

ADVANCED MODELS FOR TURBULENT SPRAY AND COMBUSTION
SIMULATIONS

By

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ABSTRACT

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A high-fidelity two-phase large eddy simulation (LES)/filtered mass density function (FMDf) model is developed and used for detailed simulations of turbulent spray breakup, evaporation and combustion. The spray is simulated with Lagrangian droplet transport, stochastic breakup, wake, collision/coalescence and finite rate heat and mass transfer submodels. The spray/droplet model is used together with a compressible LES gas flow model for numerical simulations of high pressure liquid jets sprayed into a high temperature and pressure gas chamber. Various non-evaporating and evaporating sprays at different ambient gas pressures and temperatures are simulated. The numerical results are compared with the available experimental data for global spray variables such as the spray penetration length and droplet Sauter mean diameter (SMD). A broad spectrum of droplet sizes is generated by the complex and coupled effects of the gas flow turbulence, droplet breakup and evaporation. Droplet-wake interactions are shown to play an important role in the spray evolution. The effect of subgrid turbulence model on the global spray features, like the spray penetration, is also very significant at lower gas temperatures. The interaction of the induced gas flow turbulence with the spray is studied at different chamber densities and temperatures as well as different nozzle sizes and injection pressures. It is indicated that the local rate of evaporation and its interaction with the gas density field are the key factors that control the induced gas turbulence and its interaction with the spray. It is shown that spray with a larger nozzle induces

higher turbulence due to increase in local evaporation rate of small droplets by the higher entrained gas. Our results also indicate that spray penetration remains unchanged with variation in injection pressure due to competing factors of evaporation and vapour convection. The developed spray LES model is coupled with the two-phase FMDF model for simulation of high speed spray combustion. The FMDF is a subgrid-scale probability density function (PDF) model for LES of turbulent reacting flows and is obtained by the solution of a set of stochastic differential equations by a Lagrangian Monte Carlo method. Complex skeletal kinetics models are used for the chemical reaction together with in situ adaptive tabulation (ISAT) and chemistry workload balancing for efficient parallel computations. Simulations of evaporating sprays with and without combustion indicate that the two-phase LES/FMDF results are consistent and compare well with the available experimental data for the ignition delay time and flame liftoff lengths at different ambient gas temperatures and oxygen concentrations. It is shown that for low to moderately high ambient gas temperatures, the auto-ignition occurs at the tip of spray vapour jet where there is considerable spray-induced gas turbulence and fuel-air mixing. The LES/FMDF results for ignition delay show more sensitivity to the chemical kinetics model at lower gas temperatures due to slower reaction and stronger turbulence-chemistry interactions. The spray controlled flame tends to move away from a diffusion flame structure toward a premixed one as the oxygen concentration decreases and/or the ambient gas temperature increases because of changes in spray-induced turbulence and mixing. A moderately dense droplet laden planar jet is also simulated by the LES/FMDF model for detailed study of the liquid volume fraction effects. It is indicated that the neglect of liquid volume fraction will lead to excessive evaporation and turbulence modulation. It is shown that for LES/FMDF model to be consistent and accurate, it is necessary to include the volume fraction into the FMDF equation.

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KEY TO SYMBOLS AND ABBREVIATIONS

Roman Symbols

$\mathbf{A}$	droplet surface area vector, m^2
$(\frac{A}{F})_{st}$	stoichiometric ratio of ambient gas to fuel
F_j	test level flux of kinetic energy, kg/ms^2
$B_{M\alpha}$	Spalding mass transfer number of species α
$\dot{Q}$	heat of reaction, $J/m^3.s$
$Q(\alpha)$	fragmentation spectrum
B_T	Spalding heat transfer number
U	velocity magnitude, m/s
c_ϵ	subgrid dissipation coefficient
c_ν	subgrid stress coefficient
c_k	subgrid transport coefficient
c_ϕ	subgrid scalar mixing coefficient
c_{sgs}	subgrid time scale coefficient
D	mass Diffusion coefficient m^2/s
d_p	droplet diameter, m
E	total energy, J/kg
e	internal energy J/kg
f_1	drag factor
f_2	evaporative heat transfer factor
F_L	filtered mass density function
f_j	subgrid flux of kinetic energy, kg/ms^2
Z_j	flux difference between different filters, kg/ms^2
G	filtering function, $1/m^3$
H	total enthalpy, J/kg
h	sensible enthalpy J/kg

h_v^0	vapour enthalpy of formation, J/kg
c_l	liquid specific heat capacity, J/kg.K
c_p	specific heat capacity at constant pressure, J/kg.K
H_i^{sgs}	subgrid energy flux, $J/m^2.s$
J_i^α	mass flux of species α , $kg/m^2.s$ or heat flux ($\alpha = N_s + 1$), $J/m^2.s$
k_{sgs}	subgrid kinetic energy, m^2/s^2
k_{tst}	test level kinetic energy, m^2/s^2
L_v	latent heat of evaporation, J/kg
m	mass, kg
$\dot{m}_p$	mass flow rate of droplet, kg/s
m_p	droplet mass, kg
MW	molecular weight, kg/mol
N_{core}	number of cores for parallel processing
N_G	total number of grid points
N_{MC}	total number of Monte Carlo particles
N_{PC}	total number of parcels
$N(r, t)$	number of droplets with size $\leq r$
N_s	number of species
$N(t)$	total number of droplets at time t
Nu	Nusslet number
p	pressure, Pa
Pr	Prantl number
Pr_t	turbulent Prantl number
P_{sgs}	production of subgrid kinetic energy, $J/m^3.s$
q_i	heat flux, $J/m^2.s$
R	gas constant, J/kg.K
r	droplet radius, m
$\dot{r}_s$	rate of change of droplet radius, m/s
Re_{bw}	blowing Reynolds number
Re_{sl}	slip Reynolds number

R^0	universal gas constant, J/mol.K
$\dot{S}_\alpha$	reaction rate of species α , 1/s or heat of reaction $\alpha = N_s + 1$, J/kg.s
$\dot{S}_\alpha^{sp}$	spray species α source term, kg/s.m ³
Sc	Schmidt number
$\dot{S}_\alpha^{comp}$	compressibility source term to enthalpy, J/kg.s
Sc_t	turbulent Schmidt number
$\dot{S}_E^{sp}$	energy spray source term, J/m ³ .s
$\dot{S}_h^{sp}$	enthalpy spray source term, J/m ³ .s
Sh_α	Sherwood number of species α
$\dot{S}_{Mass}^{sp}$	spray mass source term, kg/s.m ³
$\dot{S}_{ksgs}^{sp}$	spray subgrid kinetic energy source term, J/m ³ .s
S_{ij}	strain rate, 1/s
T	temperature, K
t	time, s
T_{sgs}	subgrid transport of subgrid kinetic energy, J/m ³ .s
$\mathfrak{S}$	droplet size cumulative distribution function
u_i	velocity component, m/s
u_{rel}	relative velocity of droplet, m/s
u_{relbu}	breakup relative velocity scale, m/s
u_{sgs}	subgrid velocity, m/s
u^*	stochastic subgrid velocity at droplet location, m/s
u_Θ	liquid surface velocity, m/s
V	volume, m ³
v	droplet radial internal velocity, m/s
w_p	number of droplets in a parcel
We	Weber number
dW_i	increment of Wiener process, s ^{1/2}
$w^{(n)}$	weight of Monte Carlo particle
x_i	spatial coordinate, m

Greek Symbols

α	random number between zero and one
β	non-dimensional evaporation parameter
Γ	diffusivity, <i>Pa.s</i>
Ω_m	mixing frequency, 1/s
Θ	gas identifier
ϖ	mean fractional value of free stream velocity in the wake of a sphere
χ	logarithm of ratio of radii of daughter droplet to parent drop
δ	Dirac delta function
δ_{ij}	Kronecker delta function
Δ	filtering size, m
δ_s	characteristic shear thickness, <i>m</i>
ϵ	mean viscous dissipation, <i>J/m³.s</i>
ϵ_{sgs}	dissipation of subgrid kinetic energy, <i>J/m³.s</i>
ε	mixture equivalence ratio
Λ	velocity reduction factor of droplet-wake interaction
λ	thermal conductivity, W/K
Ξ	mixture fraction
ν_t	turbulent viscosity, <i>m²/s</i>
ϕ_α	scalar α (mass fraction of species α or mixture enthalpy (J/kg))
ψ_α	sample space of scalar α (species mass fraction and enthalpy)
ρ	density, <i>kg/m³</i>
σ	surface tension, N/m
τ_{ij}	viscous stress, <i>N/m²</i>
τ_{bu}	breakup time scale, <i>s</i>
τ_L^*	subgrid time scale at droplet location, s
τ_p	droplet response time, <i>s</i>
τ_{delay}	ignition delay time, <i>s</i>
τ_{evap}	droplet evaporation time scale, <i>s</i>
τ_{ij}^{sgs}	subgrid stress, <i>N/m²</i>

τ_{sgs}	subgrid time scale, s
τ_{st}	droplet stokes time scale, s
θ	angle
ς	logarithm of fragmentation parameter
ϑ	normalized drift velocity
ξ	fine grained density
ζ_i	random numbers from standard Gaussian distribution

Subscripts

a	ambient
co	co-flow of planar jet
cr	critical
F	Fuel
g	gas
∞	free stream
inj	injection
jet	planar jet flow
lead	leading droplet
l	liquid
p	droplet
s	droplet surface

Superscripts

+	Lagrangian
sgs	subgrid scale
sp	spray

Conventions

$\langle \rangle_{az}$	azimuthal averaging operation
$\langle \rangle_L$	Favre-filtering operation
$\langle \rangle_{\hat{l}}$	test filtering operation
$\langle \rangle_l$	filtering operation
$\langle \rangle_t$	time averaging operation

Abbreviations

D	dimensional
DI	direct injection
DNS	direct numerical simulation
ECN	engine combustion network
EGR	exhaust gas recirculation
FD	finite difference
FMDF	filtered mass density function
IC	internal combustion
ISAT	in situ adaptive tabulation
K-H	Kelvin-Helmholtz
LES	large eddy simulation
MC	Monte Carlo
ODE	ordinary differential equation
PDF	probability density function
PSR	perfectly stirred reactor
P-URAN	partitioned uniform random
RANS	Reynolds averaged Navier Stokes
r.m.s	root mean square
SDE	stochastic differential equation
SGS	subgrid scale
SMD	Sauter mean diameter
TAB	Taylor analogy breakup
TCI	turbulence chemistry interaction

Chapter 1

Large Eddy Simulation of Turbulent Spray Breakup and Evaporation

1.1 Introduction

The fuel spray behaviour in combustion and propulsion systems is dependent on a significant number of parameters like the fuel supply operating pressure and temperature, the nozzle geometry, the physical and chemical properties of the liquid or droplets, the flow turbulence and all parameters controlling the heat and mass transfer between phases. For example, depending on the surface tension or Weber number, the liquid jet and droplet breakup may take place very differently through mechanisms like vibrational breakup, bag and stamen breakup, sheet stripping, or catastrophic breakup [1],[2],[3],[4] and [5]. Several different models have been proposed for the liquid breakup [6],[7]. Reitz [8] used Taylor's wave equation to estimate the wave length and growth rate of the most unstable waves on the surface of a parent drop, thereby defining the conditions where the amplification of the waves would lead to the breakup of the drop. Alternatively, the Taylor analogy breakup (TAB) model represents the oscillations of parent drops as a spring mass system, with breakup presumed to occur when the oscillations in the parent drop exceed a critical value

[9]. These two models are considered as standard models for spray breakup prediction. Recently, stochastic breakup models have gained some popularity, due to their ability to predict the essential global features of sprays without being computationally too expensive [10],[11],[12], [13] and [14]. The closure problems in the stochastic models are usually resolved with submodels for the droplet breakup frequency and the distribution of droplet radii after the breakup. Following Kolmogorov’s concept of viewing the particle breakup as a discrete random process, the atomization of liquid droplets at high liquid to gas velocity ratios may be modelled as uncorrelated breakup events, independent of the initial droplet size [15]. Gorokhovski and Saveliev [11] reformulated Kolmogorov’s discrete model of breakup in the form of a differential Fokker–Planck equation for the probability density function (PDF) of droplet radii. The probability to break each parent drop into a certain number of parts is assumed to be independent of the parent drop size, which according to central limit theorem leads to a log normal distribution for the particle size at long times. Apte et al. [12] applied this approach to non-evaporating sprays in their large eddy simulation (LES) model by relating the drop fragmentation intensity spectrum to the parent drop Weber number. They computed the breakup frequency from the droplet Stokes time and the mean viscous dissipation. Liu et al. [13] proposed a finite stochastic breakup model for pre-filming air-blast atomizers. In this model, a breakup can occur only if the size of the parent drop is larger than a critical diameter and the fragmentation generates two droplets of diameters chosen randomly from a uniform probability distribution. Jones and Lettieri [14] simulated each breakup event through a “Poisson release process.” Their breakup frequency consisted of deterministic and stochastic parts and was based on a breakup velocity, which presumed to be proportional to the difference between the surface pressure forces arising from the turbulent fluctuations and the restoring forces of surface tension. In their model,

the fragmentation generates two characteristic diameters for the daughter droplets from a surface energy distribution. Experimental studies on daughter size distributions of breaking drops ([16],[17],[18] and [19]) show that unlike bubbles, the binary breakup assumption is not reasonable for liquid drops. Therefore a breakup model capable of generating droplets with different sizes as proposed by Gorokhovski and Saveliev [11] is preferred. Following this approach, the breakup frequency is computed in this work by a breakup velocity that is based on the Lagrangian gas to droplet relative velocity fluctuations. The fragmentation intensity spectrum is assumed to be Gaussian in accordance to Kolmogorov theory [15].

Generally, there are two different types of computational models for sprays: (i) grid based Eulerian, and (ii) particle based Lagrangian models. Typical spray combustion systems often involve a dilute distribution of millions of small droplets in a turbulent environment. The liquid phase in most of these systems is then far from being a continuum and it is more appropriate to treat it as a collection of dispersed droplets. In the Lagrangian models, like that proposed by Dukowicz [20] the spray is represented by discrete computational particles which may sometimes represent individual droplets or a group of droplets possessing the same characteristic size, velocity, composition, etc. The numerical simplicity and the non-diffusive character of the Lagrangian models make them attractive for spray simulations as compared to grid based Eulerian models. However, Lagrangian spray models are often used together with an Eulerian model for the gas phase (which is normally turbulent). With such a hybrid Eulerian-Lagrangian methodology, phenomenological “submodels” are required to account for various physical processes taking place at subgrid scales. For the very dense or primary breakup region of spray, Eulerian-Eulerian computational models may be used [21]. These types of models are expected to better capture the liquid jet breakup ([22],[23] and

[24]) but they are not currently practical and cannot be employed for high speed evaporating and reacting sprays in realistic combustion systems [25], [21] and [6]. For these systems, the initial development of liquid jet is often modeled by a set of round liquid blobs injected from the nozzle with similar mass flow rate. The initial diameter and velocity of these blobs are calculated from experimental correlations that are dependent on the nozzle exit diameter and discharge coefficient [26] and/or through mechanisms of surface instabilities ([27] and [8]), drop shedding [28] and cavitation [29]. These large drops then go through a series of breakup processes to mimic the primary and secondary breakup. This is based on the reasonable assumption that the atomization and fragmentation of liquid jet, blobs or drops are indistinguishable processes within the dense liquid core region near the injector nozzle exit. The blob model is used in this work.

A key factor in the prediction of high speed liquid jet spray is the accurate modelling of gas flow interactions with the spray and droplets. For the gas flow simulations, spray models rely predominantly on the Reynolds-averaged Navier-Stokes (RANS) ([6],[30]) method. However, because of unsteady and turbulent nature of the gas flow generated by high speed sprays and other inherently transient physical and chemical processes involved in a typical engineering system, LES is expected to be more suitable than RANS, even though the latter remains to be useful for the design of practical systems. While droplet time and length scales are normally smaller than those of the resolved flow and LES grid size, they may still be larger than the smallest turbulent (Kolmogorov) scales. In this situation, the unresolved subgrid turbulent motions can have a significant effect on the droplet motion in LES. Stochastic, Langevin type models have been developed to account for these effects ([31],[32] and [33]).

Since liquid-gas interactions are important to both gas phase turbulence and droplet dis-

persion, and since droplets are interacting mostly with the gas phase turbulence at subgrid level, it is also important to properly model the physical effects of spray and droplets on the subgrid scale (SGS) flow quantities such as the SGS kinetic energy ([34] and [35]). This can be done by solving the subgrid kinetic energy equation with the added spray source terms. Patel and Menon [36] and Bharadwaj et al. [37] included the subgrid spray drag force fluctuations to the SGS kinetic energy equation. In high speed evaporating sprays like those considered in this work, the added mass due to evaporation can also be a significant source of kinetic energy at subgrid level and should be included as we have done in this work.

This chapter is focused on the development and testing of LES models for high speed evaporating sprays interacting with a high temperature and pressure turbulent gas. A stochastic SGS model is employed for the spray atomization and droplet breakup together with Lagrangian mass, momentum and energy models for the individual droplets. Compressible filtered LES equations are solved for the gas with a complete set of droplet mass, momentum and energy coupling terms and a two-phase SGS kinetic energy equation that account for spray drag force and evaporation. The stochastic LES model is applied here to both non-evaporating sprays and high speed evaporating sprays.

In the denser regions of the spray, where the droplet number density is very significant, droplets start to modify the flow around them to such an extent that droplet behaviour is also affected. These modifications should be somehow included in the spray model for improved predictions. Experimental and numerical studies of interacting spheres and droplets ([38], [39] and [40]) show that when two spherical particles are following each other along the flow direction, only the leading particle wake structure changes and the rear particle wake is much less affected by the other particle. Consequently, the vorticity field behind the leading

particle and the drag of the rear sphere are affected more by the wake effects. This of course is dependent on the Reynolds number (based on the relative velocity) and the relative position of particles. Droplet-wake interactions are neglected in the majority of previous works on multi-dimensional spray simulations. To include these effects into the droplet movement and breakup, various methods may be used. For example, Silverman and Sirignano [41] proposed a statistical model for the droplet wake effects for low Reynolds number flows in which correlation functions are introduced for various flow variables affected by the droplet wake such as the drag coefficient. Alternatively, one can apply a correction function to the felt relative velocity of gas and droplet in the definition of droplet variables like drag coefficient, rather than using a correlation function. In the present work, the aerodynamic wake effect of leading droplets on the relative velocity of the trailing droplets is implemented by the modification of relative velocity and by using correction functions which are based on the Reynolds number, droplet diameters, their positions and the direction of movement of droplets with respect to each other.

Understandably, the three dimensional flow, mass and thermal energy transport in the gas films surrounding the droplets and in the gas regions between neighbouring droplets cannot be fully computed and have to be somehow modeled in LES since they occur at SGS level. However, the heat and mass transport within the liquid droplet and its surface are important and have to be properly modeled and computed as they can have a significant effect on the spatial and temporal distribution of the fuel in the vapour phase. In most spray and combustion simulations, the modeling approach to evaporation has been that of assuming the inner droplet variables to be uniform [42]. Clearly, the presence of components with a wide range of volatility and the consequent non-monotonicity of species mass fractions and

temperature fields inside a fuel droplet demands more complex finite rate, multicomponent heat and mass transfer representation for the droplet ([44],[43]) even though an assumption of spherical symmetry is usually necessary. Torres et al. [45] provided an algorithm for efficient solution of droplet gas interface equations together with the one dimensional spherically symmetric heat and mass equations inside droplets. This algorithm is implemented in the context of LES and is employed with some extensions for the simulations of high speed evaporating sprays in this chapter..

In the following sections, the mathematical formulations for the LES and spray are presented first, followed by the description of numerical methods used for solving these equations. Next, LES results for non-evaporating and evaporating sprays for various gas and liquid jet conditions are compared with the available experimental data. The effects of various modeling assumptions and parameters on the global spray quantities are also discussed.

1.2 Mathematical Formulations and Modelling

The two phase compressible LES model has two main mathematical components: (i) the Lagrangian spray equations and submodels, and (ii) the Eulerian filtered gas equations with their SGS models and gas liquid interaction terms. These are described in two separate sections below. We will start with the spray equations.

1.2.1 Lagrangian Droplet Equations

The spray model considered in this chapter is based on the Lagrangian droplet method ([46], [47] and [44]) in which the droplet motion is computed via Basset Bousinesq Oseen

(BBO) equation [46]. Since the density of the droplet is much larger than that of the fluid and the droplet size and the droplet number density in the major portion of the spray is small, the droplet collisions are neglected in most of our evaporating spray simulations. The Basset force, the added mass term and the Saffman lift force (which are known to be small compared to drag force) are also neglected in our simulations. Under these assumptions, the Lagrangian equations describing the droplet or particle (identified by subscript p) motion are:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p, \quad (1.1)$$

$$\frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{u}_{rel}}{\tau_p}. \quad (1.2)$$

In equation 1.2, the relative velocity is $\mathbf{u}_{rel} = \mathbf{u}_g - \mathbf{u}_p$, where the gas velocity at the droplet location $\mathbf{u}_g = \langle \mathbf{u} \rangle_L + \mathbf{u}^*$ is reconstructed by adding to the filtered velocity $\langle \mathbf{u} \rangle_L$, a stochastic subgrid velocity $\mathbf{u}^*$ as described below. This SGS velocity reconstruction is important for large droplets interacting directly with the turbulence. The particle response time in equation 1.2 is defined to be

$$\tau_p = \tau_{st}/f_1(Re_{sl}), \quad (1.3)$$

where $\tau_{st} = d_p^2 \rho_l / 18 \mu_g$ is the droplet Stokes time scale and $f_1(Re_{sl})$ is the drag factor. The drag factor is the finite slip Reynolds number ($Re_{sl} = \rho_g d_p u_{rel} / \mu_g$) correction to the Stokes drag. At low Reynolds numbers ($Re_{sl} < 100$), the drag factor includes the effect of evaporation as a function of blowing Reynolds number, Re_{bw} [48] and is written as:

$$f_1 = \frac{1 + 0.0545 Re_{sl} + 0.1 Re_{sl}^{1/2} (1 - 0.03 Re_{sl})}{1 + [0.09 + 0.077 \exp(-0.4 Re_{sl})] Re_{bw}^{0.4 + 0.77 \exp(-0.04 Re_{sl})}}, \quad (1.4)$$

where the blowing Reynolds number $Re_{bw} = 2\beta/Pr$ is related to the non-dimensional evaporation parameter β defined blow. For higher Reynolds numbers ($100 < Re_{sl} < 10^5$), the evaporation effect on drag is neglected and the standard drag factor for a sphere is used [49]:

$$f_1 = 1 + 0.15Re_{sl}^{0.687} + 0.0175Re_{sl}/(1 + 4.25 \times 10^4 Re_{sl}^{-1.16}). \quad (1.5)$$

The drag factor is modified for a distorting drop, using the simple assumption that the drag coefficient of a distorting drop should lie between the lower limit of a rigid sphere and the upper limit of a disk where the distortion is computed using the TAB model [50].

The subgrid velocity $\mathbf{u}^*$, used in the droplet transport equation together with the resolved velocity, is calculated along the particle path. For very large particles, the model should have no short time effect on the particle motion. A reasonable assumption in LES is to consider the subgrid turbulent motion to be locally homogenous and isotropic, suggesting that the SGS velocity is related to the SGS kinetic energy as $u_{sgs} = \sqrt{2k_{sgs}/3}$. Pozorski and Apte [33] assumed that the residual velocity seen by the particle to be governed by the following Langevin equation:

$$du_i^* = -\frac{u_i^*}{\tau_L^*} dt + \sqrt{\frac{2u_{sgs}^2}{\tau_L^*}} dW_i, \quad (1.6)$$

where dW_i is an increment of the Wiener process [51]. In equation 1.6, the time scale of the flow seen by the particle at SGS level is estimated to be:

$$\tau_{sgs} = c_{sgs} \frac{\bar{\Delta}}{u_{sgs}}. \quad (1.7)$$

Here, the model constant is taken to be 0.1 [33]. Additionally, the characteristic time scales for large droplets differ in the directions parallel and perpendicular to the mean relative

velocity as captured by the following models:

$$\tau_{L||}^* = \frac{\tau_{sgs}}{\sqrt{1 + \vartheta^2}}; \tau_{L\perp} = \frac{\tau_{sgs}}{\sqrt{1 + 4\vartheta^2}}. \quad (1.8)$$

Here, the Eulerian and Lagrangian time scales of the gas field are assumed to be the same and $\vartheta = |\langle \mathbf{u} \rangle_L - \mathbf{u}_p|/u_{sgs}$ is the normalized drift velocity. This choice of time scales means that the SGS fluid velocity seen by the droplet is auto-correlated over the time scale of the residual motion. The residual velocity then is found along the droplet path according to the following equation

$$u_i^{*(n+1)} = (1 - \frac{\Delta t}{\tau_L^*})u_i^{*(n)} + u_{sgs}\sqrt{\frac{2\Delta t}{\tau_L^*}}\zeta_i, \quad (1.9)$$

where Δt is the time interval of the droplet calculations and ζ_i are random numbers from the standard Gaussian distribution. This equation is used when $\Delta t < \tau_L^*$, for very large time scales, the residual velocity is $u_i = u_{sgs}\zeta_i$.

