not feasible.