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Coupling multicomponent droplet evaporation and tabulated chemistry combustion models for large-eddy simulations

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ABSTRACT

An evaporation model for multicomponent fuels and emulsions is implemented in OpenFOAM within the Euler–Lagrangian formulation. The model is suitable for pressures typical of heavy duty gas turbines, up to 30 bar, and considers an increased evaporation rate of the most volatile component when the droplet temperature reaches its boiling temperature. Evaporation of emulsion droplets is modeled following a shell approach, assuming that the water in the droplet core does not evaporate. A diffusivity model is introduced to account for the transport of the dispersed phase from the core to the outer shell. The combustion model is based on the Flamelet Generated Manifold approach. The mixture fraction is calculated from the species mass fractions to couple it with the evaporation model. Flamelet tables are created for different enthalpies and mixture fractions so that they can be used in non-premixed simulations. The thermo-chemistry model considers up to two fuel components by using 4-D tables. Experimental data for n-decane droplets are used to validate the evaporation model. Results from the combustion model are compared with the detailed chemistry solutions. Following the separate evaluation of each model, 1-D spray simulations for 0% and 10% initial water contents are performed to verify the coupling between the models, so that they can be applied to partially pre-vaporized spray flames.

1. Introduction

Numerical simulations of heavy duty gas turbines combustion systems are an important part of the development process. They can provide an insight of the physics involved within the system and aid the design. Particularly with the use of liquid fuels, due to the more complex physics involved than those in gas operation. The present article focuses on the evaluation and coupling of a multicomponent droplet evaporation model and a tabulated chemistry combustion model. This model chain aims to predict the shape and the stability of a partially pre-vaporized diluted emulsified spray flames at heavy duty gas turbine conditions.

In the simulation of liquid sprays within the Euler–Lagrangian formulation, the injection and atomization models result in a statistical distribution of particles sizes downstream the injection point. As the volatility of the fuel increases, either because of the use of a lighter fuel component or an increased droplet temperature, the use of an evaporation model becomes necessary due to the phase change of the liquid phase. The objective of this model is to predict the amount of evaporated mass from each liquid species transferred to the gas phase and the heat absorbed by the liquid phase. This is done based on the properties of the liquid and gas phases as well as on the flow structure inside and around the droplet.

In evaporation modeling, gas phase quasi-steadiness and spherical symmetry is usually assumed [1,2]. The classical evaporation model was proposed by Godsave [3] and Spalding [4], considering a steady state evaporation by assuming a constant droplet temperature. This model is also know as the d^2-law.

Unsteady effects were investigated by Law [5] and Hubbard et al. [6], assuming a spatially uniform time-varying droplet temperature (infinite liquid conductivity). A non-uniform temperature inside the droplet was modeled by Sazhin [7], assuming a polynomial profile. The 1-D model by Abramzon and Sirignano [8] uses an effective liquid conductivity in the energy equation to account for internal recirculation, which is calculated assuming a Hill vortex flow inside the droplet. Influence of natural and force convection are accounted by using correlations for the Sherwood and Nusselt numbers ([9,10]), or by applying corrective factors to the model to account for the formation of a film layer around the droplet [11]. Non-unity Lewis number of the gas phase, Stephan flow and spray interaction effects can also be accounted for [8,2].

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Nomenclature

Symbols

A	parameter of the Peng–Robinson equation of state
B	parameter of the Peng–Robinson equation of state
b	molar fraction of oxygen in air
B_m	mass transfer number
c	flame progress variable
C_nH_m	primary hydrocarbon species
C_p	heat capacity at constant pressure
C_pH_q	secondary hydrocarbon species
CO	carbon monoxide
CO_2	carbon dioxide
D	diffusivity
d	droplet diameter
dx	axial cell size of a 1-D mesh
F	artificial flame thickening factor
f	fugacity
g	gravity acceleration
Gr	Grashof number
h	sum of the sensible and the chemical enthalpies
H_2	hydrogen
H_2O	nitrogen
K	coefficient to account for the dispersed phase convective transport to the droplet shell
k_B	Boltzmann constant
L_v	latent heat of vaporization
M	molecular weight
m	number of hydrogen atoms in a molecule of the primary fuel species
M_d	droplet mass
n	number of carbon atoms in a molecule of the primary fuel species
N_2	nitrogen
Nu	Nusselt number
O_2	oxygen
P	pressure
p	number of carbon atoms in a molecule of the secondary fuel species
q	number of hydrogen atoms in a molecule of the secondary fuel species
Sc	Schmidt number
Sh	Sherwood number
Su	laminar flame speed
T	temperature
t	time
U	velocity magnitude
V	volume
W	secondary species mass fraction to mixture fraction ratio
Y	mass fraction
Z	mixture fraction
Z_c	compressibility factor

Greek symbols

α	thermal conductivity
β	amount of moles of the CO product species
χ	molar fraction
δ	amount of moles of the H_2 product species
$\dot{\omega}$	source term
ϵ	amount of moles of the CO_2 product species
η	amount of moles of the H_2O product species
γ	activity coefficient
μ	dynamic viscosity
ν	amount of moles of the secondary fuel species
Φ	fugacity coefficient
ϕ	equivalence ratio
ρ	density
Ξ	wrinkling coefficient
ζ	amount of moles of the O_2 product species

Abbreviations

AFR	air-to-fuel ratio
BC	boundary conditions
DNS	direct numerical simulation
EBU	eddy break-up
FGM	flamelet generated manifold
HLB	hydrophilic–lipophilic balance
O/W	oil-in-water
PDF	probability density function
SCRS	simple chemical reacting system
W/O	water-in-oil

Subscripts

∞	at the far field
a	air
b	burnt mixture
$boil$	at the boiling point
$core$	in the core region of an emulsion droplet
d	droplet
eff	effective
eq	equilibrium conditions
exp	experiments
f	fuel
FC	forced convection
$frac8$	fraction
g	gas phase
$h,lagr$	enthalpy transferred from the lagrangian parcels
i	each species of the droplet composition
in	at the inlet boundary
j	species whose boiling temperature equals the droplet temperature
l	liquid phase
lam	laminar flame
$M,lagr$	mass transferred from the lagrangian parcels
NC	natural convection
s	at the droplet surface
sat	at the saturation pressure
sgs	sub-grid scale
$\sim$	simulation
st	stoichiometric conditions
$U,lagr$	momentum transferred from the lagrangian parcels
ub	unburnt mixture
w	water species
$Y,lagr$	species mass fraction transferred from the lagrangian parcels

Additionally, ambient pressure plays a significant role in droplet evaporation, especially when it is near or above the liquid critical pressure [12], since it affects the liquid and gas phase properties, as well as the vapor–liquid equilibrium. Several authors [13,12,14–17] employ the Peng–Robinson equation of state to calculate the fugacity of the liquid and gas phases to solve the vapor–liquid equilibrium. A model for evaporation of oxygen droplets at sub-, trans- and supercritical conditions was developed by Delplanque and Sirignano [18] and applied to the evaporation of parallel droplet streams in [19]. A numerical investigation on the evaporation oxygen droplets at several high temperatures and pressures, from subcritical to supercritical conditions, was