To consider the effect of droplet collision, the improved version [52] of the model proposed by Munnannur and Reitz [53] is used in some of our simulations. Four possible collision outcomes of bouncing, coalescence, reflexive separation and stretching separation are considered. Fragmentations in stretching and reflexive separations are modeled by assuming that the interacting droplets form an elongating ligament that either breaks up by capillary wave instability, or retracts to a single satellite droplet. Droplet collision/coalescence happens mostly away from the primary breakup region. Therefore, the initial blobs are allowed to break first into smaller droplets before going through collision.

With the assumptions of Fourier heat conduction and Fickian mass diffusion, the following spherically symmetric, one dimensional, multicomponent unsteady continuity, energy and

species equations [45] inside each individual droplet are solved together with the gas and liquid-gas interface equations for obtaining the droplet variables at each time step.

$$\frac{\partial \rho_l}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_l v_l) = 0 \quad (1.10)$$

$$\frac{\partial(\rho_l \phi_{l\alpha})}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_l v_l \phi_{l\alpha}) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_l D_l \frac{\partial \phi_{l\alpha}}{\partial r}) \quad (1.11)$$

$$\frac{\partial(\rho_l T_l)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_l v_l T_l) = \frac{1}{c_p r^2} \frac{\partial}{\partial r} (r^2 \lambda_l \frac{\partial T_l}{\partial r}) \quad (1.12)$$

The internal droplet circulation, caused by the relative motion of gas and liquid, and its effect on the droplet variables are accounted for by changing the effective mass and thermal liquid diffusivities [54]. The mass and energy conservations provide the necessary droplet interface equations as well as the global droplet mass and energy changes which affect the gas phase such as the total change in the droplet internal energy $d(me)_p/dt$. For a multicomponent droplet, the mass flux of species at the droplet interface may be written as

$$\dot{m}_\alpha = \phi_{ls\alpha} 2\pi r_s \rho_{gs} D_{g\alpha} Sh_\alpha \ln(1 + B_{M\alpha}), \quad (1.13)$$

where the Spalding mass transfer number, defined as,

$$B_{M\alpha} = \frac{\phi_{gs\alpha} - \phi_{\infty\alpha}}{\phi_{ls\alpha} - \phi_{gs\alpha}}, \quad (1.14)$$

relates the liquid and gas interface mass fractions ($\phi_{ls\alpha}$ and $\phi_{gs\alpha}$) to the free stream (with respect to droplet) mass fraction $\phi_{\infty\alpha}$. For the heat and mass transfer between droplet and surrounding gas, the well known Ranz-Marshall correlations for the Sherwood and Nusselt

numbers are used.

$$Nu^* = 2 + 0.552Re_{sl}^{1/2}Pr^{1/3}; Sh_{\alpha}^* = 2 + 0.552Re_{sl}^{1/2}Sc_{\alpha}^{1/3} \quad (1.15)$$

To account for the surface blowing effect of the evaporated liquid, Sherwood and Nusselt numbers are modified based on the film model of Abramzon and Sirignano [54] as:

$$Sh_{\alpha} = 2 + \frac{0.552Re_{sl}^{1/2}Sc_{\alpha}^{1/3}}{F(B_{M\alpha})}, F(B_{M\alpha}) = (1 + B_{M\alpha})^{0.7} \frac{\ln(1 + B_{M\alpha})}{B_{M\alpha}}, \quad (1.16)$$

$$Nu = 2 + \frac{0.552Re_{sl}^{1/2}Pr^{1/3}}{F(B_T)}, F(B_T) = (1 + B_T)^{0.7} \frac{\ln(1 + B_T)}{B_T}, \quad (1.17)$$

where, the Spalding heat transfer number $B_T = e^{\beta} - 1$ is calculated based on the non-dimensional evaporation parameter:

$$\beta = -\frac{3}{2}Pr\tau_{st}\frac{\dot{m}_p}{m_p}. \quad (1.18)$$

The overall mass flow rate at the droplet surface is

$$\dot{m}_p = 4\pi r_s^2 \rho_{ls} (\dot{r}_s - v_{ls}), \quad (1.19)$$

where the surface regression rate is found by summing over all species

$$(\dot{r}_s - v_{ls}) = \frac{\rho_{gs} \sum_{\alpha} \phi_{ls\alpha} D_{g\alpha} Sh_{\alpha} \ln(1 + B_{M\alpha})}{2r_s \rho_{ls}}. \quad (1.20)$$

Finally, the inter-phase coupling effects are represented by the conservation of mass for

species α and energy at the droplet interface as

$$2r_s\rho_{ls}(v_{ls} - \dot{r}_s)(\phi_{gs\alpha} - \phi_{ls\alpha}) + 2r_s\rho_{ls}D_{ls}\frac{\partial\phi_\alpha}{\partial r}|_{ls} - \rho_{gs}D_{g\alpha}Sh_\alpha\ln(1 + B_{M\alpha}) = 0, \quad (1.21)$$

$$2r_s \sum_i L_{v\alpha}\rho_{ls}[(\dot{r}_s - v_{ls})\phi_{ls\alpha} + D_{l\alpha}\frac{\partial\phi_\alpha}{\partial r}|_{ls}] - 2r_s\lambda_l\frac{\partial T}{\partial r}|_{ls} + \lambda_g Nu(T_{g\infty} - T_s) = 0. \quad (1.22)$$

1.2.1.1 Droplet Wake Model

The wake effect of an upstream droplet on a trailing droplet makes the felt relative velocity by the trailing droplet smaller than the free stream flow. However, this effect disappears at downstream locations from the leading droplet. Here, the correction factor due to multi-droplet wake interactions is computed by taking into account the relative position and size of droplets. Looking for the effect of nearby droplets, three possible upstream droplets (among those in the same cell or neighbouring cells) with the lowest relative angle, minimum distance and maximum relative size are considered. To find the nearest upstream droplets, the droplet indices are sorted according to the cell in which they are and for each droplet, the search is carried out only among the droplets residing in the same cell and neighbouring cells. Subsequently, the inner product of the distance vector between the two droplets and the relative velocity vector of the concerned droplet is used to find the distance and position angle (θ_{pp}) between droplets. Only droplets upstream of the concerned droplet closer than 10 times of their diameters are taken into account. The upstream droplet must be moving in the same direction as the concerned droplet to have the maximum wake interactions. This is found by using the angle between the relative velocities of the two droplets (θ_{upp}). The correction factor for the relative velocity of the droplet affected by an upstream droplet is based on the difference between these two angles, ($\Delta\theta = \theta_{pp} - \theta_{upp}$) and is written as

[41]:

$$\Lambda' = [1 + (\varpi - 1) \cos(\Delta\theta)], \quad (1.23)$$

where ϖ is the average fraction of the free stream velocity, obtained as a function of Reynolds number and distance from the experimental data [55]. It may be observed that the reduction factor is more significant when $\Delta\theta$ is closer to zero which happens when droplets are aligned with respect to their relative velocity directions. With this alignment, depending on the distance between droplets, the relative velocity of the trailing droplet is clearly reduced when droplets have the same size. However, if the leading droplet is smaller than the one affected by the wake, the effect is much smaller. To take into account the size effect, we do a correction to the wake model and the reduction factor Λ' based on the portion of the area of the concerned droplet wetted by the wake of the smaller upstream droplet according to the following equation when the leading droplet is smaller than the trailing one:

$$\Lambda = [1 + (\frac{d_{p,lead}}{d_p})^2(\Lambda' - 1)]. \quad (1.24)$$

Finally, the corrected relative velocity is used in the droplet Reynolds number for computing the drag factor, Nusselt and Sherwood numbers modified by the wake.

1.2.1.2 Stochastic Droplet Breakup Model

As mentioned before, a stochastic breakup model ([15] and [11]) capable of generating a broad range of droplet sizes at high Weber numbers is used in this chapter for predicting the new droplet formation. In this model, the size distribution of droplets generated by the breakup is based on the solution of a Fokker Planck equation whose main parameters are breakup

frequency and the first two moments of the fragmentation intensity spectrum. The breakup frequency and consequently the evolution of droplet diameter are controlled by the relative velocity fluctuations between the gas and liquid phases which is an important parameter and is obtained from a Lagrangian model. Let $N_{tot}(t)$ and $N(r, t)$ represent the total number of breaking droplets and droplets with size less than or equal to r , respectively, at discrete time instants $t^* = 0, 1, 2, \dots$. These time moments are scaled by the breakup frequency ($1/\tau_{bu}$, τ_{bu} is the time at which breakup occurs). Their corresponding expectations are given as $\bar{N}_{tot}(t^*)$ and $\bar{N}(r, t^*)$, respectively. Consider the breakup of a given particle with size r within the time interval $[t^*, t^* + 1]$. Let $Q(\alpha)$ be the mean number of secondary particles produced with size less than or equal to αr , with $0 < \alpha < 1$. According to Kolmogorov's hypotheses, the probability to break each parent particle into a given number of fragments is independent of the parent particle size. In other words, $Q(\alpha)$ does not depend on the history of breakup and is not influenced by other parent droplets. It then follows that

$$\bar{N}(r, t^* + 1) = \int_0^1 \bar{N}\left(\frac{r}{\alpha}, t^*\right) dQ(\alpha). \quad (1.25)$$

By introducing $\chi = \ln(r/r_0)$, where r_0 is the parent drop size, Kolmogorov showed that

$$\mathfrak{S}(\chi, t^*) = \frac{\bar{N}(e^\chi, t^*)}{\bar{N}_{tot}(t^*)} = \frac{N(e^\chi, t^*)}{N_{tot}(t^*)}. \quad (1.26)$$

Equation 1.26 can be rewritten as

$$\mathfrak{S}(\chi, t^* + 1) = \int_{-\infty}^0 T(\chi - \varsigma) dS(\varsigma), \quad (1.27)$$

where $\varsigma = \ln(\alpha)$ and $Q(\alpha) = Q(1)S(\varsigma)$. The entire spectrum $Q(\alpha)$ is unknown. However, in the limit of large time ($t^* > 1$), equation 1.27 can be replaced by the following Fokker-Planck equation in which only the first two moments of $Q(\alpha)$ are important.

$$\frac{\partial \mathfrak{S}(\chi, t^*)}{\partial t} = -\frac{\langle \varsigma \rangle}{\tau_{bu}} \frac{\partial \mathfrak{S}(\chi, t^*)}{\partial \chi} + \frac{1}{2} \frac{\langle \varsigma^2 \rangle}{\tau_{bu}} \frac{\partial^2 \mathfrak{S}(\chi, t^*)}{\partial \chi^2}. \quad (1.28)$$

The moments $\langle \varsigma \rangle = \int_{-\infty}^0 \varsigma S(\varsigma) d\varsigma$ and $\langle \varsigma^2 \rangle = \int_{-\infty}^0 \varsigma^2 S(\varsigma) d\varsigma$ are the first two moments of the breakup intensity spectrum which are related to the stochastic nature of the breakup process in the general cascade of breakup events. Apte et al. [12] related them to parent drop Weber number. In the present work, $Q(\alpha)$ is assumed to be Gaussian and independent of droplet size; consequently the two moments will be $\langle \varsigma \rangle = -0.36$ and $\langle \varsigma^2 \rangle = 0.14$ [56]. Furthermore, Gorokhovski and Saviliev [11] showed that the initial delta-function for the logarithm of radius of the parent droplet evolves into a steady state distribution that is a solution to the Fokker-Planck equation

$$\mathfrak{S}(r) = \frac{1}{2} [1 + \operatorname{erf}(\frac{\ln(r/r_0) - \langle \varsigma \rangle}{\sqrt{2\langle \varsigma^2 \rangle}})]. \quad (1.29)$$

In our simulations, the number and size of new droplets are determined by a stochastic sampling procedure that conserves the liquid mass. The generated droplet velocity is computed by adding a factor w_{bu} to the parent drop velocity. The additional velocity is randomly distributed in a plane normal to the relative velocity vector between the gas and parent drop $w_{bu} = r_0/\tau_{bu}$. This is based on the physical picture of parent drops being torn apart by aerodynamic forces, giving momentum to the newly formed droplets in the direction normal to the relative velocity between the gas and parent drops [9].

The droplet breakup is associated with the instabilities on the surface of the droplet, induced by relative velocity fluctuations of the gas and droplet and occurs when the age of the droplet exceeds the inverse of breakup frequency. The natural frequency $1/\tau_{bu}$ of a droplet, subjected to aerodynamic instability on its surface is [9]:

$$\tau_{bu} = \sqrt{3} \sqrt{\frac{\rho_l}{\rho_g} \frac{r_p}{u_{rel_{bu}}}}, \quad (1.30)$$

in which $u_{rel_{bu}}$ is the relative velocity for the breakup. Apte et al. [12] assumed $u_{rel_{bu}}$ to be the root mean square of relative velocity fluctuations and computed it from the mean viscous dissipation and Stokes time scale as $u_{rel_{r.m.s}} = \sqrt{\epsilon \tau_{st}}$. This estimate however is limited to low Reynolds number droplets interacting with the gas turbulence at inertial scales. However, it is reasonable to believe that the extent of droplet deformation that leads to breakup is dependent on the duration and intensity of droplet motion in the gas flow [2]. This suggests that the use of time averaged relative velocity fluctuations for the breakup frequency is justified. Here, we have averaged the relative velocity fluctuations along the droplet path as

$$\langle \mathbf{u}_{rel} \rangle_t = \frac{1}{age} \sum \mathbf{u}_{rel} \Delta t. \quad (1.31)$$

In the above equation, “age” is the total time of droplet exposure to the gas. The relative velocity fluctuation is assumed to be the Lagrangian root mean square (r.m.s.) of the relative velocity,

$$u_{rel_{r.m.s}} = \sqrt{\frac{|\mathbf{u}_{rel} - \langle \mathbf{u}_{rel} \rangle_t|^2 \Delta t}{age}}. \quad (1.32)$$

The breakup proceeds for the new born droplets till they reach a stable or critical radius. The critical radius for breakup can be obtained by a balance between the disruptive hydrodynamic

and capillary forces as:

$$r_{cr} = \frac{We_{cr}\sigma}{\rho g u_{rel}^2}. \quad (1.33)$$

Here, the critical Weber number We_{cr} is around six over a wide range of Ohnesorge numbers [1], [2].

Whenever the number of droplets becomes very significant, the grouping approach of Apt. et al. [12] is used in which the droplets generated by the breakup are grouped into parcels. These parcels are allowed to break, meaning that the number of particles in the parcels will increase and the diameter is decreased without creating new parcels. PDFs of the droplet number densities in each parcel are constructed based on the droplet numbers and diameters. The grouping process through parcels, does not change the mass, momentum and energy of the droplets and is used for controlling the computational cost.

1.2.2 Filtered Gas Equations

For the very high speed sprays simulated in this chapter, the induced gas flow by the spray is very significant and turbulent. This gas flow is simulated by solving the following compressible Favre-filtered continuity, momentum, energy and species mass fraction (scalar)

equations.

$$\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_i} = \langle \dot{S}_{Mass}^{sp} \rangle_l, \quad (1.34)$$

$$\frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_j} = -\frac{\partial \langle p \rangle_l}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle_l}{\partial x_j} - \frac{\partial (\tau_{ij}^{sgs})}{\partial x_j} + \langle \dot{S}_{mi}^{sp} \rangle_l, \quad (1.35)$$

$$\begin{aligned} \frac{\partial \langle \rho \rangle_l \langle E \rangle_L}{\partial t} + \frac{\partial (\langle \rho \rangle_l \langle E \rangle_L + \langle p \rangle_l \langle u_i \rangle_L)}{\partial x_i} = & -\frac{\partial (\langle q_i \rangle_l + H_i^{sgs})}{\partial x_i} + \langle \dot{Q} \rangle_l + \langle \dot{S}_E^{sp} \rangle_l, \\ & + \frac{\partial [(\langle \tau_{ij} \rangle_l - \tau_{ij}^{sgs}) \langle u_j \rangle_L]}{\partial x_i} \end{aligned} \quad (1.36)$$

$$\frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial (\langle J_i^\alpha \rangle_l + J_i^{\alpha sgs})}{\partial x_i} + \langle \rho \dot{S}_\alpha \rangle_l + \langle \dot{S}_\phi^{sp} \rangle_l. \quad (1.37)$$

In Equations 1.34 to 1.37, $\langle \rangle_l$ and $\langle \rangle_L$ represent filtered and Favre-filtered operations, respectively. The primary variables are filtered density $\langle \rho \rangle_l$, the Favre filtered velocity $\langle u_i \rangle_L$, the Favre filtered total energy $\langle E \rangle_L = \langle e \rangle_L + \frac{1}{2} \langle u_i \rangle_L \langle u_i \rangle_L$ and the Favre filtered scalar mass fraction $\langle \phi_\alpha \rangle_L$. The equations are closed with the filtered equation of state for a perfect gas, $\langle p \rangle_l = \langle \rho \rangle_l \langle R \rangle_L \langle T \rangle_L$, which relates filtered density and pressure to the Favre-filtered temperature, $\langle T \rangle_L$ through mixture gas constant $\langle R \rangle_L$. The filtered viscous stress tensor $\langle \tau_{ij} \rangle_l$ is a linear function of the filtered strain rate $\langle S_{ij} \rangle_L$, and the filtered heat flux vector $\langle q_i \rangle_l$ and species diffusion $\langle J_i^\alpha \rangle$ are evaluated based on Fourier and Fick's laws. The Favre-averaged rate of change of species α due to chemical reaction $\langle \rho \dot{S}_\alpha \rangle_l$ and the Favre-filtered heat of reaction $\langle \dot{Q} \rangle_l$ are zero for a non-reacting flow.

The discretization of the carrier gas equations is based on the compact parameter finite difference scheme, which yields up to sixth order spatial accuracy. The time differencing is based on a third order low storage Runge Kutta method ([57],[58]). A low pass, high order, spatial implicit filtering operator is used for both interior and near boundary values to remove the numerical noise generated by the growth of numerical error at very high wave

number modes. Five overlap points between blocks are considered to maintain accuracy across grid block boundaries in the parallel computations [59].

The effects of droplets on the carrier gas are included via a series of source/sink terms in the gas conservation equations. These terms are evaluated by volumetric averaging and interpolation of the Lagrangian droplet quantities as:

$$\langle \dot{S}_{Mass}^{sp} \rangle_l = - \sum_p \frac{w_p}{\Delta V} \dot{m}_p, \quad (1.38)$$

$$\langle \dot{S}_{mi}^{sp} \rangle_l = - \sum_p \frac{w_p}{\Delta V} \left[m_p \frac{du_{pi}}{dt} + \dot{m}_p u_{pi} \right], \quad (1.39)$$

$$\langle \dot{S}_E^{sp} \rangle_l = - \sum_p \frac{w_p}{\Delta V} \left[\frac{d(me)_p}{dt} + \frac{1}{2} \dot{m}_p \mathbf{u}_p^2 + m_p \mathbf{u}_p \cdot \frac{d\mathbf{u}_p}{dt} \right], \quad (1.40)$$

$$\langle \dot{S}_\alpha^{sp} \rangle_l = - \sum_p \frac{w_p}{\Delta V} \dot{m}_\alpha. \quad (1.41)$$

Note that equation 1.40 is the spray source term to the total energy equation. Alternatively, one can obtain the spray source term to enthalpy as:

$$\langle \dot{S}_h^{sp} \rangle_l = \langle \dot{S}_E^{sp} \rangle_l - \langle u_i \rangle_L \langle \dot{S}_{mi}^{sp} \rangle_l + \frac{\langle u_i \rangle_L \langle u_i \rangle_L}{2} \langle \dot{S}_{Mass}^{sp} \rangle_l. \quad (1.42)$$

1.2.2.1 Subgrid-Scale Models

The unclosed SGS terms in the filtered equations are closed here by gradient type closures [60]-[61]. In these closures, the characteristic length and velocity for defining the eddy viscosity are provided by the local grid size $\bar{\Delta}$ and the subgrid kinetic energy k_{sgs} as $\nu_t = c_\nu \bar{\Delta} \sqrt{k_{sgs}}$. The subgrid stress τ_{ij}^{sgs} is assumed to be proportional to the eddy viscosity ν_t

as

$$\tau_{ij}^{sgs} = -2\langle\rho\rangle_l \nu_t (\langle S_{ij}\rangle_L - \frac{1}{3}\langle S_{kk}\rangle \delta_{ij}) + \frac{2}{3}\langle\rho\rangle_l k_{sgs} \delta_{ij}. \quad (1.43)$$

The SGS velocity correlations in the energy and scalar equations are also modeled with similar gradient type closures:

$$H_i^{sgs} = -\langle\rho\rangle_l \frac{\nu_t}{Pr_t} \frac{\partial\langle H\rangle_L}{\partial x_i}, \quad (1.44)$$

$$J_{\alpha i}^{sgs} = -\langle\rho\rangle_l \frac{\nu_t}{Sc_t} \frac{\partial\langle\phi_\alpha\rangle_L}{\partial x_i}, \quad (1.45)$$

where $\langle H\rangle_L = \langle E\rangle_L + \langle p\rangle_l/\langle\rho\rangle_l$ is the total filtered enthalpy, Pr_t and Sc_t are turbulent Prantl and Schmidt numbers, respectively. The subgrid kinetic energy is obtained from the following transport equation:

$$\frac{\partial\langle\rho\rangle_l k_{sgs}}{\partial t} + \frac{\partial\langle\rho\rangle_l \langle u_i\rangle_L k_{sgs}}{\partial x_i} = P_{sgs} + T_{sgs} - \epsilon_{sgs} + \langle\dot{S}_{ksgs}^{sp}\rangle_l. \quad (1.46)$$

The production term in k_{sgs} equation, $P_{sgs} = -\tau_{ij}^{sgs}\langle S_{ij}\rangle_L$ is closed and readily computable with a model for τ_{ij}^{sgs} . The dissipation of k_{sgs} is evaluated based on the characteristic length and velocity scales of the SGS turbulence as $\epsilon_{sgs} = c_\epsilon \langle\rho\rangle_l \sqrt{k_{sgs}^3/\bar{\Delta}}$, in analogy with the Kolmogorov's energy cascade concept. The transport term T_{sgs} consists of diffusion of k_{sgs} due to subgrid fluctuations in kinetic energy (often referred to as the triple velocity correlation), subgrid fluctuations in viscous stresses and subgrid fluctuations in pressure, which are also closed by gradient type closures as

$$T_{sgs} = \frac{\partial}{\partial x_i} [\tau_{ij}^{sgs} \langle u_i\rangle_L + \langle\rho\rangle_l (\nu + c_k \bar{\Delta} \sqrt{k_{sgs}}) \frac{\partial k_{sgs}}{\partial x_j}] + \langle\rho\rangle_l \frac{\nu_t}{Pr_t} \langle R\rangle_L \frac{\partial\langle T\rangle_L}{\partial x_j}. \quad (1.47)$$

The model coefficients in equation 1.46 are suggested by Yoshizawa and Horiuti [62] to be $c_\nu = 0.05, c_\epsilon = 1.0$ and c_k equal to c_ν . Here, c_ν and c_k are computed dynamically using the variable density version of the method employed by Ghosal et al. [61]. However, due to difficulty in obtaining the energy dissipation rate from the resolved scales [61], c_ϵ is assumed to be constant and unity. The transport term $\partial(\tau_{ij}^{sgs}\langle u_i\rangle_L)/\partial x_j$ in equation 1.47 may be absorbed in the model for the triple correlation. However, since c_k is found dynamically and since the dynamic procedure used for k_{sgs} transport by subgrid turbulence accounts for the unclosed part of the triple correlation, this term is kept in the modeled equation when dynamic method is used. The dynamic procedure used for computing the SGS stresses and coefficients in the SGS kinetic energy equation is well developed. Here, we only describe this procedure, as an example, for evaluation of the triple velocity correlation term in the SGS kinetic energy equation,

$$-\frac{1}{2}\langle\rho\rangle_l(\langle u_i u_i u_j\rangle_L - \langle u_i u_i\rangle_L \langle u_j\rangle_L) + \langle\rho\rangle_l(\langle u_i u_j\rangle_L - \langle u_i\rangle_L \langle u_j\rangle_L) \langle u_i\rangle_L. \quad (1.48)$$

The second part of the triple correlation term is already closed by a model for the subgrid stresses. The unclosed triple correlation part which reflects the SGS flux of kinetic energy is calculated by the ‘‘Germano identity’’ [63], relating the grid level SGS kinetic energy flux f_j to the corresponding flux at the test level F_j as:

$$Z_j = (F_j - \langle f_j\rangle_{\hat{l}}), \quad (1.49)$$

$$Z_j = \langle\langle\rho\rangle_l\rangle_{\hat{l}}\langle\langle u_j\rangle_L\rangle_{\hat{l}}\langle\frac{1}{2}\langle u_i\rangle_L\langle u_i\rangle_L + k_{sgs}\rangle_{\hat{l}} - \langle\langle\rho\rangle_l\langle u_j\rangle_L(\frac{1}{2}\langle u_i\rangle_L\langle u_i\rangle_L + k_{sgs})\rangle_{\hat{l}}, \quad (1.50)$$

$$F_j = c_k \hat{\Delta} \langle\langle\rho\rangle_l\rangle_{\hat{l}} k_{tst}^{1/2} \frac{\partial k_{tst}}{\partial x_j}; f_j = c_k \bar{\Delta} \langle\rho\rangle_l k_{sgs}^{1/2} \frac{\partial k_{sgs}}{\partial x_j}. \quad (1.51)$$

Using the least square method of Liliy [64], c_k is calculated as

$$c_k = \frac{Z_j[F_j - \langle f_j \rangle_l]}{[F_j - \langle f_j \rangle_l][F_j - \langle f_j \rangle_l]}. \quad (1.52)$$

The numerator and denominator of equation 1.52 are averaged separately over the test filtering domain.

