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Physical modelling and advanced simulations of gas–liquid two-phase jet flows in atomization and sprays

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ABSTRACT

This review attempts to summarize the physical models and advanced methods used in computational studies of gas–liquid two-phase jet flows encountered in atomization and spray processes. In traditional computational fluid dynamics (CFD) based on Reynolds-averaged Navier–Stokes (RANS) approach, physical modelling of atomization and sprays is an essential part of the two-phase flow computation. In more advanced CFD such as direct numerical simulation (DNS) and large-eddy simulation (LES), physical modelling of atomization and sprays is still inevitable. For multiphase flows, there is no model-free DNS since the interactions between different phases need to be modelled. DNS of multiphase flows based on the one-fluid formalism coupled with interface tracking algorithms seems to be a promising way forward, due to the advantageous lower costs compared with a multi-fluid approach. In LES of gas–liquid two-phase jet flows, subgrid-scale (SGS) models for complex multiphase flows are very immature. There is a lack of well-established SGS models to account for the interactions between the different phases. In this paper, physical modelling of atomization and sprays in the context of CFD is reviewed with modelling assumptions and limitations discussed. In addition, numerical methods used in advanced CFD of atomization and sprays are discussed, including high-order numerical schemes. Other relevant issues of modelling and simulation of atomization and sprays such as nozzle internal flow, dense spray, and multiscale modelling are also briefly reviewed.

Contents

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Nomenclature

a	parent droplet or blob radius
A	surface area
A_f,A_p	droplet/particle frontal area
A_R	Arrhenius kinetics constant
b	collision impact parameter
b_R	Arrhenius kinetics constant
B_0, B_1	"wave" breakup model constants
B_M	mass transfer number
c	specific heat
C	constant
C_D	drag coefficient
C_p, C_v	specific heats at constant pressure and volume
C_s	Smagorinsky constant
C_ν, C_ε	constants in the subgrid turbulent kinetic energy equation
d	particle cloud diameter
D	diffusion coefficient; energy dissipation rate; droplet diameter; distribution function
$\mathcal{D}$	rate of deformation tensor
e	specific total energy
E	error
f	function; flow variable
$\boldsymbol{f}$	arbitrary vector field
F	fuel; force
$\mathbf{F}$	force
$\mathbf{g}$	specific body force (gravitational acceleration)
G	scalar in the level-set method
h	heat flux; heat transfer coefficient; grid size
$h_{v,s}$	evaporated enthalpy at droplet surface
H	heaviside function
I	specific internal energy; indicator function
k	turbulent kinetic energy
k_R	reaction rate
l	eddy size
L	large (integral) length scale
L_v	latent heat for vaporization
m	mass
$\boldsymbol{m}$, $\boldsymbol{n}$	unit normal vector
n, N	number
Nu	Nusselt number
O	oxidizer
p	probability
P	product; probability density function; weighted projection
Pr	Prandtl number
q	random number between (0, 1); random scalar
Q	heat transfer rate; storage locations
$\dot{Q}$	heat release source term
r	droplet radius
R	time rate of change of droplet radius; gas constant
R_c, R_v	carrier gas and vapor gas constants
Re	Reynolds number
S	strain rate tensor; source term; surface area
Sc	Schmidt number
Sh	Sherwood number
t	time
T	Taylor parameter; gas temperature
T_A	activation temperature
T_d	droplet temperature
$\dot{T}_d$	time rate of change of temperature
$\mathbf{u}$	gas-phase velocity vector
U	gas velocity at the liquid surface
v	particle velocity
$\mathbf{v}$	droplet velocity vector
V	droplet volume; domain; diffusion velocity
Vol	volume of the cell
w	weighting
$\mathbf{w}$	local relative velocity between the droplet and the surrounding gas ($\mathbf{v}-\mathbf{u}$)
W	molecular weight
$\dot{W}^s$	subgrid turbulence effects due to spray
We	Weber number
x	droplet position vector
X	mole fraction; random number
x_p	particle centroid
X_i	droplet transient location
y	droplet distortion from sphericity
Y	mass fraction
$\dot{y}$	time rate of change of the droplet distortion (oscillation velocity)
$\ddot{y}$	time rate of change of oscillation velocity
Z	Ohnesorge number

Greek

α	(laminar) thermal diffusivity; linking parameter; droplet variable
β	heat transfer correction coefficient
χ	molar fraction
δ	Kronecker delta function
δ_ε	smoothed delta function
Δ	incremental amount
∇	gradient operator
ε	dissipation rate of turbulent kinetic energy
γ	drop radius ratio (r_1/r_2); ratio of specific heats
Γ	Fickian diffusion coefficient; interface
η_K	Kolmogorov scale
κ	von Karman constant; curvature
θ	diffusive mass flux
λ	frequency of subgrid stirring; thermal conductivity
Λ	wavelength
μ	dynamic viscosity
ν	kinematic viscosity
ν_{12}	collision frequency
ρ	density
σ	surface tension
Π	velocity–pressure gradient correlation
Θ	viscous work
τ	breakup time; wall shear stress; time scale
ϕ	area flux
Φ	species mass flux; volume fraction