The last term in the SGS kinetic energy equation (equation 1.46) is the spray term, $\langle \dot{S}_{ksgs}^{sp} \rangle_l$ which is very important in high speed spray simulations. This term represents the effects of droplet force and evaporation on k_{sgs} . The part due to droplet force can be decomposed into two parts $\mathbf{F}_p \cdot \mathbf{u}_p = \mathbf{F}_p \cdot \mathbf{u}_g - \mathbf{F}_p \cdot \mathbf{u}_{rel}$. The first part affects the total kinetic energy of the gas field, the second part appears in the internal energy equation. The droplet force contribution to k_{sgs} can be closed as

$$\langle \dot{S}_{sgsF}^{sp} \rangle_l = -[\langle \mathbf{F}_p \cdot \mathbf{u}_g \rangle_l - \langle \mathbf{F}_p \rangle_l \cdot \langle \mathbf{u} \rangle_L] \approx -[\langle \mathbf{F}_p \cdot \langle \mathbf{u} \rangle_L \rangle_l - \langle \mathbf{F}_p \rangle_l \cdot \langle \mathbf{u} \rangle_L]. \quad (1.53)$$

For evaporating droplets, there is also a change in kinetic energy due to mass transfer. The total energy transfer from the evaporated liquid to gas field can be written as

$$\dot{m}_p \frac{\mathbf{u}_p^2}{2} = \dot{m}_p \left[\frac{\mathbf{u}_{rel}^2}{2} + \left(\frac{\mathbf{u}_g^2}{2} - \mathbf{u}_{rel} \cdot \mathbf{u}_g \right) \right]. \quad (1.54)$$

The first term on the right hand side of 1.54 is due to particle dissipation to internal energy and the second term is the source term to the total kinetic energy equation, that, when filtered, can be written as

$$\langle \dot{m}_p \left(\frac{\mathbf{u}_g^2}{2} - \mathbf{u}_{rel} \cdot \mathbf{u}_g \right) \rangle_l = \langle \dot{m}_p \left(\frac{\langle \mathbf{u} \rangle_L^2}{2} + k_{sgs} \right) \rangle_l - \langle \dot{m}_p \mathbf{u}_p \cdot \mathbf{u}_g \rangle_l. \quad (1.55)$$

The source term due to evaporation to the subgrid kinetic energy equation is the subgrid part of the above term, which may be written as [65]:

$$\langle \dot{S}_{sgsMass}^{sp} \rangle = -[(\langle \dot{m}_p(\frac{\langle \mathbf{u} \rangle_L^2}{2} + k_{sgs}) - \langle \dot{m}_p \rangle_l \frac{\langle \mathbf{u} \rangle_L^2}{2}) - (\langle \dot{m}_p \mathbf{u}_p \cdot \langle \mathbf{u} \rangle_L \rangle_l - \langle \dot{m}_p \mathbf{u}_p \rangle \cdot \langle \mathbf{u} \rangle_L)]. \quad (1.56)$$

By adding all the liquid effects, the droplet source term to the subgrid kinetic energy can be written in the following final form

$$\langle \dot{S}_{ksgs}^{sp} \rangle_l = (\langle \dot{S}_{mi}^{sp} \langle u_i \rangle_L \rangle_l - \langle \dot{S}_{mi}^{sp} \rangle_l \langle u_i \rangle_L) - (\langle \dot{S}_{Mass}^{sp} k_{total} \rangle_l - \langle \dot{S}_{Mass}^{sp} \rangle_l \frac{\langle u_i \rangle_L \langle u_i \rangle_L}{2}). \quad (1.57)$$

1.3 Results and Discussions

The spray and LES models described above are used together to simulate a series of non-evaporating and evaporating sprays. Few non-evaporating spray cases are considered in this chapter for comparison with the experiment. However, the focus is on the high speed evaporating sprays. These are discussed in two separate sections below.

1.3.1 Non-Evaporating Sprays

The classical non-evaporating spray experiment of Hiroyasu and Kadota [66] is first used in this chapter for the overall assessment of the droplet transport and breakup models. In this experiment, a high speed, solid cone, liquid jet of diesel fuel is sprayed into an enclosed cylindrical apparatus filled with constant temperature (293 K) stagnant nitrogen. The injector is a single hole nozzle with orifice diameter of 300 μm and nozzle opening

pressure of 9.9MPa. The diesel fuel density is 840kg/m^3 . Global spray/droplet variables such as the spray penetration length and droplet Sauter mean diameter (SMD) are measured at varying chamber pressures. Since the chamber temperature is not high, we refer to this experiment as non-evaporating spray.

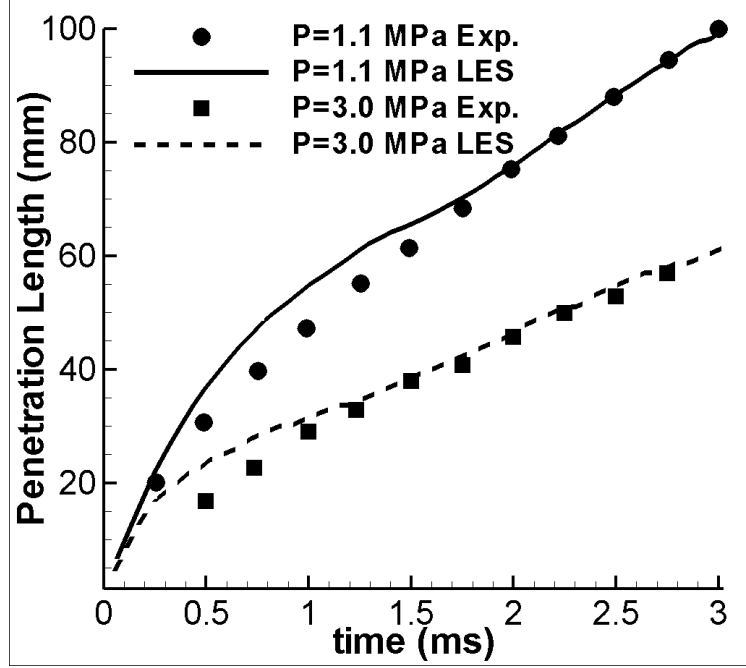


Figure 1.1: Comparison of non-evaporating spray penetration depth, obtained by the LES/Spray model with the experimental data at different times for two chamber pressures.

In the simulations considered in this chapter, large liquid “blobs” with diameter of $300\mu\text{m}$ are injected with similar velocity and mass flow rates (obtained from injection velocity, nozzle diameter, and injection period) to the liquid jet in the experiment. Two chamber pressures of 1.1 and 3.0 MPa are considered. The blob’s injected velocities are computed to be 102.0 and 90.3 m/s for the two chamber pressures. The uniform grid size used in the gas LES calculations is 0.75 mm. Figure 1.1 shows the spray penetration lengths predicted by the LES model at different times as compared with the experimental data. Overall, the numerical spray penetrations are in good agreement with the measured data. However, simulations

seem to capture better the experimental trend at later times. The much earlier values of the liquid penetration are significantly dependent on the details of the very complex liquid jet breakup close to the nozzle which is modeled here by the breakup of big injected blobs. The model is not expected to be fully accurate in this flow region; however it can capture the droplet behaviour further away from the nozzle and the longer time trends. The penetration length decreases with an increase in gas pressure as seen in Figure 1.1. This is attributed not only to the decreased injection velocity, but also to higher breakup frequency in the denser gas. As droplet breakup rate is higher at higher chamber pressures, the numerical penetration values approach to the experimental values in a shorter time at higher pressures.

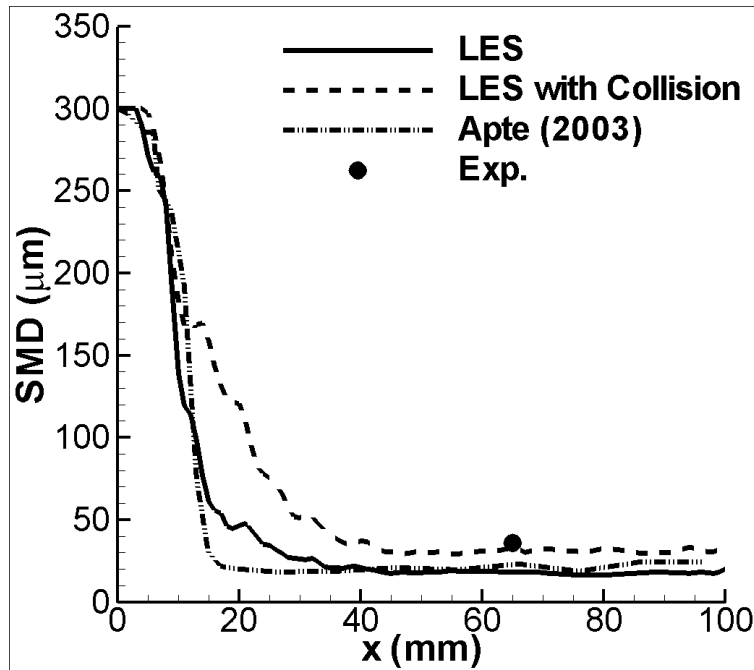


Figure 1.2: Variations of Sauter mean diameter (SMD) in the non-evaporating spray along the spray direction for chamber pressure of $P=1.1$ MPa.

Figure 1.2 shows the droplet SMD at different axial locations as predicted by the present LES/spray model with and without collision and coalescence submodels and by that of Apte et al. [12] for the chamber pressure of 1.1 MPa. Figure 1.2 also shows the experimental

SMD measured by Hiroyasu and Kadota [66] at $x=65$ mm from the nozzle for the same spray. Only one experimental point is shown as the experimental SMD at other available downstream positions are virtually the same as that shown in Figure 1.2 which is consistent with the trends in numerical simulations. Several investigators have compared their model predictions with this experiment as summarized by Apte et al. [12] and Jones and Lettieri [14]. However, only the model results of Apte et al. is presented in Figure 1.2 as this model is the closest one to our model. Close to the nozzle, the SMD predicted by LES corresponds to the size of largest injected blobs or drops and is comparable to the nozzle diameter. But it decreases rapidly over a short distance from the injector and remains more or less constant further downstream. While the results obtained by our LES model and that of Apte et. al. [12] are similar without any collision/coalescence model, those obtained by our LES with the collision model show a slower decrease in SMD and better prediction of the experimental results at locations far from the nozzle, where the collision and coalescence are important. The under-prediction of experimental SMD by LES models is expected when no collision/coalescence model is used. After the rapid decrease in SMD near the nozzle exist, caused by the dominant breakup process, there is a mild gradual increase in SMD when the collision/coalescence of droplets becomes more significant than their breakup. It has been shown that close to the injector the stochastic models of the type used in [12] and [14] generally perform better than the traditional models ([8],[9],[67]). The results obtained by latter models are however slightly better at locations far away from the injector mainly because they use collision/coalescence models. Collision/coalescence has not been considered in previous simulations conducted by stochastic models but is considered here in some of our simulations. However, the collision/coalescence is only important in the non-evaporating sprays at long distances from the nozzle, where the local liquid/gas volume fraction is still

significant. This is in contrast to evaporating sprays in which the dispersed flow region at the tip of the spray is reasonably dilute [68]. Based on these observations, one may conclude that the collision and coalescence do not have a dominant effect on the global evaporating spray variables like the spray penetration length. This conclusion is supported by the evaporating spray results presented below.

1.3.2 Evaporating Sprays

The evaporating sprays simulated in this chapter are similar to those considered in the experiments performed at Sandia National Laboratory [69] - [70]. In these experiments, the fuel spray behaviour in a closed combustion chamber is studied for a variety of spray and gas conditions. A schematic view of the combustion chamber is shown in Figure 1.3. The chamber is about 105 mm in length and is filled with Nitrogen. The Nitrogen temperature and density are varied between 700 K to 1300 K and 3 to 60 kg/m^3 to study the effect of ambient gas temperature and density on the spray. We have simulated the sprays for all gas temperatures and densities and compared the liquid penetration lengths computed from the LES data with the experimental data. The liquid penetration length is the maximum extent of spray, defined to be the axial location at which % 97 of the liquid mass exists in the LES. While the initial gas temperature, density and pressure are uniform and same as experiment, the injected droplet velocity is calculated from the Bernoulli's equation with a correction coefficient as $u_{p,inj} = c_V \sqrt{2p_{inj}/\rho_l}$ (c_V varies from 0.7 to 1.0 according to the experiment). The initial diameters of droplets are calculated from the mass flow rate by using the nozzle diameter and its area contraction coefficient. The spray spreading angle is also computed from the following empirical correlation [70] as

$$\tan(\theta_{sp}/2) = c_{noz}[(\frac{\rho_g}{\rho_l})^{0.19} - 0.0043\sqrt{\frac{\rho_l}{\rho_g}}],$$

where c_{noz} depends on the nozzle diameter.

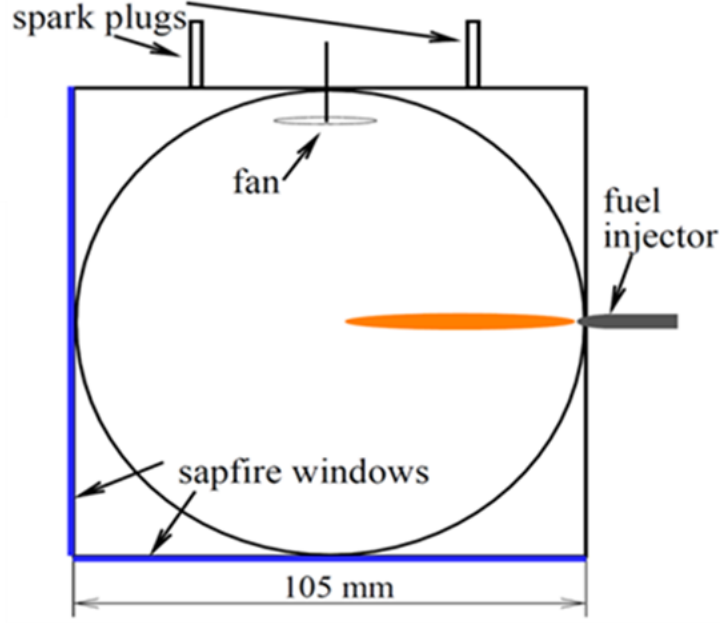


Figure 1.3: Schematic picture of Sandia's closed chamber spray apparatus. For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this dissertation.

The fuel properties are obtained from data and correlations presented by Poling et al. [71]. A rectangular chamber is assumed for the numerical simulations with a length of 105 mm in axial direction and 100 mm in the lateral directions. Table 1.1 summarizes the computational parameters for the most of simulations. The grid size in LES is 0.5 mm at spray location and gradually increases in lateral directions to 1 mm at the outer edges of the chamber. The fuel is Hexadecane and is injected with a constant temperature of 436 K and pressure of 138 MPa through a nozzle with diameter of 0.246 mm. The injection duration is 3 ms. The LES spray penetration length and droplet statistics calculated at or after $t=1.0$ ms are shown to be the same, indicating that the spray reaches to a “steady state” condition at or before $t=1.0$ ms. The vapour jet, however, keeps on penetrating during the spray injection,

N_{core}	32
N_{PC}	50,000 to 100,000
N_G	3,500,000
Δ (mm)	0.500
d_{noz} (mm)	0.246

Table 1.1: Computational parameters for LES of turbulent spray breakup and evaporation

thereby making the spray gas flow a transient process. The instantaneous gas flow results shown in this chapter are at $t=2.0\text{ms}$ when the spray induced flow is already developed.

Figure 1.4 shows the spray evolution and droplet pattern at different times, obtained by LES for intermediate gas density of 14.8 kg/m^3 and temperature of 700 K. The region close to injector mostly consists of large drops accompanied by small stripped droplets, resembling ligament like liquid structures. Further away from the nozzle close to the spray axis, there is a dense pack of both large and small droplets; moving together and deflected outward by the spray generated flow as the spray grows. The breakup proceeds to the tip of the spray where droplets are shown to be well atomized and hence evaporate and disappear quickly. These well atomized small droplets carry less inertial of the initial spray momentum and are significantly affected by the very strong turbulent gas flow created as a result of not only the drag of droplets but also by the kinetic energy of the evaporated fuel. To correctly simulate a high speed spray of the type considered in this chapter, it is important that the flow/turbulence generated by the spray is also properly simulated.

Figure 1.5 compares the numerically predicted liquid penetration lengths with the experimental values as a function of gas density for different gas temperatures. The agreement of simulated results with the experiment is fairly good in all cases. As shown, the penetration length decreases rapidly with the gas density; this is mainly due to more droplet drag and breakup and is more pronounced at lower gas density range. On the other hand, the liquid

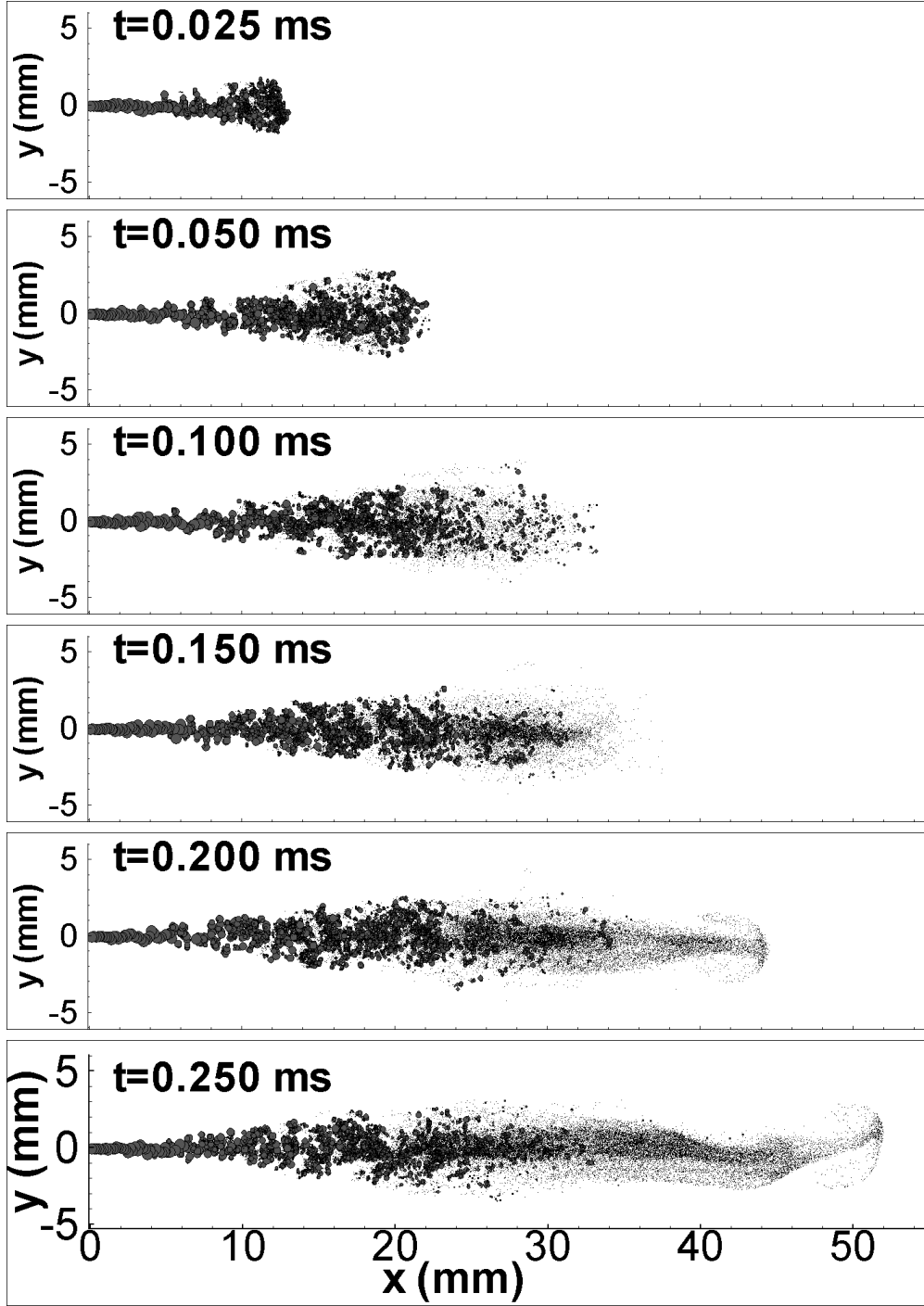
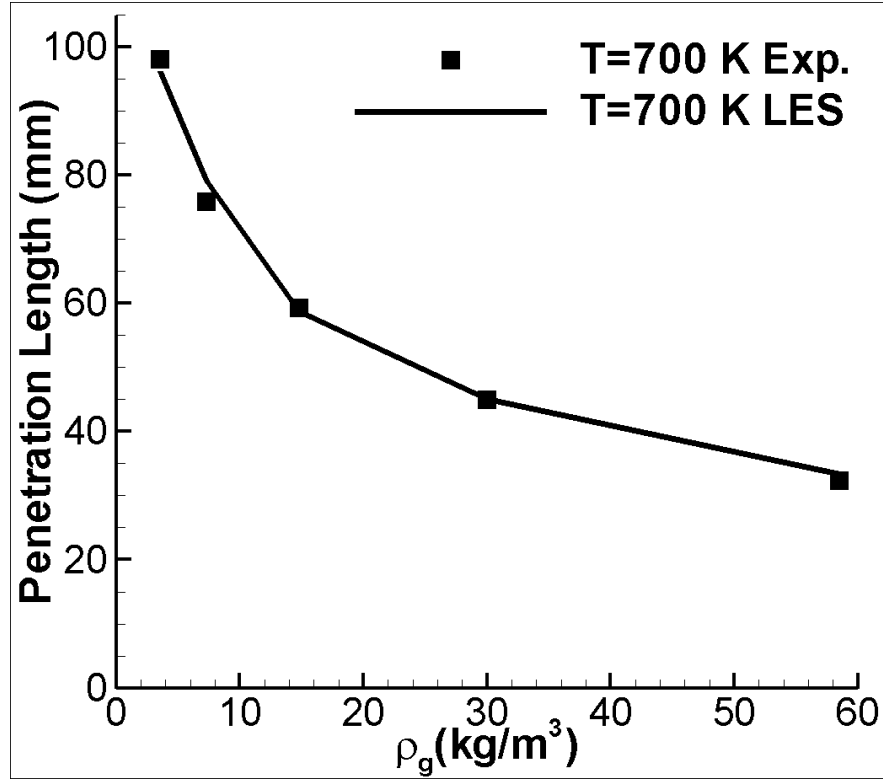
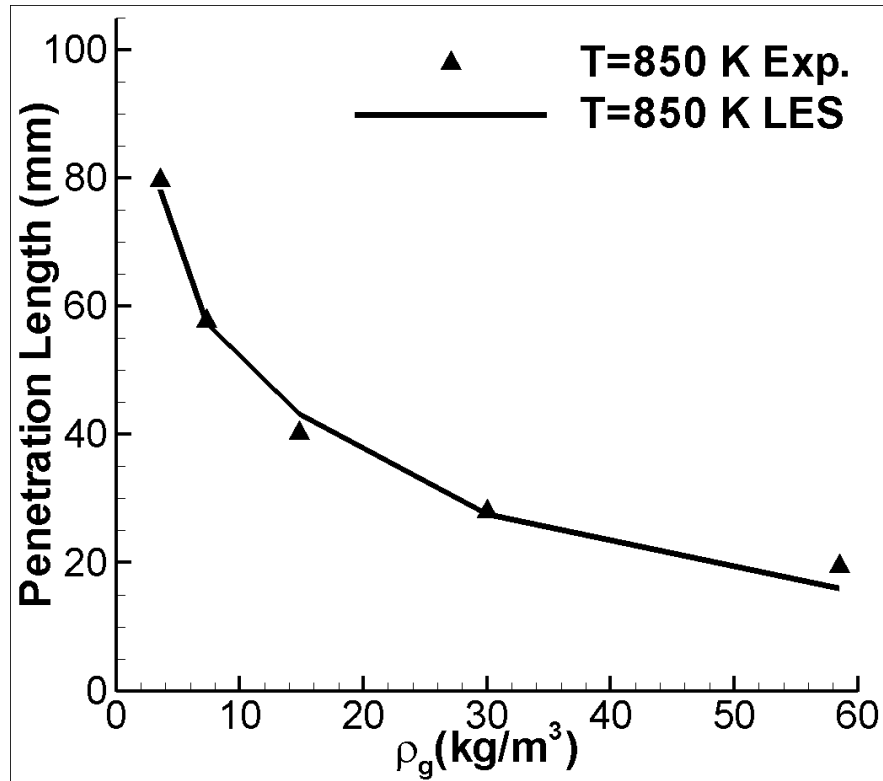


Figure 1.4: Evolution of the evaporating spray at $T = 700K$, $\rho = 14.8kg/m^3$ as shown by sample of droplets at different times.

penetration decreases with an increase in gas temperature which is mainly due to higher heat transfer and evaporation of the droplets and is expected. At very high, supercritical



(a) $T=700$ K

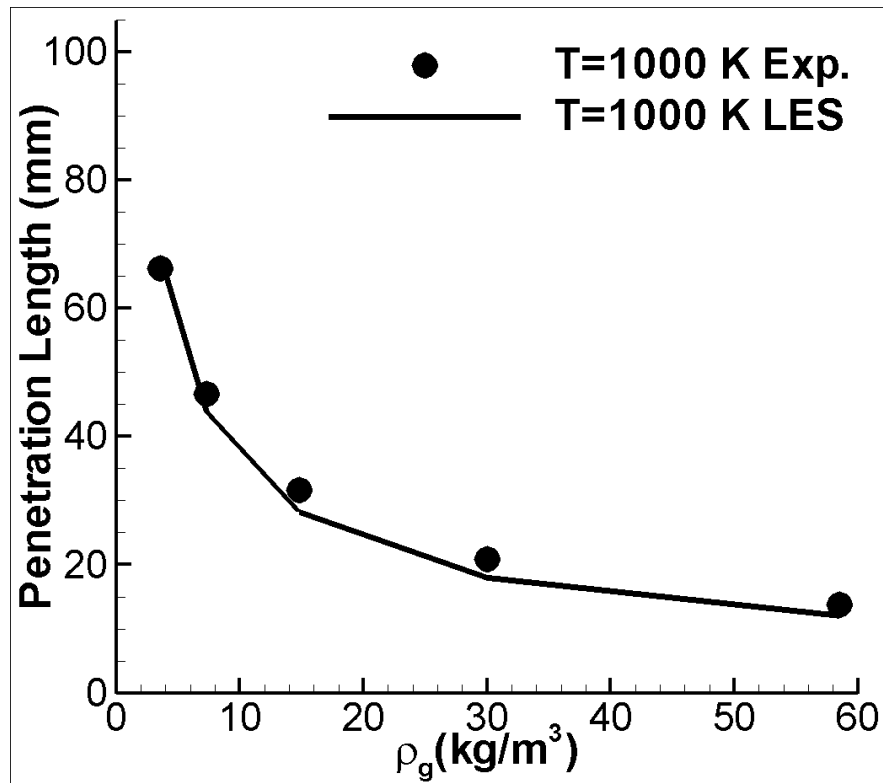


(b) $T=850$ K

Figure 1.5: Comparison of simulated and measured liquid penetration for different ambient conditions.

Figure 1.5: (cont'd)

(c) T=1000 K



(d) T=1150 K

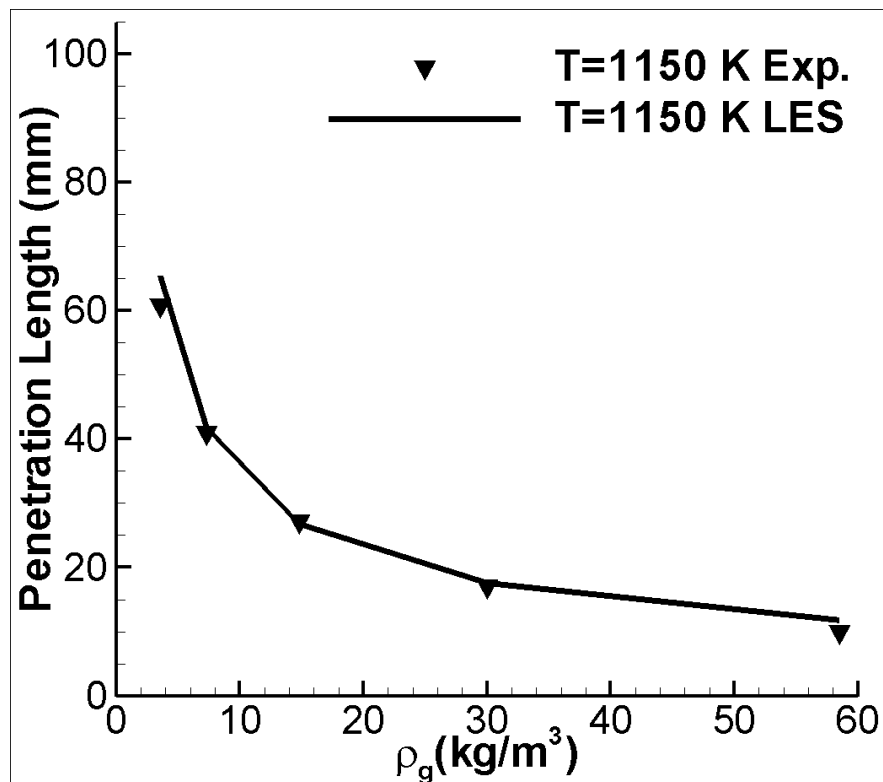
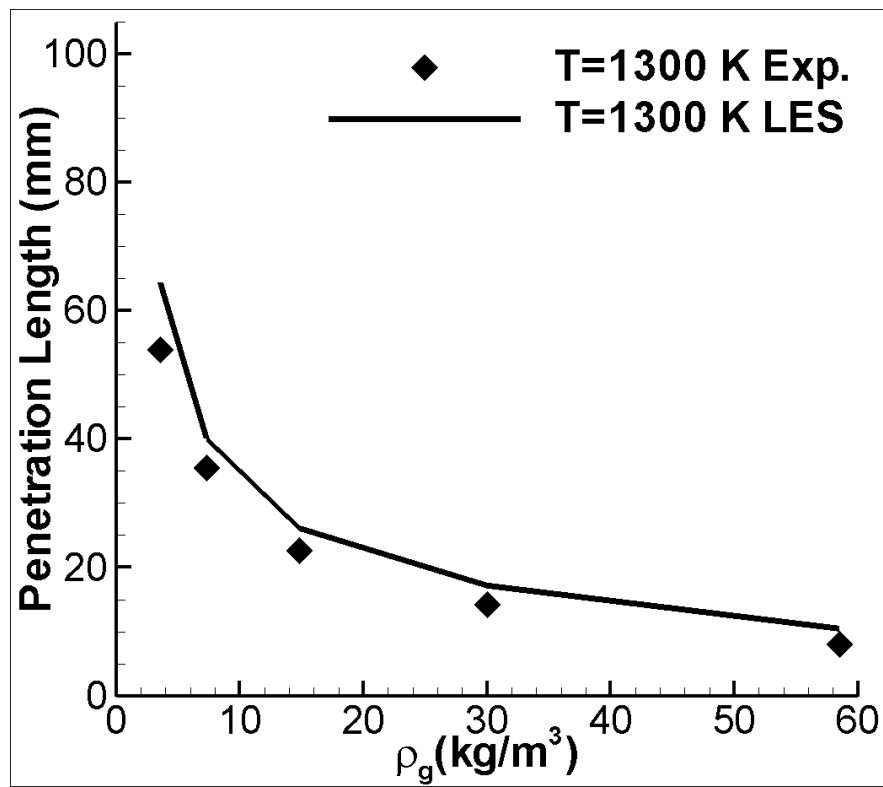


Figure 1.5: (cont'd)

(e) $T=1300$ K



gas temperatures and densities, some of droplets may reach to supercritical conditions. In the absence of a reliable supercritical model in the present calculations, the evaporating spray variables such as the penetration length could start to deviate from the experiment as the supercritical effects become more important. Figure 6 shows the percentage of error for the liquid penetration length for different gas temperatures and densities. It is clear that the error is the most at the highest temperatures and densities.

The increase in ambient gas pressure beyond the critical pressure for the droplets at supercritical temperatures first hinders the evaporation but for even higher gas/droplet temperature, the increase in pressure or density can actually promote the evaporation. At elevated pressures, the liquid-gas phase equilibrium is considerably changed by the ambient gas pressure, normally causing the droplet temperature to rise in the later stages of the evaporation. This means that more heat is transferred to the droplet's interior, because evaporation is hindered at high gas pressures and less heat is needed for the vaporization. However at higher ambient gas temperatures, the droplet heating is fast and the most influential factor determining the phase equilibrium is no longer the ambient gas pressure but the droplet temperature [72]. As shown in Figure 1.6, at supercritical ambient gas temperature of 1000K, the penetration length is slightly underpredicted by the LES at higher gas densities which confirms that higher pressures can hinder the evaporation. By further increase in the gas temperature to 1150K, the effect of pressure fades away and LES results become virtually identical with the experiment. At gas temperature of 1300 K, the high pressure facilitates the evaporation, leading to the overprediction of experimental results. It is clear that there is almost no clear distinction between the liquid penetration lengths predicted by LES for the last two temperatures. This suggests that the supercritical phase equilibrium and gas dissolution into

the liquid droplets are indeed significant. The overprediction of experimental values at gas temperature of 1300 K can also be partially attributed to the transition from the subcritical liquid breakup to the supercritical breakup at elevated supercritical temperatures and pressures as suggested by Segal and Polikhov [73].

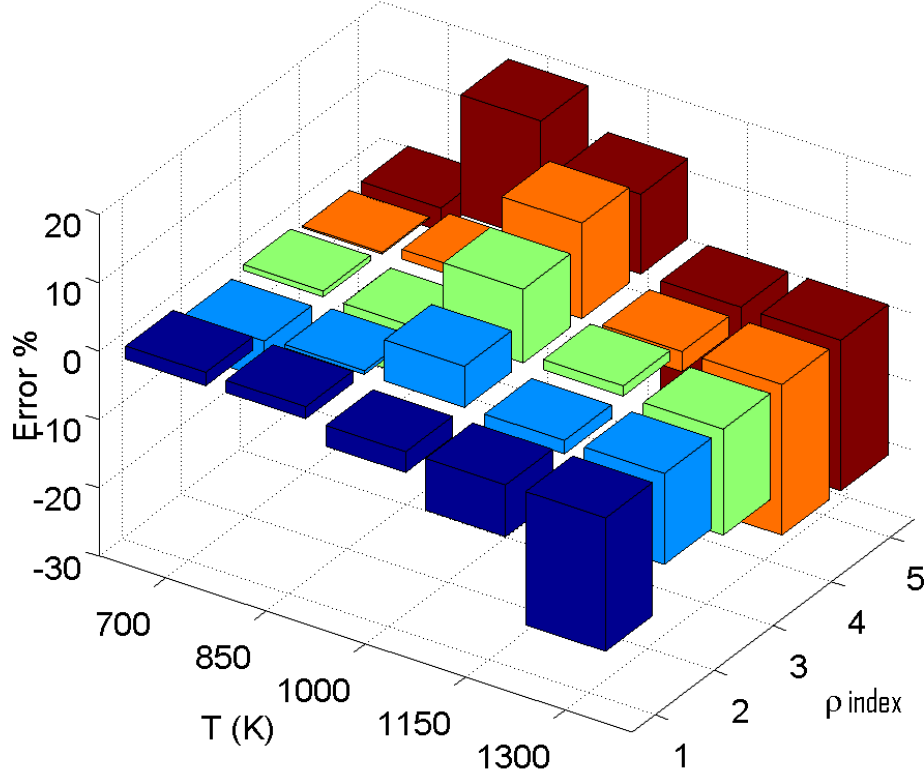


Figure 1.6: Percentage error of liquid penetration prediction for five chamber gas densities at different chamber temperatures.

The global behaviour of the simulated evaporating sprays as parameterized by the liquid penetration length are obviously dependent on the ambient conditions such as the gas chamber density and temperature as well as the gas flow velocity and turbulence. The latter effects seem to be adequately captured by the LES and its SGS models as LES results in Figure 1.5 are generally in a good agreement with the experimental data for all tested gas conditions. To explain this consistency and the trends in the liquid penetration length at different ambient gas and spray conditions, various factors affecting the spray and the computational

model are investigated in more details in the next several sections.

1.3.2.1 Effect of Grid Resolution

Figure 1.7 compares the liquid penetration length for different gas densities and temperatures predicted with several grid sizes ranging from 1.0 to 0.5 mm. Any further grid refinement leads to relatively high liquid volume fractions in the denser part of the spray which requires the reformulation of the carrier gas equations to include the finite liquid volume effect. This is not however the focus of this chapter and is the subject of future work. Nevertheless, the spray penetration lengths obtained by LES at higher gas temperature of 1000 K are nearly the same for all grids. At lower gas temperature of 700 K, as Figure 1.7 shows, the spray length is different and dependent on the grid resolution for coarser grids but is nearly the same for the two finest grids. At this temperature, the evaporation is dependent more on the gas flow and the correct prediction of the near nozzle gas flow, its transition and the induced gas turbulence are all important to the prediction of spray behaviour. Evidently, with $\Delta=1.0$ mm grid LES over-predicts the experimental data at lower gas densities and under-predicts them at higher gas densities. These can be attributed to the lower induced gas velocity and turbulence by the coarser grid which causes different behaviour of spray at low and high gas densities. Simulations conducted with $\Delta=0.75$ mm grid slightly overpredict the experimental values, while the finest grids with $\Delta=0.625$ and 0.500 mm both generate results close enough to experiment to conceive grid convergence. A more detailed discussion of the spray evaporation behaviour at different gas densities is presented below.

The azimuthally averaged radial profiles of the axial gas velocity and its normalized variance for the gas density and temperature of $\rho = 14.8 \text{ kg/m}^3$ and $T=700$ K at $x = 20d_{noz}\sqrt{\rho_l/\rho_g}$ in

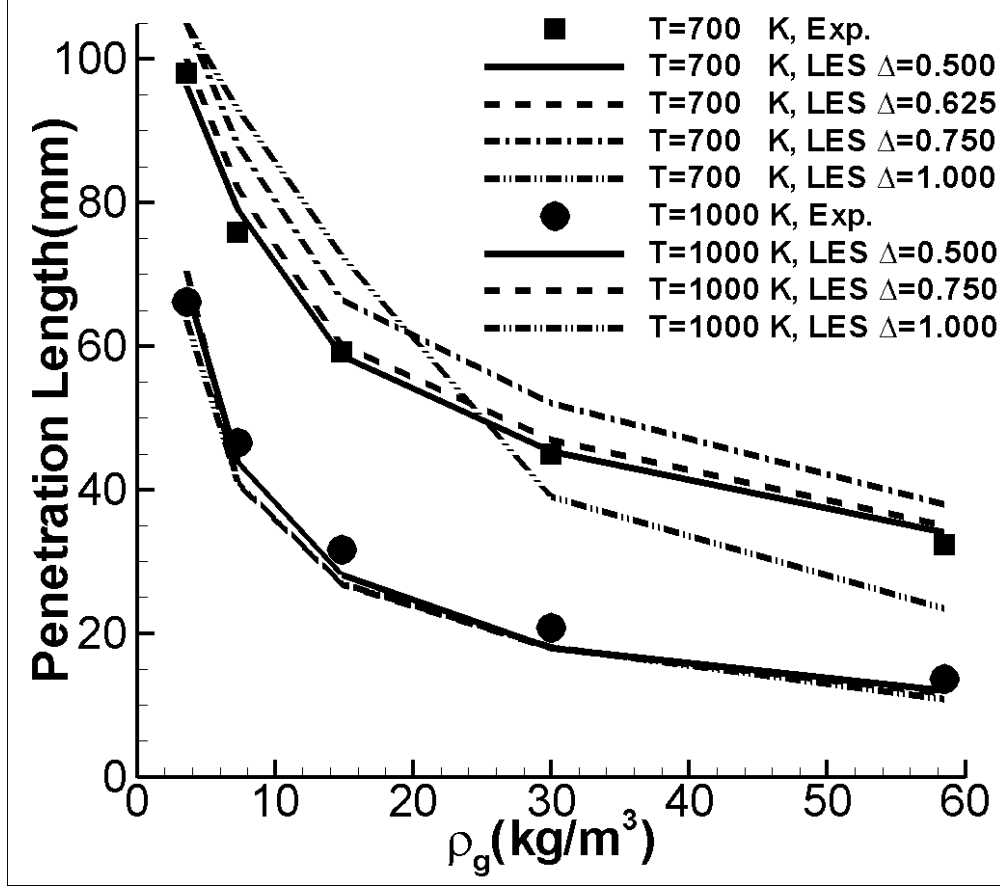
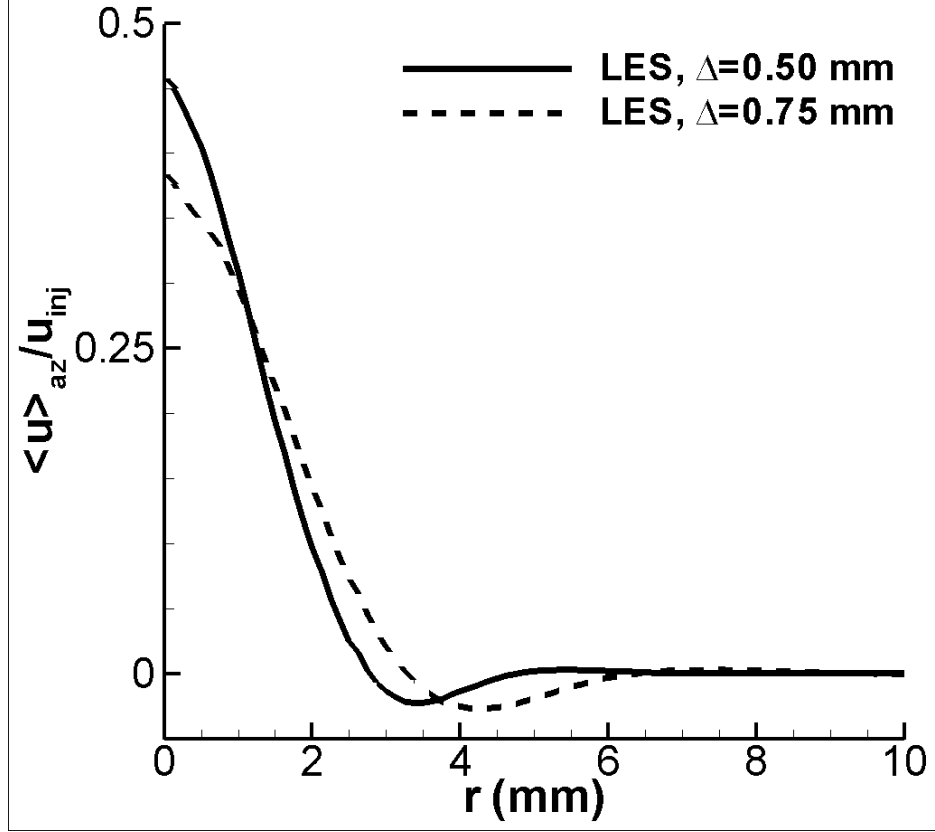


Figure 1.7: Grid size effect on liquid penetration length as a function of density for different temperatures.

Figure 1.8 indicate that with the 0.75 mm grid, the interphase coupling is not fully captured, causing the maximum induced gas velocity to be lower and the velocity profiles more diffused. More importantly, the peak values of the axial velocity variance are comparatively higher for the finer grid of size $\Delta = 0.5$ mm. The higher fluctuations in the inducted gas cause more instability and faster transition to the turbulence in the main gas stream.

Figure 1.9 compares contours of the evaporated vapour in the gas for different LES grid resolutions at the same gas conditions considered in Figure 1.8. For the coarser grid, the vapour concentrations are somewhat diffused due to weaker inter-phase coupling. With the grid refinement, the gas flow instability and turbulence appear further upstream closer to



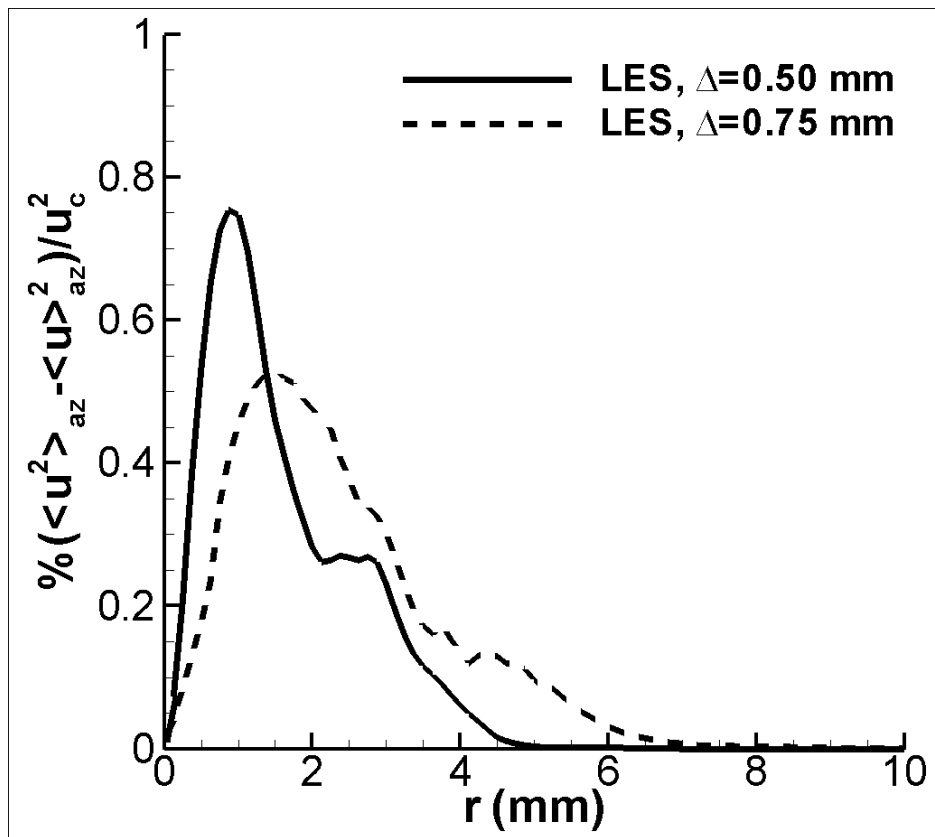
(a)

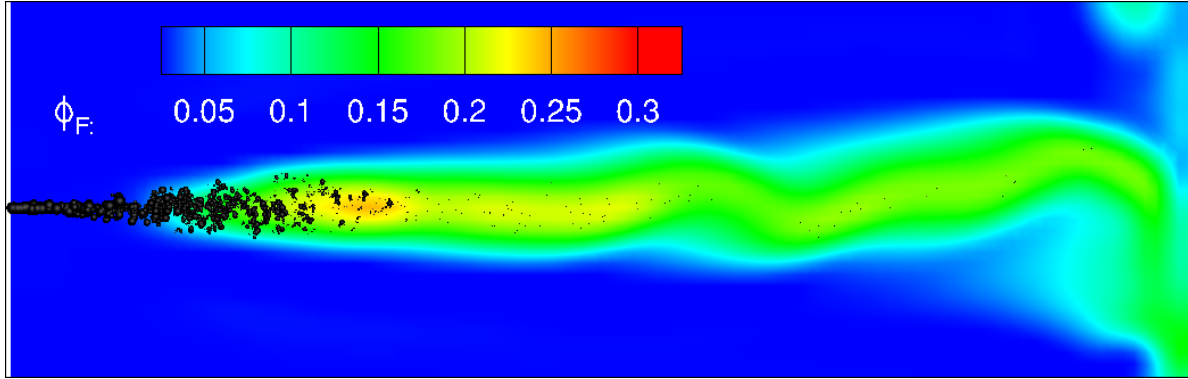
Figure 1.8: Grid size effect on (a) azimuthally-averaged induced gas velocity and (b) its fluctuations at non-dimensional distance of 20 from injector for $\rho = 14.8 \text{ kg/m}^3$ and $T = 700 \text{ K}$.

the nozzle. Subsequently, more significant multi-scale flow structures are generated by the spray with finer grids while the small scale flow is also better captured by the LES. For capturing the near nozzle flow instability a fine grid is required which in some cases may become so small that the gas to liquid volume fraction effects has to be included in the LES formulation and models.

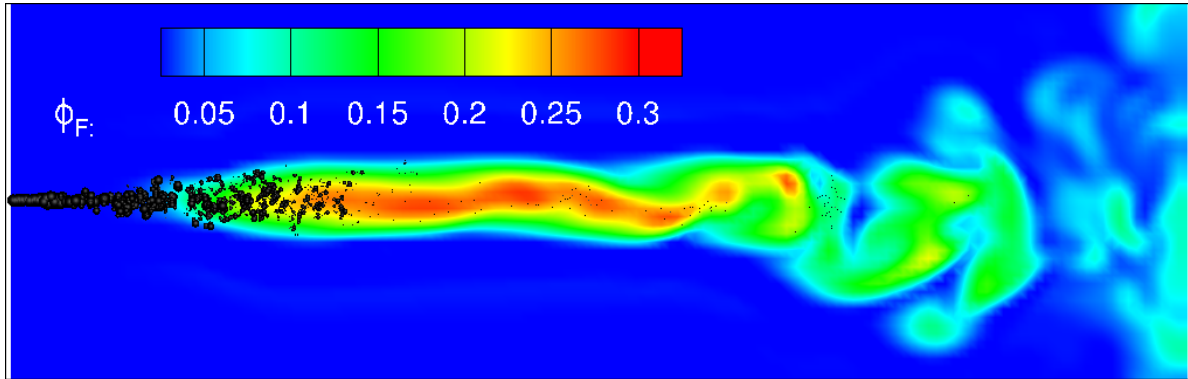
Figure 1.8: (cont'd)

(b)





(a) $\Delta = 1.00$ mm

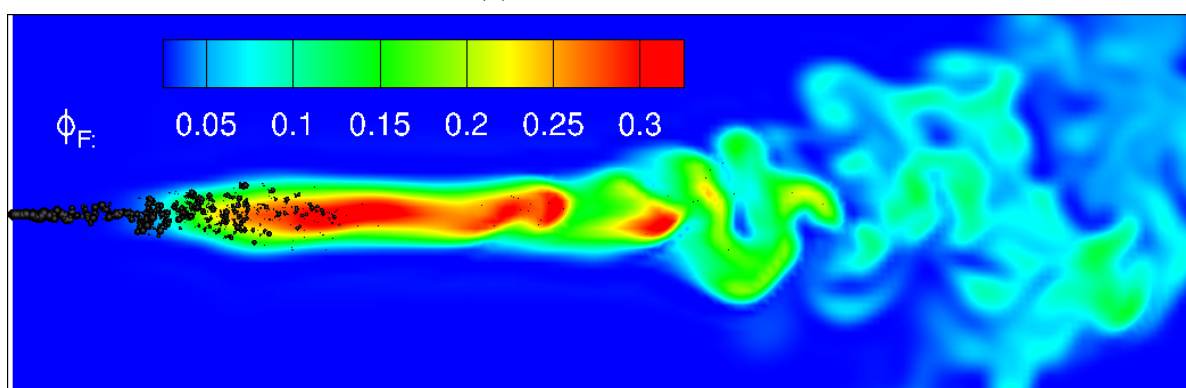


(b) $\Delta = 0.750$ mm

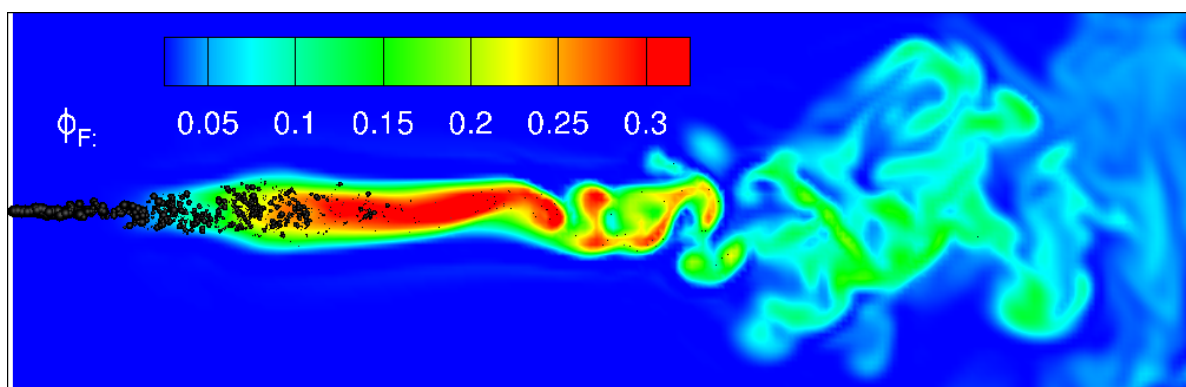
Figure 1.9: Grid size effect on evaporated vapour contours obtained by LES with different grid sizes for $\rho = 14.8 \text{ kg/m}^3$ and $T = 700$ K.

Figure 1.9: (cont'd)

(c) $\Delta = 0.625$ mm



(d) $\Delta = 0.500$ mm



1.3.2.2 Effect of Ambient Gas Conditions

A good parameter for measuring the evaporation in liquid sprays is the non-dimensional evaporation parameter β (equation 1.18). Figure 1.10 shows the effect of ambient gas temperature on the mass averaged β predicted by LES as a function of droplet diameter for the temperature range considered in the experiment. Only small droplets are considered in Figure 1.10 as a major part of mass transfer in the spray is due to the evaporation of these droplets. For the lower temperatures of 700 and 850 K, a considerable part of spray consists of small droplets which survive the evaporation. At these temperatures, the heating rate of colder liquid droplets is not high enough for a “rapid” evaporation of the droplets. The cooling effects of spray on the gas also delay the evaporation and keep the values of β low for all droplet diameters. The cooling effect of droplets stems from not only the latent heat of evaporation, but also from the (sensible) heating of the relatively “cold” fuel vapour released to the ambient gas. The vaporizing gas energy requirement is dependent on the liquid and vapour fuel properties and can be very different for different fuels depending on the relative importance of the two factors mentioned above. It increases with an increase in gas temperature as the phase change energy rate and the amount of “cooler” evaporated gas both increase. Also, with an increase in ambient gas temperature, the evaporation occurs in a shorter distance away from the injector, where the droplets are larger in size and the local relative velocity and temperature difference for droplets is higher. However, despite an increase in the evaporative cooling effects and temperature gradients, droplets will warm up and evaporate considerably faster at gas temperatures of 1000 K or more. At these temperatures, much less number of smaller droplets survive the evaporation as the high values of β in Figure 1.10 suggest. The changes in evaporation cause the gas turbulence induced

by the high speed spray and evaporative gas to be very different and more important to the overall spray behaviour. At lower gas temperatures of 700 or 850K, the dynamics of flow and turbulence generated by the spray are very important and have to be properly considered in the spray and flow/turbulence models as evaporation of small droplets at the tip of spray is dependent on the mixing of vapour saturated, cold induced gas jet with the surrounding unsaturated hot gas. At gas temperatures of 1000 K or more, small droplets evaporate quickly and disappear as they are born, so the evaporation is much less dependent on the turbulence and mixing in the gas.

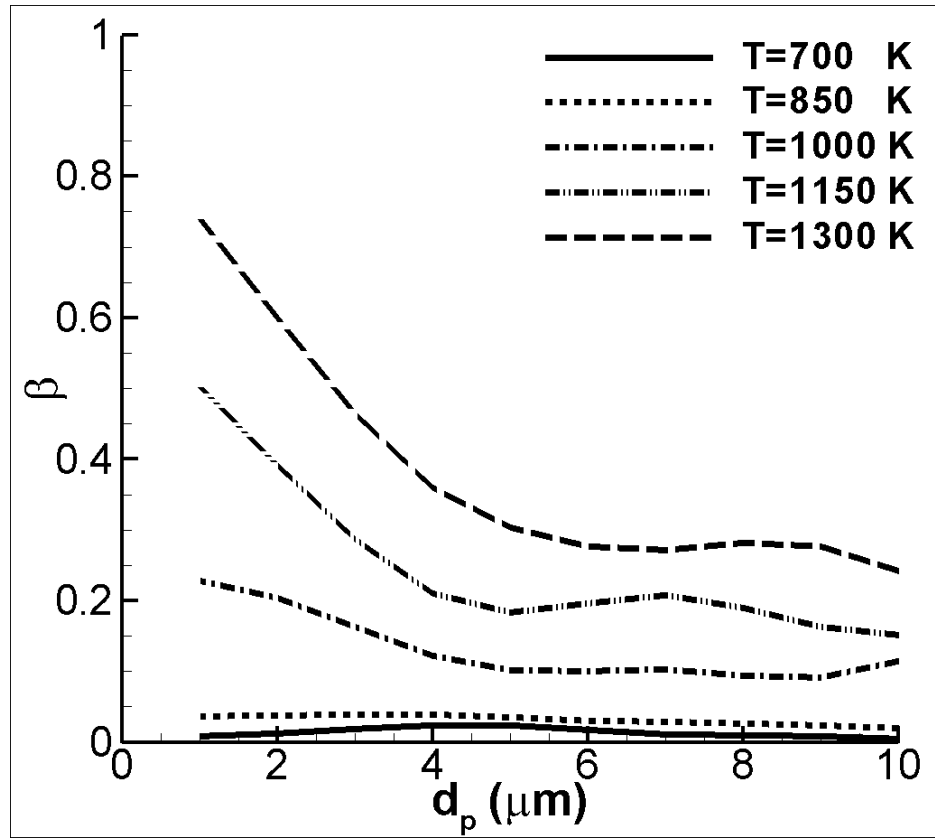


Figure 1.10: Evaporation rate of small droplets for different gas temperatures at $\rho = 14.8 \text{ kg/m}^3$.

Figure 1.11 compares the predicted β values for different gas densities as a function of droplet diameter at the same gas temperature of 700 K. It is clear that the evaporation of

small atomized droplets is considerably reduced with an increase in gas density. A higher gas density should enhance the heat and mass transfer between phases simply because more gas mass is available at the spray location. However, for a high injection pressure spray with very fast liquid jet and droplet velocities, and very significant droplet relative velocity, relative temperature and relative composition, the spray dynamics play a dominant role in controlling the evaporation. At lower gas densities the gas “inertia” will be less and the spray effect on the gas flow velocity, temperature and composition will be more.

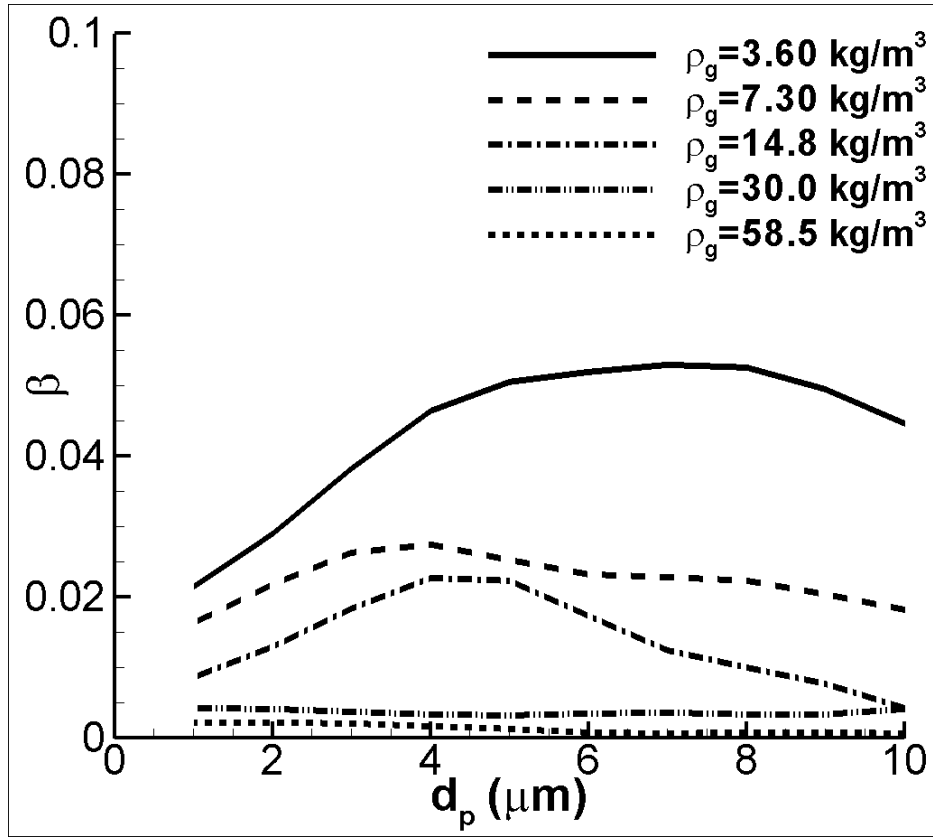
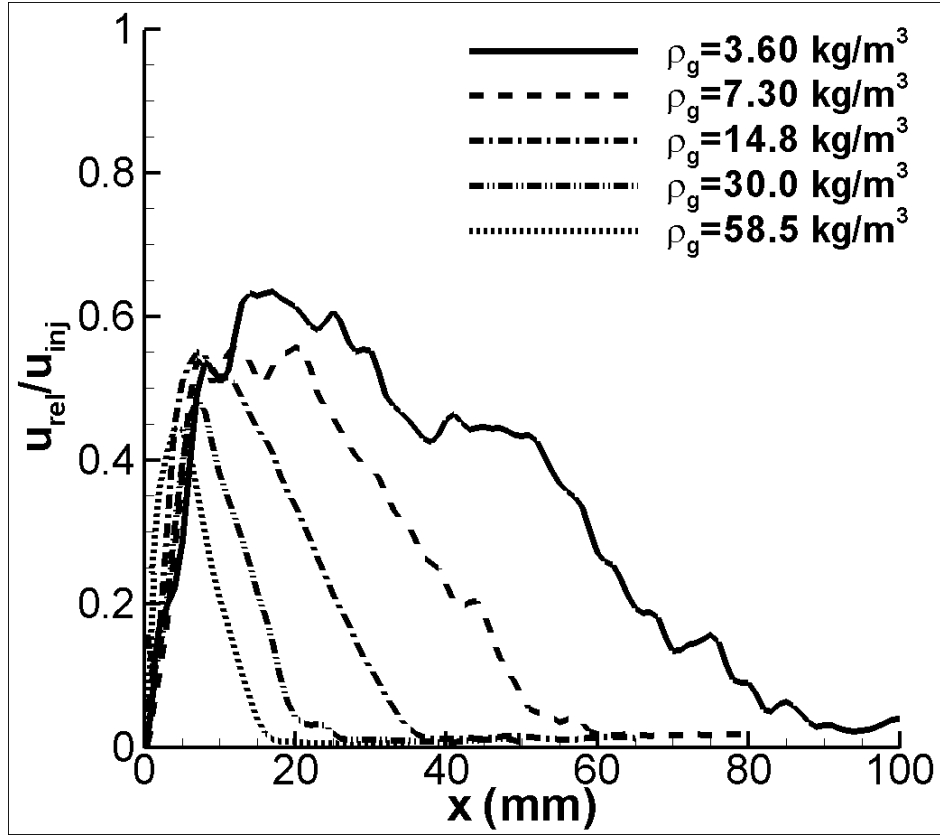


Figure 1.11: Evaporation rate of small droplets for different gas densities at $T=700 \text{ K}$.

To better understand and explain the spray behaviour at different gas densities, the mass averaged relative liquid/spray velocity as a function of axial distance from injector and the azimuthally averaged radial gas velocity profiles at the same non-dimensional distance from the injector ($x = 20d_{noz}\sqrt{\rho_l/\rho_g}$) are compared in Figure 1.12 for different gas densities

at the lower gas temperature of 700 K. Both velocities are normalized with the injection liquid jet velocity for a better comparison. For any gas density, Figure 1.12a shows that the relative velocity between phases first increases in the near injector region where large blobs or drops (representing the liquid jet) are present. By the breakup of this liquid jet and formation of smaller droplets with lower inertia, the relative velocity decreases. There are some oscillations in the relative velocity profiles at lower gas densities which can be attributed to more small scale, gas induced turbulence effect at lower gas densities. Expectedly, there is more resistance in the denser gas against the spray and consequently a decrease in the relative velocity. A higher gas density increases the breakup frequency according to equation 1.30. Consequently, lower relative velocity fluctuations can cause breakup at higher gas densities. This is consistent with the decreasing trend of relative velocity with the gas density as the relative velocity fluctuations scale with the relative velocity itself. Figure 1.12b shows that the radial profiles of the induced gas velocity also becomes narrower at higher gas densities, while the augmented negative gas velocity shows the formation and growth of a much stronger recirculating flow pattern in the gas at higher gas densities. It is to be noted here that the induced gas velocity is more significant at lower gas densities not just because the high speed droplets push better a lower density gas, but also because of larger mean droplet size in the lower gas densities with higher drag forces. The induced gas velocity also helps the evaporation by convecting away the vapour fuel and by preventing the saturation condition in the gas that hinders the evaporation. This is another reason for the higher evaporation rate of small droplets at lower gas densities. Also note that due to smaller average droplet size at any (axial) location from the nozzle for higher gas densities, the overall evaporation rate is higher and the liquid penetration is shorter at higher gas densities.

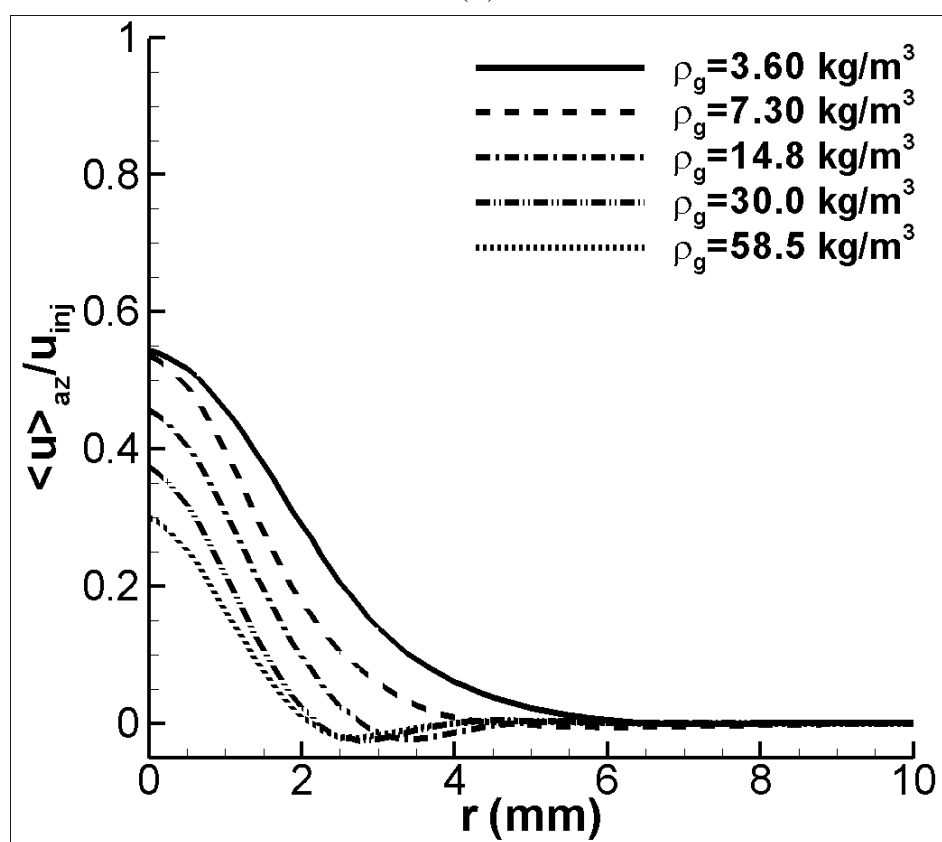


(a)

Figure 1.12: Effect of gas density on (a) mass-averaged relative velocity profile of the spray and (b) the radial profile of azimuthally-averaged, spray-induced gas axial velocity, at the non-dimensional distance of 20 from injector.

Figure 1.12: (cont'd)

(b)



1.3.2.3 Effect of Droplet Wake

When the wake effects of droplets are considered in the model, the drag, the breakup and the evaporation of a considerable number of droplets are changed in the simulations. For these droplets, the relative velocities are lowered by the wake of other droplets, leading to a significant change in the liquid penetration length at nearly all gas temperatures and densities (Figure 1.13). To directly show the effects of droplet wakes on the droplet relative velocity, the normalized values of the relative velocities and relative velocity fluctuations, obtained by LES with and without wake models, are compared in Figure 1.14. The results in Figure 1.14a show that close to the nozzle the relative velocities of big blobs or drops are very small when wake effects are included in the model. As these drops travel downstream in the main liquid spray region, their relative velocities grow due to more exposure to the gas until they become so significant that the breakup occurs. At this point, the relative velocities of daughter droplets start to decrease due to higher drag and also further breakup. However, in the absence of a wake model, the relative velocities of big blobs/drops are already very large and comparable to the spray injection velocity near to the nozzle and only decrease when they break to smaller and smaller droplets. Figure 1.14b shows that the fluctuations or r.m.s. values of the relative velocity are also decreased as bigger drops break into smaller droplets. However, in contrast to the relative velocity trends in Figure 1.14a, the r.m.s. of relative velocity of large drops is much more significant when the wake effects are considered. In other words, while the relative velocity magnitude is decreased, its fluctuations are actually increased by the wake effect such that the breakup occurs earlier. This is especially important for the large drops in the main liquid spray core. By including the wake interactions, these big drops experience considerably higher relative velocity fluctuations when their relative

velocity is reduced due to wakes of leading blobs.

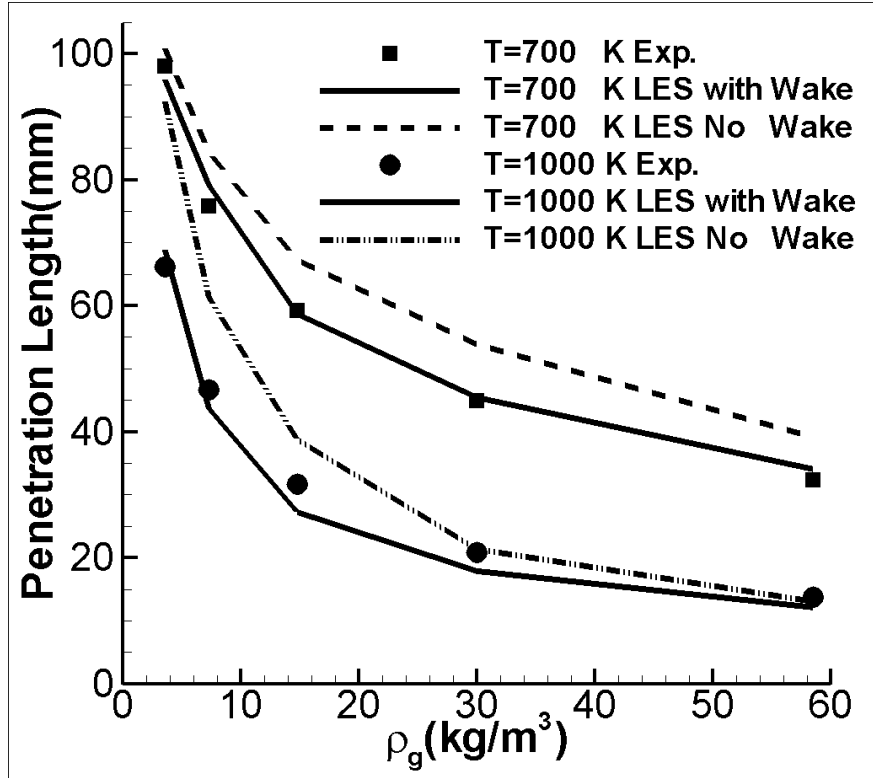
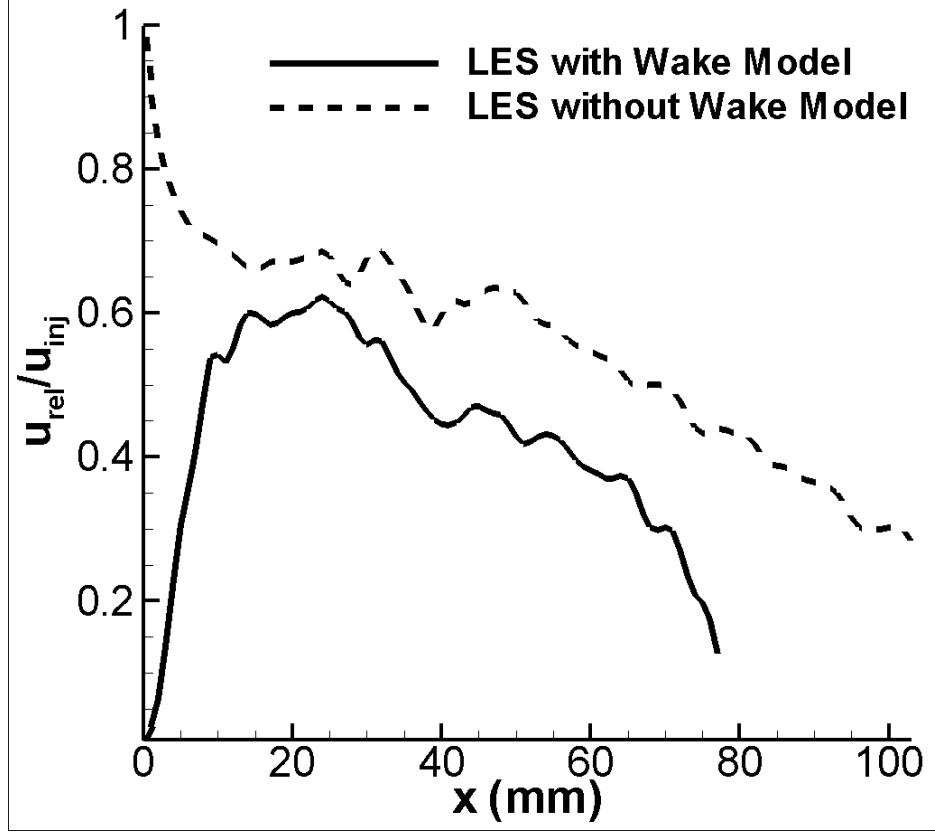


Figure 1.13: Liquid penetration lengths, obtained from experimental data and by LES with and without wake model at different gas densities and temperatures.

At higher gas temperature of 1000 K, the wake effect tends to decrease the penetration length when the gas density is not high. At this temperature, the evaporation is fast and therefore less important to the prediction of spray penetration length in comparison to the spray dynamics and breakup. The wake effect is very significant at low gas densities where mean droplet breakup frequency is lower but fades away as gas density and breakup frequency increases. These are confirmed by the results in Figure 1.15 which shows the droplet SMD profiles for two different gas densities at $T=1000$ K. As observed in this figure, for the lower gas density of 3.6 kg/m^3 , the liquid jet core is predicted to be much longer and the droplet breakup to take place more slowly along the main spray axis when the wake model is not included. The wake effect is understandably less significant away from the main liquid jet



(a)

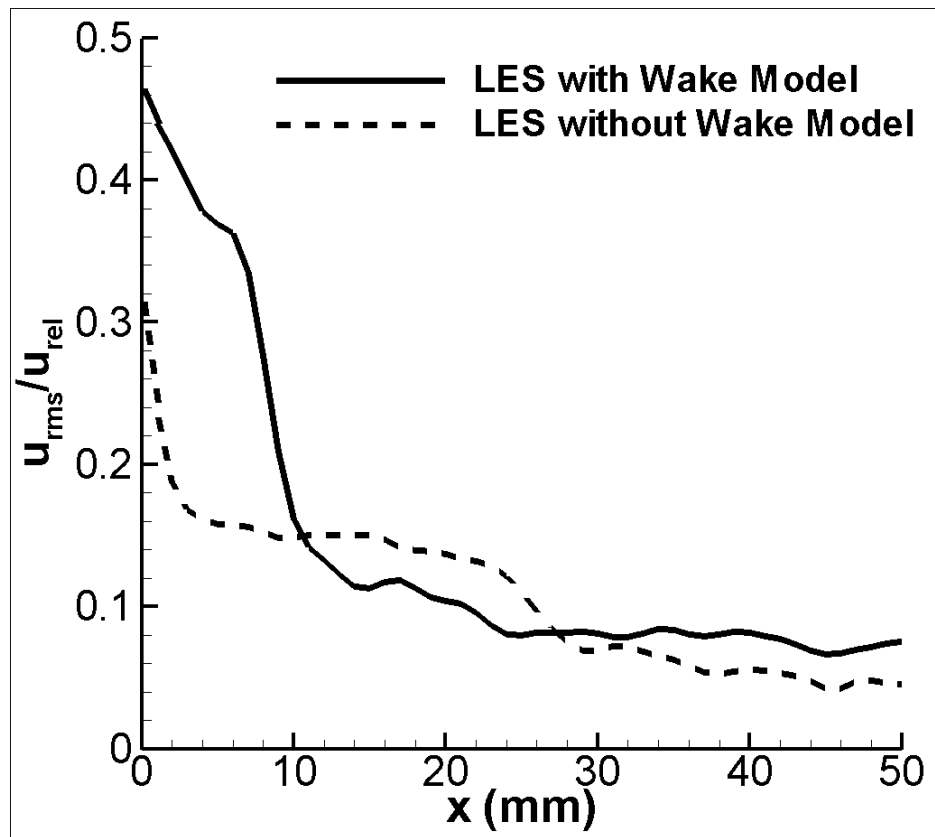
Figure 1.14: Effects of droplet-wake interactions on (a) relative velocity profile of the spray and (b) relative velocity fluctuations for gas density of 3.6 kg/m^3 and temperature of 1000 K.

core where the spray is less dense. At much higher gas density of 30 kg/m^3 , Figure 1.15 shows that the droplet SMD plots obtained with and without wake models are very close to each other. This is partly due to higher evaporation rate which cancels the promoting effect that the droplet wake model has on the breakup. As shown in Figure 1.16a, the evaporation of small droplets, measured by the evaporation parameter β , is much more significant when the wake interactions are not included in the simulations, even though the relative velocities are lower for droplets with no wake interactions (Figure 1.16b).

Keeping other parameters the same, the higher relative velocity is expected to increase the evaporation rate, yet the evaporation rate is shown to be lower when the wake interactions

Figure 1.14: (cont'd)

(b)



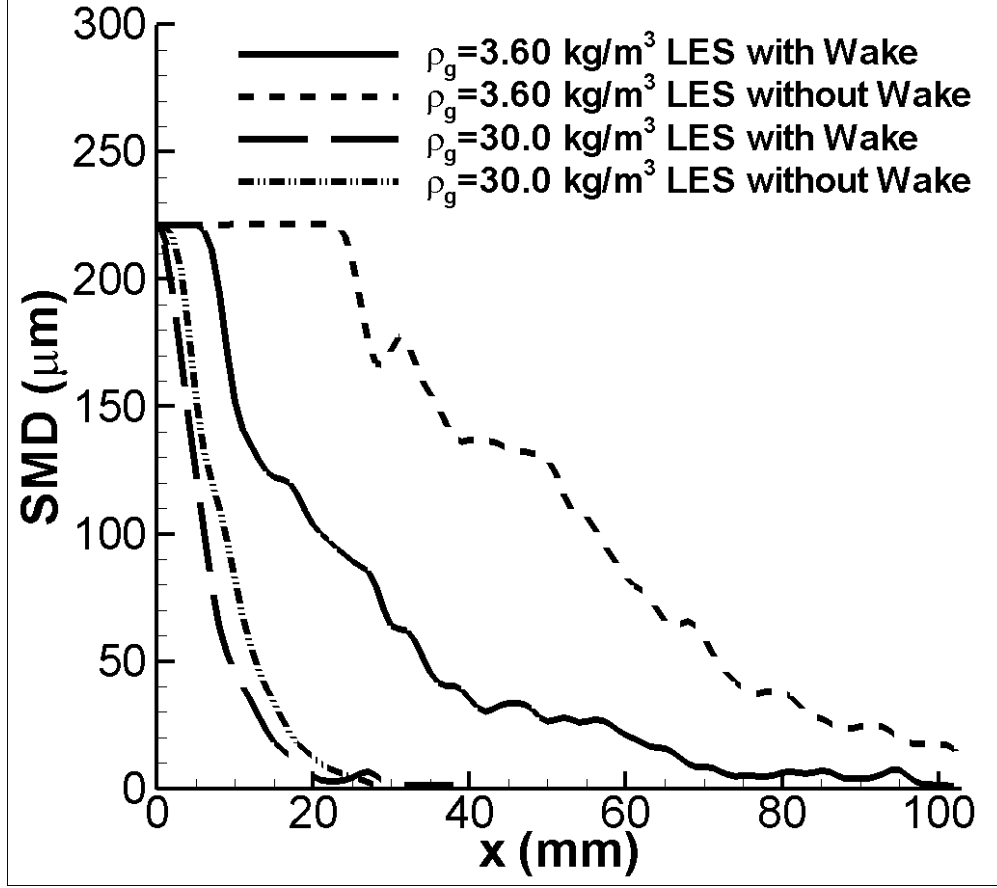
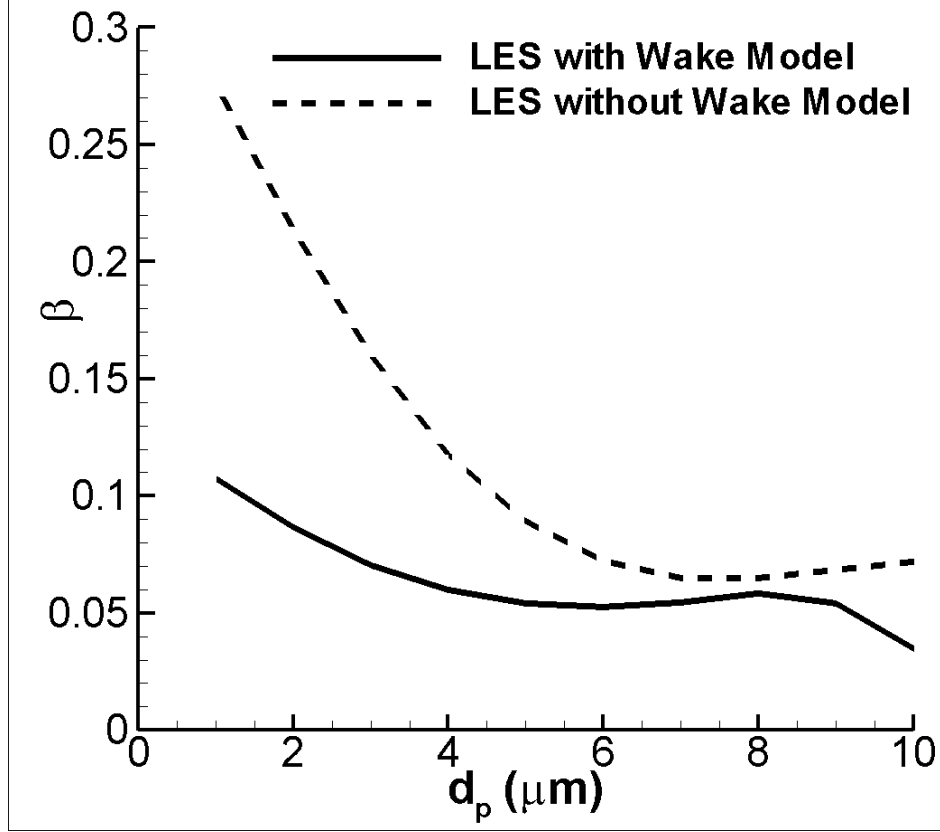


Figure 1.15: Effect of droplet-wake interactions on SMD profiles of spray for different gas densities at temperature of 1000 K.

are considered. To explain this, the radial profiles of the azimuthally averaged induced gas velocity and vapour concentration at axial distance of $x = 20d_{noz}\sqrt{\rho_l/\rho_g}$, obtained by LES with and without the wake model, are compared in Figure 1.17. Evidently, the evaporated vapour fuel concentration is much lower without wake model. The lower vapour concentration in the gas surrounding the droplets paves the way for further evaporation and as a result, the evaporation rate increases. The lower vapour concentration is due to higher induced gas velocity predicted by the LES when the wake interactions are not included. When these interactions are taken into account, the droplet drag force is reduced and consequently the momentum transfer to the gas and the gas induced velocity are decreased.



(a)

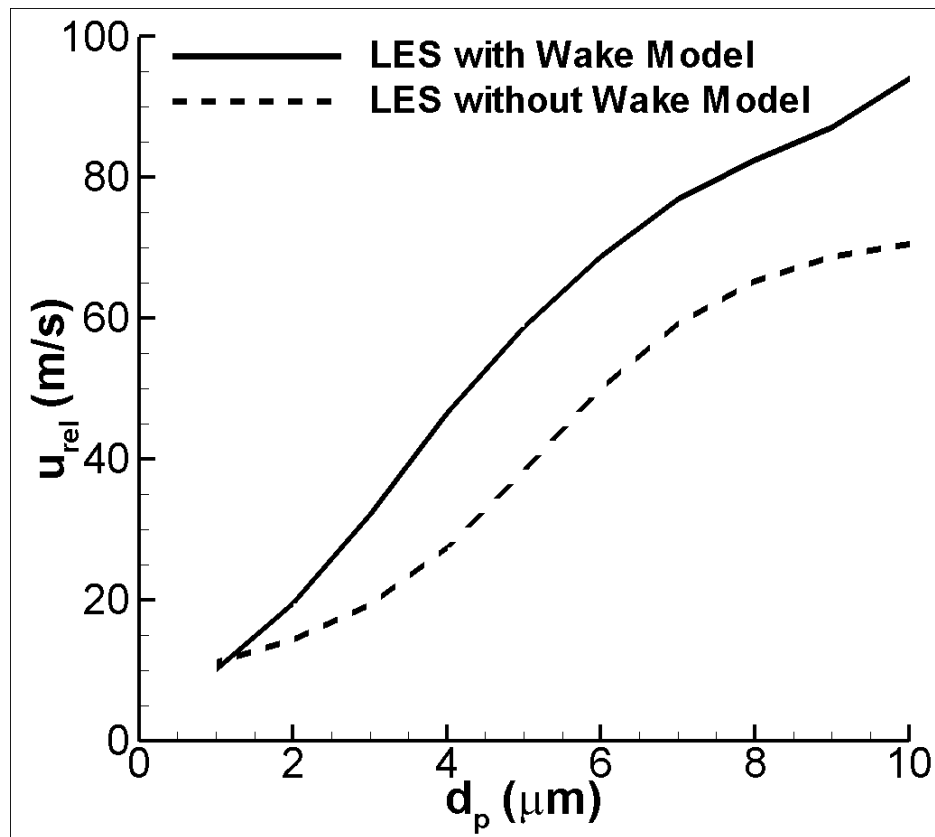
Figure 1.16: Effect of droplet-wake interactions on (a) mass-averaged evaporation rate and (b) mass- averaged relative velocity of small droplets at $\rho = 7.3 \text{ kg/m}^3$ and $T = 1000 \text{ K}$.

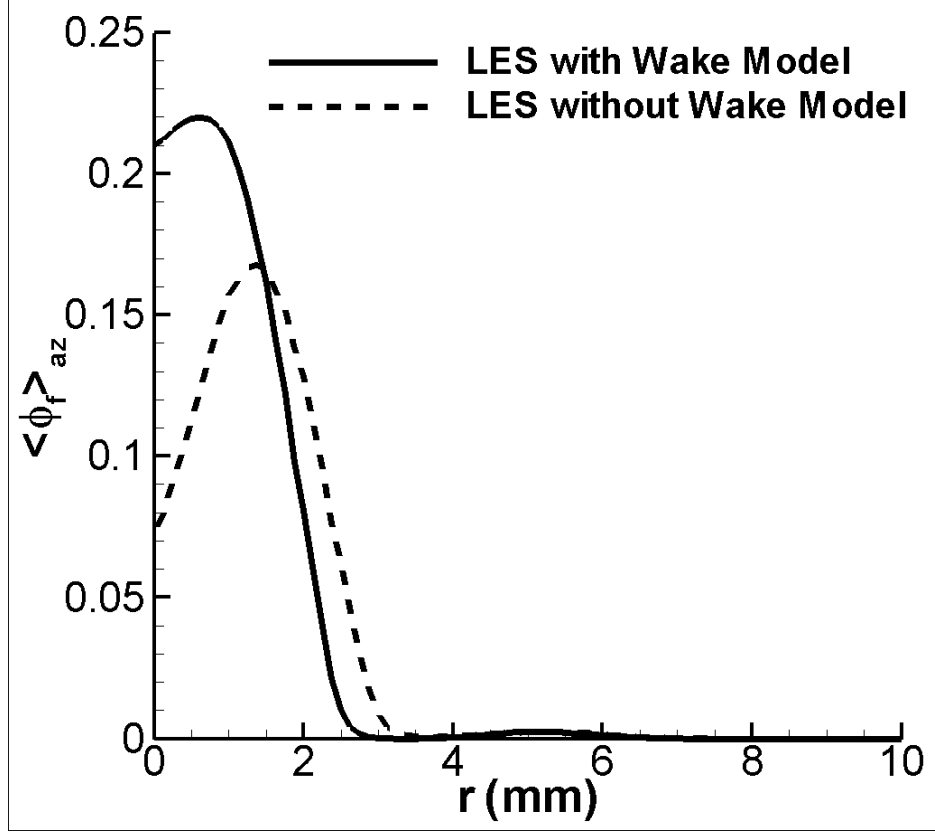
This lower induced velocity is less efficient in convecting the evaporated fuel away from the spray/droplets, resulting in a net decrease in the evaporation rate. For the gas density range considered in the experiment, the LES model seems to always overpredict the experimental penetration length at gas temperature of 700 K when the droplet-wake interactions are not considered (Figure 1.13). The difference between the numerical and experimental values can be attributed to the presence of smaller droplets and more dependency of the spray penetration length to the evaporation than the droplet dynamics and breakup at gas temperature of 700 K.

Figure 1.18 shows the vapour concentration contours obtained by LES with and without

Figure 1.16: (cont'd)

(b)





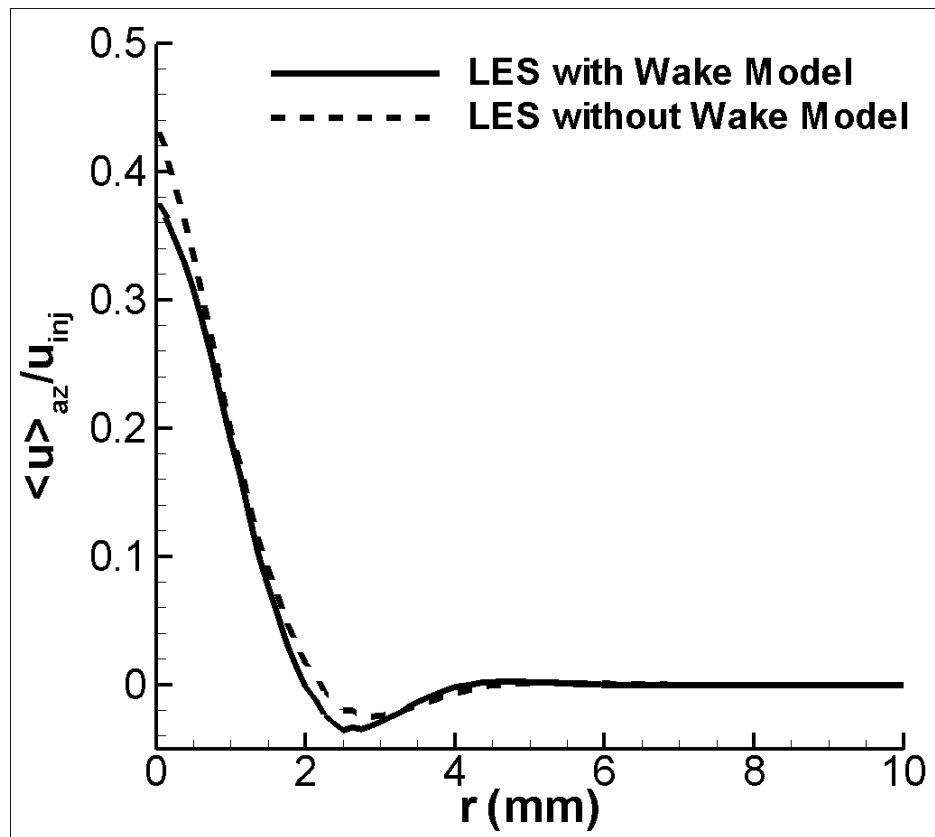
(a)

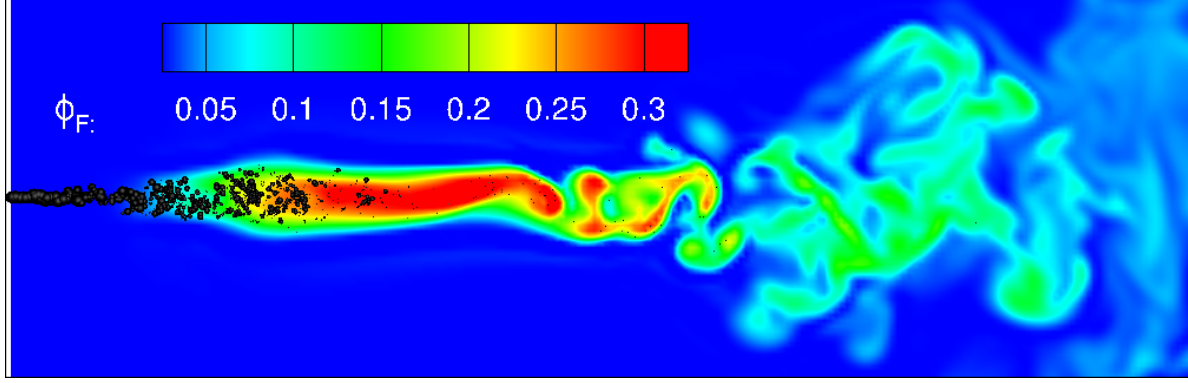
Figure 1.17: Effect of droplet-wake interactions on radial profiles of (a) azimuthally-averaged evaporated fuel mass fraction and (b) azimuthally-averaged induced axial velocity for $\rho=30 \text{ kg/m}^3$ and $T=1000 \text{ K}$ at non-dimensional distance of 15 from injector.

droplet wake model for the lower temperature of 700 K. Due to mass and momentum transfer from spray to the gas, a high speed gas jet is induced along the axis of spray. The induced gas flow is due to droplet drag and the added high kinetic energy fuel vapour and becomes highly unsteady and turbulent at downstream locations. The “potential core” of the gas jet is an important environment for the surviving droplets. At the gas temperature of 700 K, this potential core is predicted by LES to be longer without the droplet wake model as opposed to that with the model (Figure 1.18). The vapour concentration contours in Figure 1.18 show that although the evaporation rate of individual droplets are higher without wake interactions, the overall evaporation in the spray is lower simply because there are

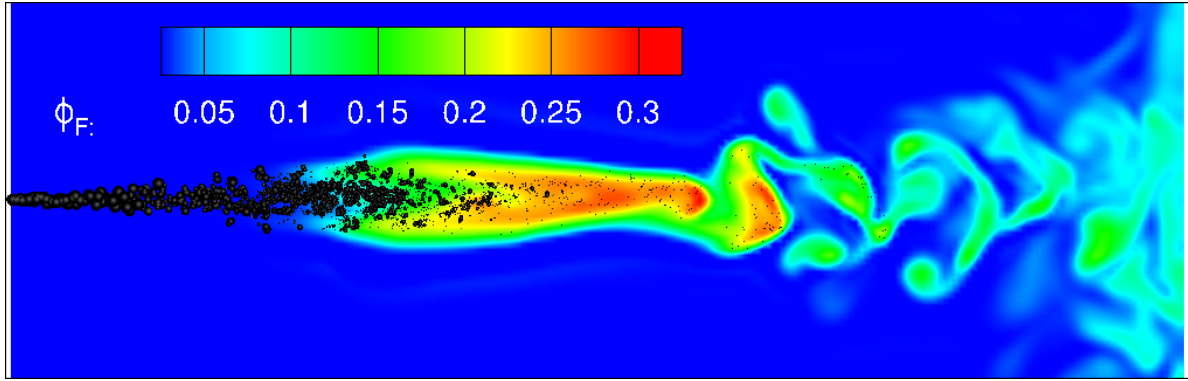
Figure 1.17: (cont'd)

(b)





(a)



(b)

Figure 1.18: Vapour concentration contours with and without wake interactions for gas density of 14.8 kg/m^3 and temperature of 700 K. (a) With droplet-wake interactions, (b) without droplet-wake interactions.

larger number of bigger droplets in the spray simulated by LES without wake model. When the droplet-wake interactions are included, the added mass of high kinetic energy vapour promotes the turbulence in the gas jet. Without the wake effect and with less added mass, the gas jet experiences slower transition to the turbulence. As a result, droplets survive longer and hence the liquid penetration length is predicted to be longer.

1.3.2.4 Effect of Subgrid Turbulence and Particle Models

Figure 1.19 compares the liquid penetration lengths obtained by LES with constant and dynamic coefficient subgrid turbulent kinetic energy (k_{sgs}) equation models with the ex-

perimental data for various gas densities at two different gas temperatures. At higher gas temperature of 1000 K, the SGS model seems to play a less significant role on the spray evolution as the penetration lengths predicted by LES with dynamic and constant coefficient SGS kinetic energy models are not very different. This trend has been observed in all of our simulations for all tested turbulence models and numerical methods. The effect of SGS turbulence model on the global spray results is also not very important at lower gas temperature of 700K when the gas density is relatively low but becomes very significant at higher gas densities at this temperature. To explain the results in Figure 1.19, the axial variations of the SGS kinetic energy, k_{sgs} and its production (which is the SGS dissipation of the resolved flow) are shown along the spray axis in Figure 1.20 for gas density and temperature of 30 kg/m^3 and 700 K. Evidently, the SGS kinetic energy itself, and more importantly its production are both predicted to be more significant when constant coefficient SGS kinetic energy equation model is employed. This indicates that the LES with the constant coefficient model can generate significant small scale turbulent motions downstream of the main liquid jet core, contrary to the fact that in this region the mean relative velocity of droplets is large and the momentum transfer between phases mainly occurs at large scales. Associated with the much higher SGS kinetic energy production in the LES model due to constant c_ν , is the enhanced SGS energy dissipation and also enhanced diffusion due to constant c_k which ultimately lowers the large scale and global gas jet velocity. It is, therefore, clear that not all of the extra energy transferred to the subgrid scales by the constant coefficient model affects k_{sgs} since part of this energy is dissipated and diffused by higher dissipation and diffusion predicted by the constant coefficient model.

Figure 1.21 compares the evaporation rates of small droplets for two gas densities of 14.8 and

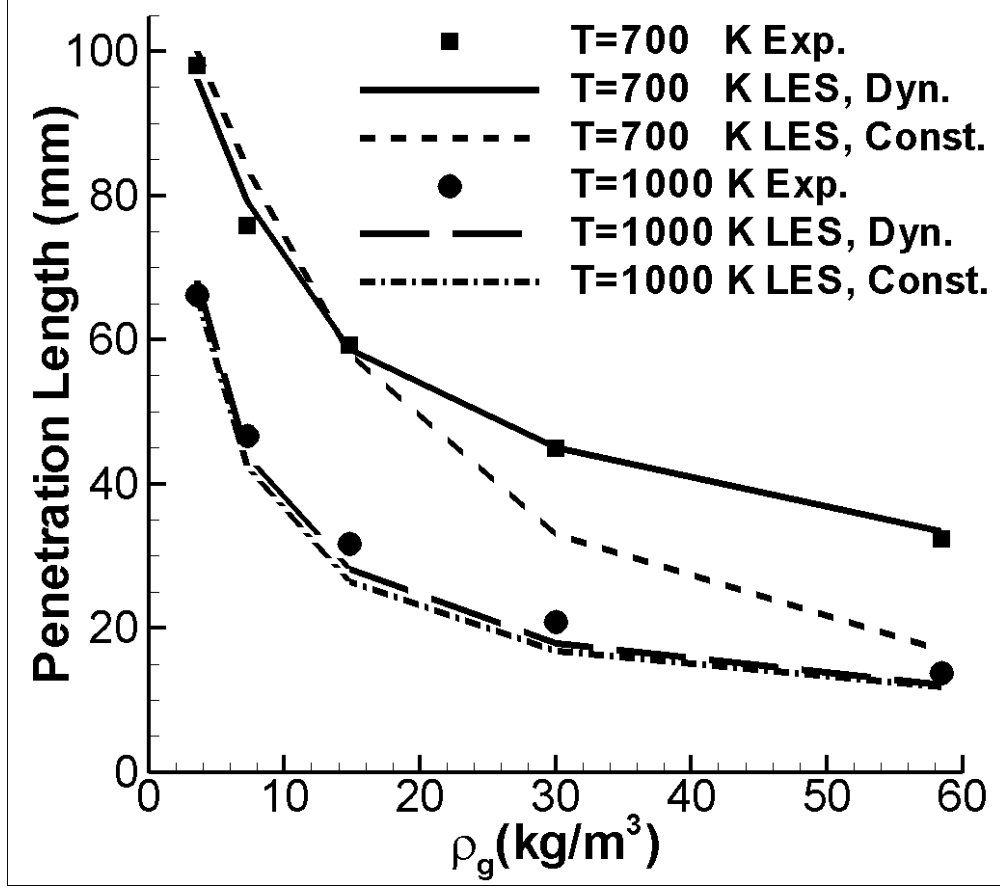
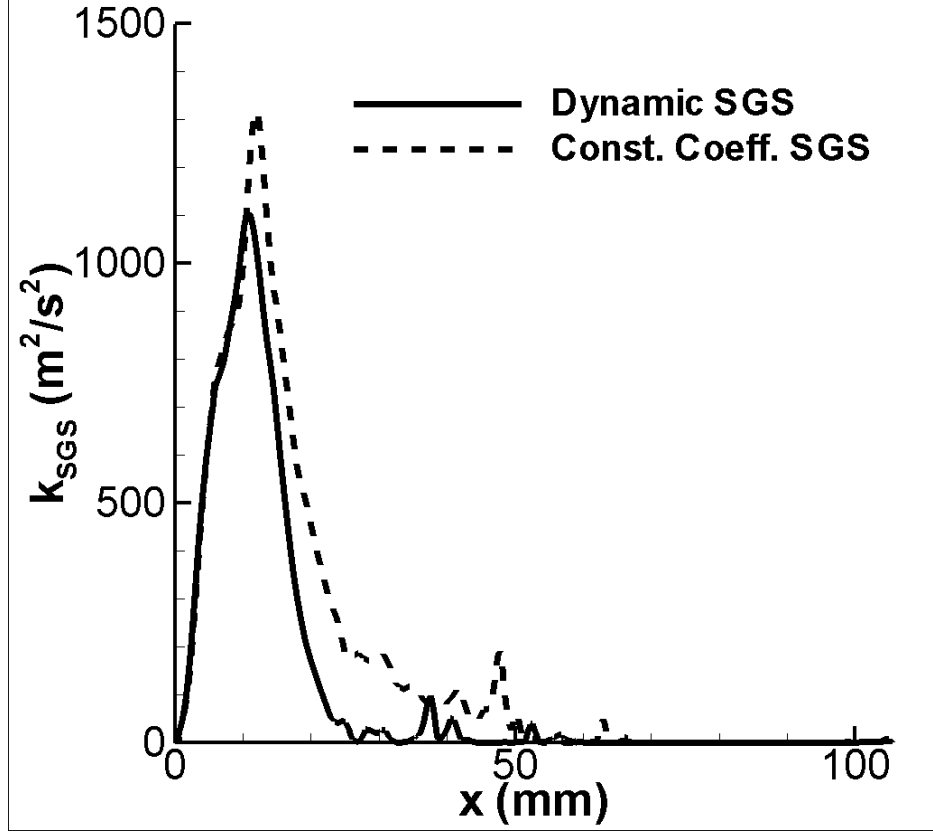


Figure 1.19: Penetration length v.s. gas density as predicted by LES with constant coefficient and dynamic coefficient SGS kinetic energy equation models at different gas temperatures.

30 kg/m^3 at $T=700 \text{ K}$. It is clear that the LES with dynamic subgrid model predicts less evaporation than the LES with constant coefficient model at the lower gas density. However, the difference in evaporation rate is much more pronounced at the higher gas density. The weaker large scale/global gas velocity computed by LES with constant coefficient subgrid model (due to more energy transfer to subgrid scales) cause comparatively higher relative velocity and more evaporation for droplets. This is illustrated in Figure 1.22, where the mass averaged relative velocity of small droplets obtained by the constant coefficient and dynamic subgrid turbulence models are compared. As pointed out earlier, the spray generated gas velocity depends on the gas density as the evaporation induces more velocity in the gas



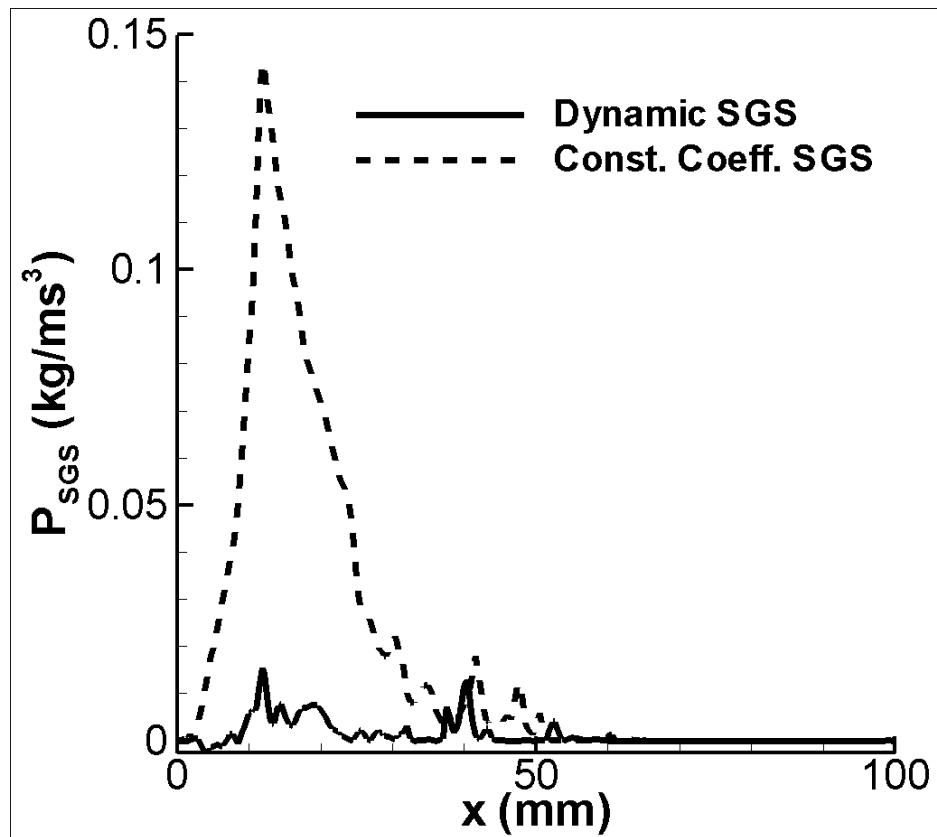
(a)

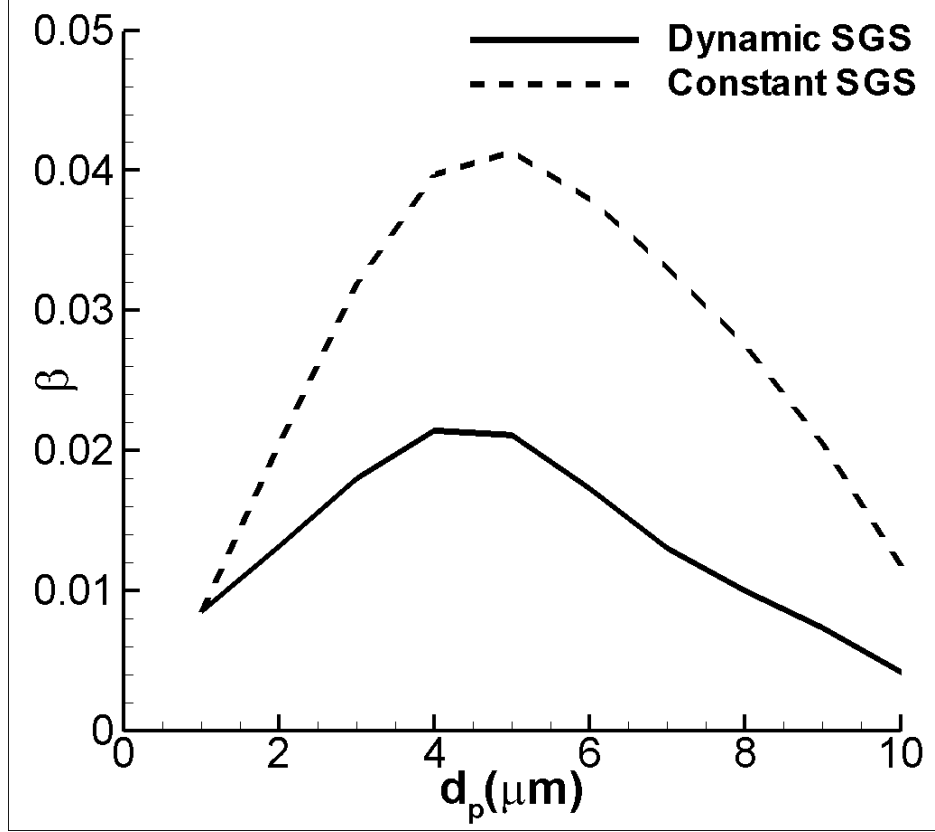
Figure 1.20: Axial variations of the subgrid kinetic energy and its production for constant coefficient and dynamic coefficient SGS kinetic energy equation model at gas temperature and density of $T=700$ K and $\rho = 30 \text{ kg/m}^3$. (a) Subgrid kinetic energy and (b) production of SGS kinetic energy.

at lower gas densities. On the other hand, the higher evaporation rate predicted by LES with constant coefficient k_{sgs} model induces more velocity in the gas and lowers the relative velocity of droplets at sufficiently low gas densities. The lower relative velocity in turn hinders the evaporation. The net effect will be a balance between the two competing factors. At higher gas densities, the higher evaporation rate by the constant coefficient subgrid model induces weaker gas velocity; therefore droplets can maintain higher relative velocities which lead to more significant evaporation. The relative velocity has a much more significant effect on the evaporation at elevated gas densities as shown and explained before. Thus, the net

Figure 1.20: (cont'd)

(b)





(a) $\rho = 14.8 kg/m^3$

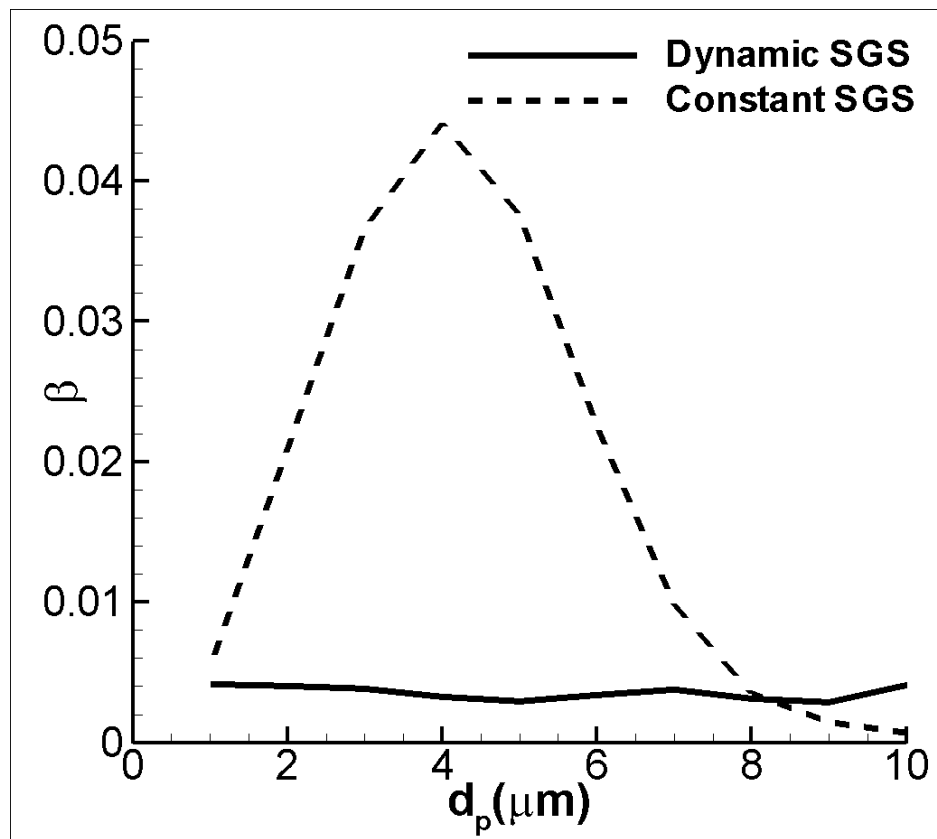
Figure 1.21: Evaporation rate parameter of small droplets predicted by LES with constant and dynamic coefficient SGS kinetic energy equation model for gas temperature of $T=700$ K and different gas densities.

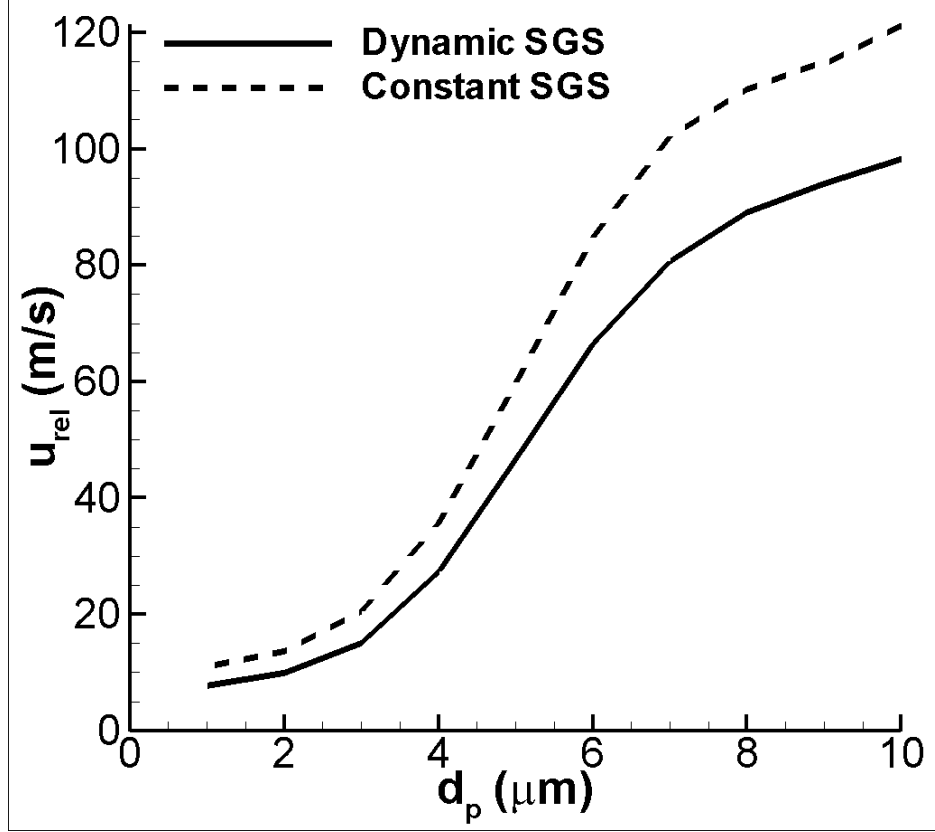
effect is such that the relative velocity and evaporation are higher when constant coefficient subgrid kinetic energy equation model is employed, especially at higher gas densities. The increase in droplet evaporation leads to a shorter penetration length at sufficiently high gas densities and low gas temperatures. The same gas droplet momentum interactions occur at higher gas temperatures, but they are less important simply because atomized droplets warm up and disappear much faster and their evaporation is less dependent on the gas flow dynamics at higher ambient gas temperatures.

To show the effect of subgrid turbulence model on the evaporation and liquid vapour, in Figure 1.23 the vapour contours obtained by the dynamic and constant coefficient models

Figure 1.21: (cont'd)

(b) $\rho = 30.0 kg/m^3$





(a) $\rho = 14.8 \text{ kg/m}^3$

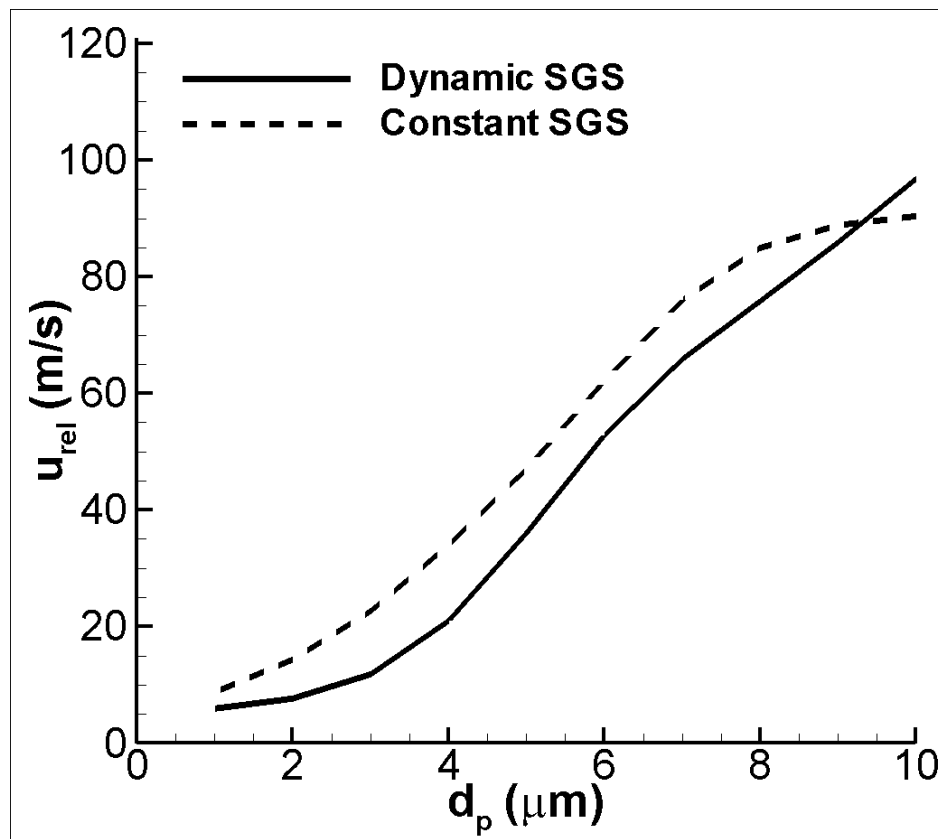
Figure 1.22: Relative velocity of small droplets as predicted by LES with constant and dynamic coefficient SGS kinetic energy equation model for gas temperature of $T=700 \text{ K}$ and different gas densities.

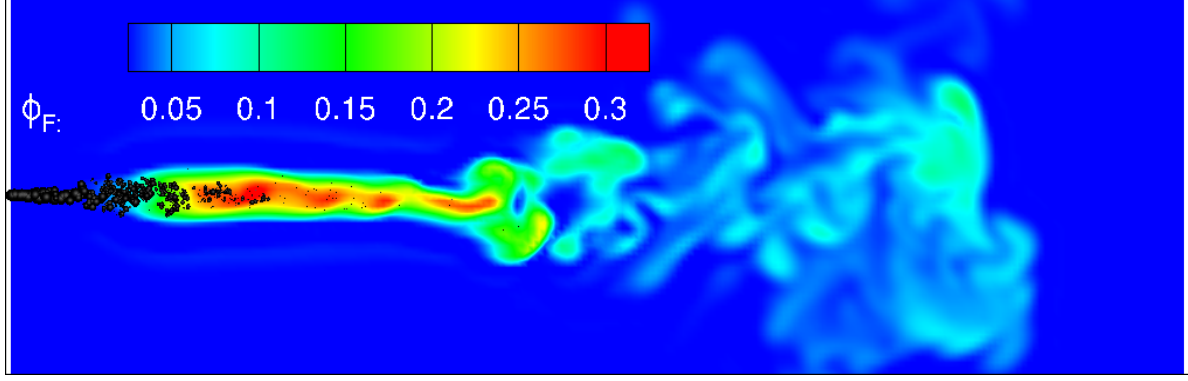
for gas density and temperature of 30 kg/m^3 and $T=700 \text{ K}$ are compared. As shown, with the more accurate dynamic model the spray induced gas jet breaks down at a relatively shorter distance from the injector and upon breaking, it creates more small scales compared to the case with constant coefficient model. While the breaking point of the gas jet predicted by LES with dynamic model correlates well with the liquid penetration length; with the constant coefficient subgrid model the evaporation is artificially increased such that the liquid length is predicted to be much shorter than the gas jet breaking point at higher gas densities.

Figure 1.24 shows the effect of subgrid droplet dispersion model on the liquid penetration length at different gas densities and temperatures. It is observed that the subgrid dispersion

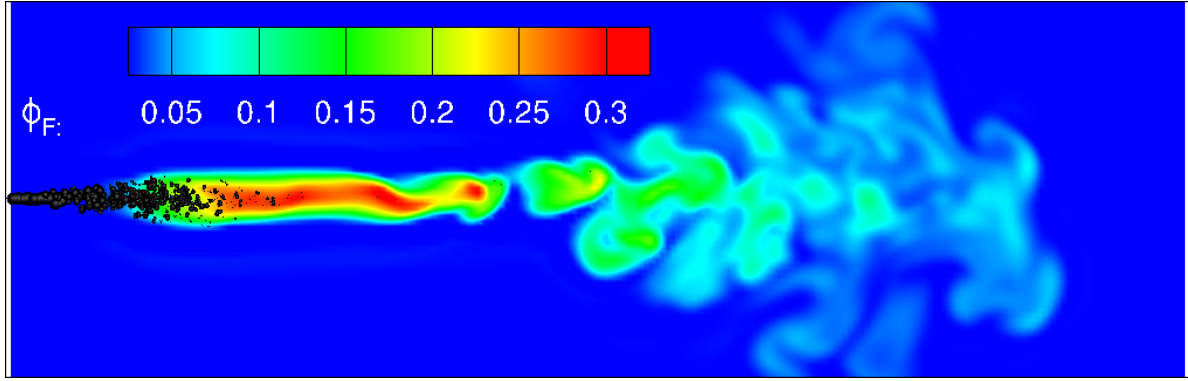
Figure 1.22: (cont'd)

(b) $\rho = 30.0 \text{ kg/m}^3$





(a)



(b)

Figure 1.23: Contours of the evaporated fuel vapour in a mid spanwise plane for gas density and temperature of $\rho = 30 \text{ kg/m}^3$ and $T=700 \text{ K}$. (a) Dynamic SGS model, (b) constant coefficient SGS model.

model does not have a substantial effect on the liquid penetration length. This can be an indication of well prediction of the droplet-gas flow and turbulence. Expectedly, the overall effect of the subgrid dispersion model is to reduce the liquid penetration. This is more pronounced at lower gas temperature of 700 K at which the liquid penetration length is more sensitive to the droplet gas flow dynamics. The minor reduction in the liquid penetration by the subgrid dispersion model is due to a slight increase in relative velocity for small droplets as depicted in Figure 1.25. The results in this figure for the intermediate gas density of 14.8 kg/m^3 and relatively low temperature of 700 K show a slightly more evaporation for a slightly higher relative velocity.

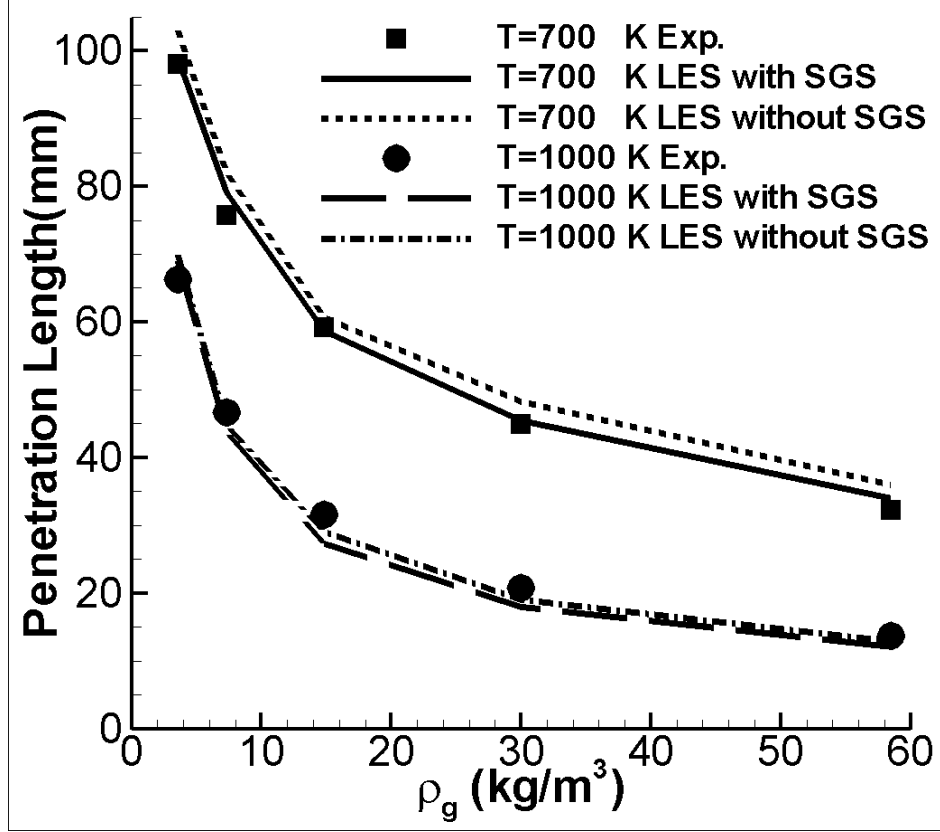


Figure 1.24: Effect of subgrid dispersion on liquid penetration at different gas densities and temperatures.

As stated above, the effect of droplet collision/coalescence on the spray is dependent on the evaporation and is expected to be secondary when evaporation is significant. To better understand this, liquid penetration length obtained by LES with and without collision/coalescence models are compared in Figure 1.26 for the lower ambient gas temperature of 700 K and intermediate gas density of 14.8 kg/m^3 . The droplet-droplet interactions are expected to be more pronounced at these conditions due to longer penetration and relatively lower evaporation rate. As shown in Figure 1.26, after the spray reaches to its pseudo-steady condition, the mean liquid penetration length is slightly shorter when collision and coalescence models are included. This may be attributed to the slightly wider spray as a result of mostly bouncing and grazing collisions of droplets and also slightly faster local evaporation due to

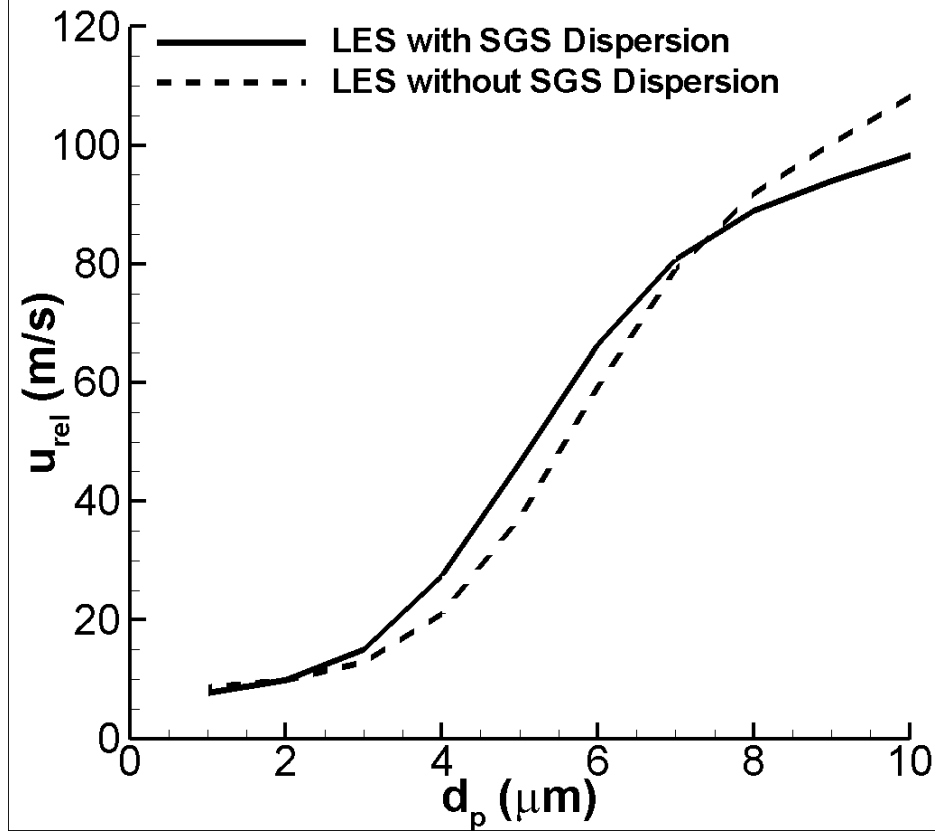


Figure 1.25: Effect of subgrid dispersion model on the relative velocity of small droplets for gas density and temperature of $\rho = 30\text{kg/m}^3$ and $T=700$ K.

fragmentations and satellite droplet formation by the reflexive and stretching separations [74]-[75]. Figure 1.27 compares the predicted SMD profiles and the evaporation parameter β for small droplets by LES with and without collision/ coalescence models. As expected, the evaporation rates for small droplets are higher, while the overall SMD profiles remain almost the same. The higher local evaporation rate for small droplets explains the slight decrease in liquid penetration length. The vapour mass fraction contours in Figure 1.28 indicate that while evaporation rates are higher locally for some of small droplets when collision and coalescence are included, the overall evaporation of spray does not significantly change by the inclusion of these models.

While the droplet subgrid dispersion and collision/coalescence models do not seem to have

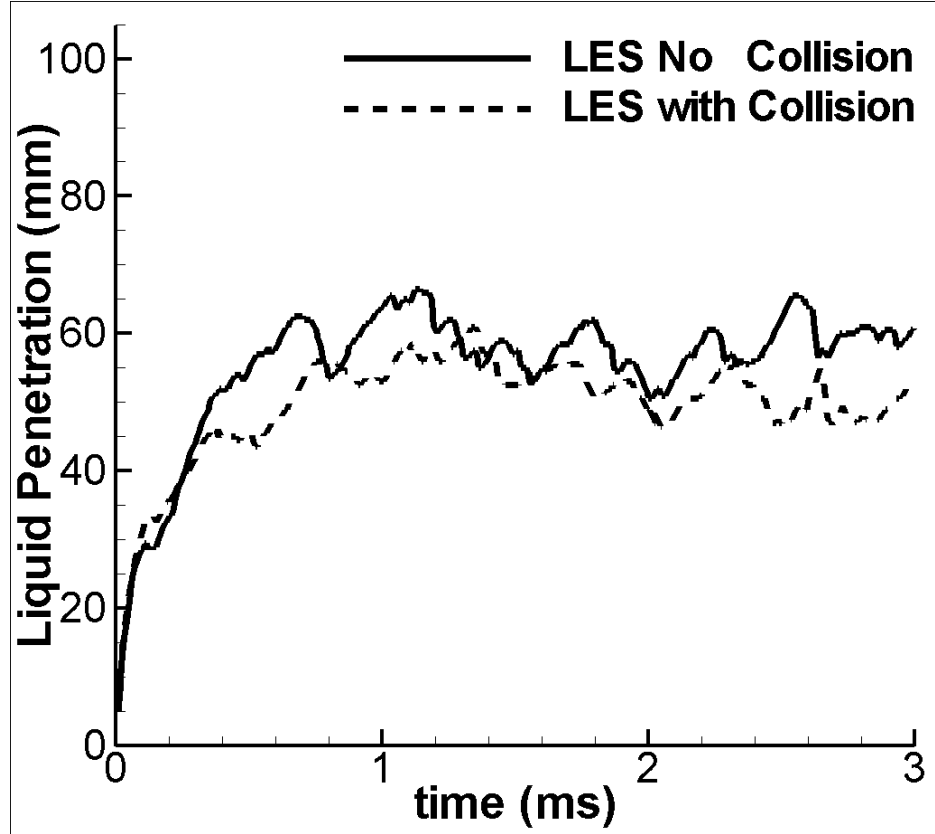
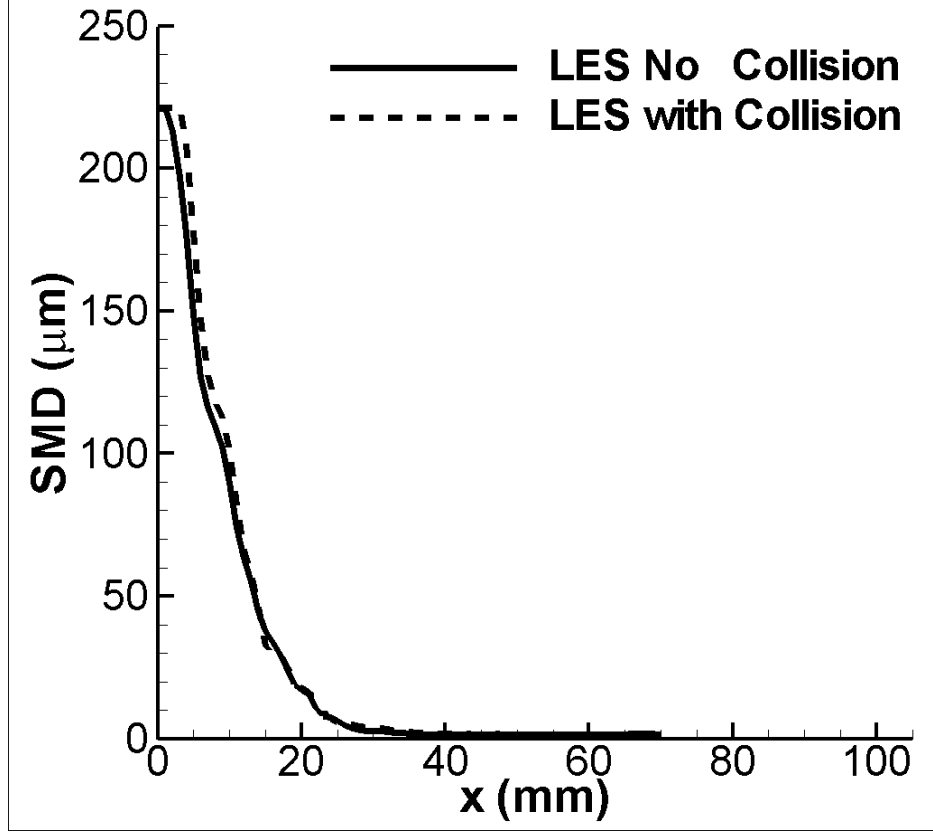


Figure 1.26: Liquid Penetration predicted by LES with and without collision/coalescence models for gas density and temperature of $\rho = 30 \text{ kg/m}^3$ and $T=700 \text{ K}$.

a significant effect on the overall spray behaviour, the model used for computing the heat and mass transfers inside the droplet does [76]. This is illustrated in Figure 1.29, where the liquid penetration length obtained with two different droplet heat and mass transfer models are shown. The finite rate model directly solves the temperature and species equations for any multicomponent liquid inside each individual droplet and is obviously superior to the lumped model which only assumes the interior droplet temperature and species concentration to be uniform. The former model is used in all of our simulations discussed in this chapter. However, to show the significance of the finite rate droplet heat and mass transfer models in the simulated high speed evaporating sprays, we have also considered the spray with the lumped model [42] in the results shown in Figure 1.29 for ambient gas temperature of 1000



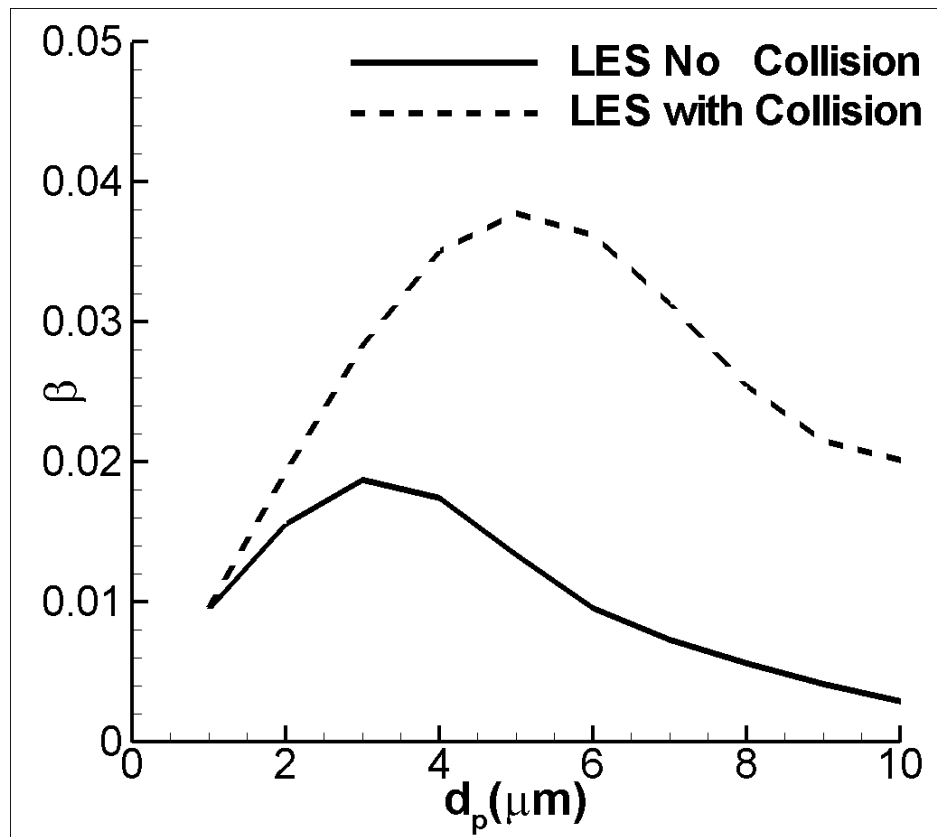
(a)

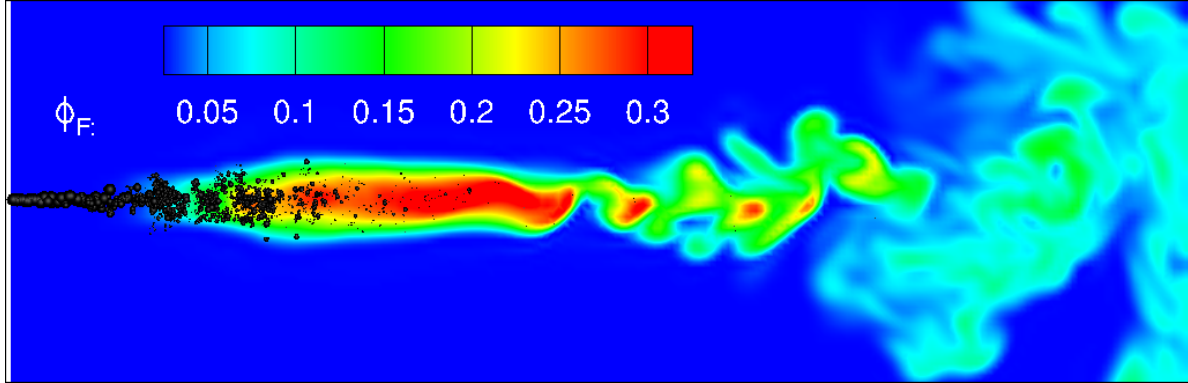
Figure 1.27: Spray variables obtained by LES with and without collision/coalescence models for gas density and temperature of $\rho = 7.3 \text{ kg/m}^3$ and $T=700\text{K}$. (a) SMD, (b) evaporation parameter for small droplets.

K and intermediate density of 14.8 kg/m^3 . Evidently, the lumped model causes significant error in the spray calculations at gas temperature of 1000 K. The effect is much less at lower gas temperature of 700 K (not shown). At higher gas temperatures, the rate of heat and mass transfer between phases is obviously higher, giving less time to the droplet interior to adjust to the time variations of the droplet surface (interface) conditions. Thus, more finite rate heat and mass transfer effects are expected. The lumped model does not include the finite rate effects and as a result liquid penetration is dependent on large scale mixing in the gas. For this reason, we observe more large scale oscillations in the penetration length data in Figure 1.29.

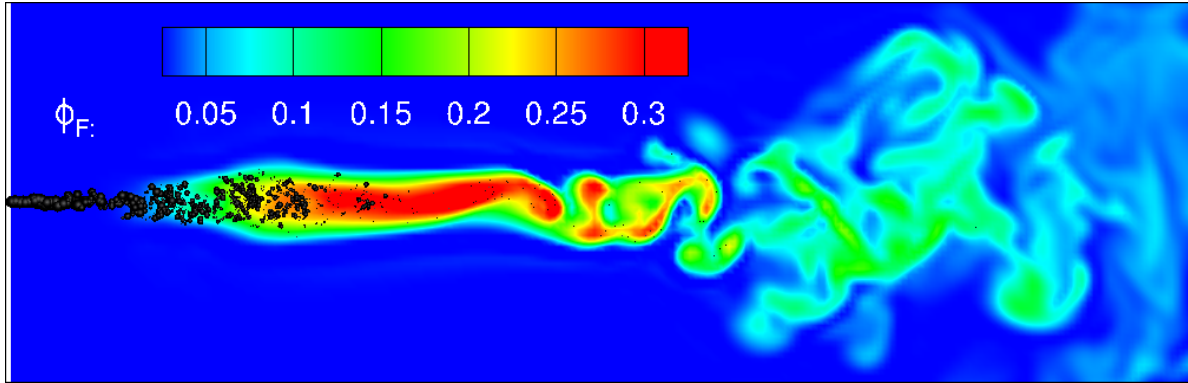
Figure 1.27: (cont'd)

(b)





(a)



(b)

Figure 1.28: Vapour concentration contours obtained with and without collision/coalescence models for gas density of $\rho = 30 \text{ kg/m}^3$ and $T=700 \text{ K}$. (a) With collision/coalescence model, (b) without collision/coalescence model.

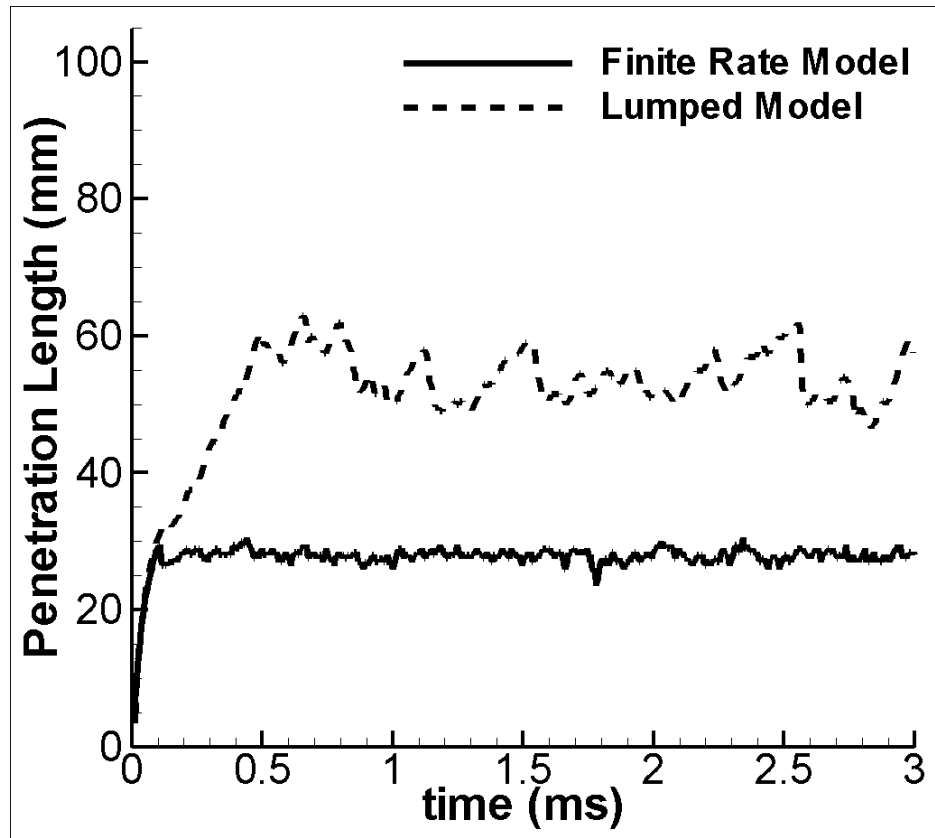


Figure 1.29: Liquid penetration predicted by finite-rate and lumped inner droplet heat and mass transfer models for gas density and temperature of $\rho = 30 \text{ kg/m}^3$ and $T = 1000 \text{ K}$.

1.4 Summary and Conclusions

Large eddy simulations of very high speed evaporating sprays issuing into a quiescent gas chamber are performed with a hybrid Eulerian-Lagrangian mathematical/ computational model. For the gas phase, the Favre-filtered Navier-Stokes, energy and fuel mass fraction equations are solved together with the dynamic subgrid turbulent kinetic energy equation. The liquid spray simulations are based on a Lagrangian model in which the atomization process is viewed as a discrete random process with uncorrelated breakup events, independent of the initial droplet size. The size and number density of the newly produced droplets by the breakup is assumed to be governed by a Fokker-Planck equation used for the evolution of the PDF of droplet radii. The droplet breakup frequency is based on the fluctuations of the local relative velocities of the gas and droplet which is found by Lagrangian time averaging of data along the droplet path. The modification of droplet and gas aerodynamics by the wake of nearby droplets is taken into account through corrections to the relative velocity. Also, the finite rate droplet heat and mass transfer are taken into account by solving the spherically symmetric conservation equations inside individual droplets together with the interface equations for the phase coupling.

The global spray results generated with the hybrid Eulerian-Lagrangian LES/spray model (e.g. the liquid penetration length) were found to be in good agreement with the experimental data for different ambient gas pressures for non-evaporating sprays and different gas densities and temperatures for the very high speed evaporating sprays considered in this work. For non-evaporating sprays, higher breakup frequencies at higher pressures are shown to shorten the liquid penetration length. For evaporating sprays, the increase in gas density is shown to substantially increase the breakup of droplets through faster decrease in mean

droplet size along the spray axis. The gas temperature through its effect on evaporation was shown to decrease the effect of gas/droplet flow dynamics when increased, making the numerical predictions by the LES/spray model to become less sensitive to the turbulence models at higher temperatures. Moreover, our simulations indicate that the droplet-wake interactions have a significant effect on the global spray behaviour and spray variables like the liquid penetration length through their effects on the droplet aerodynamics, breakup and evaporation. It is shown that due to slower evaporation, longer spray penetration length is predicted by the LES/spray model when the droplet-wake interactions are ignored. This was related to different gas flow and turbulence induced by the spray which experiences weaker atomization without droplet-wake interactions.

The evolution of spray and gas flow for different grid resolutions indicate that the global spray variables such as the penetration length is insensitive to the grid resolution at high gas temperatures. However, the fair prediction of gas flow and turbulence is shown to be important at lower gas temperatures where the evaporation is slower. The effects of the droplet and gas flow subgrid turbulence are also studied for a range of gas densities and temperatures. It was found that for sprays at higher gas densities and lower gas temperatures, the subgrid turbulence model is important to the prediction of overall spray variables like the spray penetration. Our results also indicate the significance of the inner droplet heat and mass transfer models at higher gas temperatures. However, the effect of subgrid droplet dispersion and droplet collision/coalescence is shown to be insignificant provided that the turbulent flow is captured well by the LES.

Chapter 2

Evaporating Spray Turbulence Interaction

2.1 Introduction

Sprays and their two-way mass, momentum and energy interactions with the gas flow turbulence play a crucial role in advanced combustion systems. In such a gas-liquid system, the interactions between phases occur over a vast range of length and time scales. The fractional volume and mass of the dispersed liquid with respect to carrier gas are two of the critical parameters that determine the level of interaction between phases. Flows containing very small (in comparison to Kolmogorov scales) droplets with small volume fractions have gas flow and turbulence structure similar to that of a single-phase flow. However, with larger droplets and higher volume fractions the liquid effects on gas turbulence production, dissipation and stresses become important ([35],[44] and [46]). This, of course, depends on the spray speed and the level of background gas turbulence. When the liquid is sprayed with low to moderate speeds into a quiescent chamber, the gas turbulence remains to be insignificant. However, at high injection pressures and for high speed sprays (typically several hundred meters per second) the droplets can become a significant source of gas turbulence. This is partly due

to drag of liquid droplets but can also be caused by the evaporated liquid gas as shown below. Balachandar and Eaton [35] indicated the main mechanisms for the flow/turbulence modifications by droplets to be: (i) the drag of larger droplets causing enhanced dissipation, (ii) the transfer of droplet kinetic energy to the gas, (iii) the wakes and vortex shedding behind large droplets and (iv) the buoyancy induced instabilities due to density variations arising from the preferential concentration of droplets. For evaporating sprays issuing into a quiescent chamber with high injection pressures, the droplet wake and enhanced dissipation mechanisms play lesser role and the turbulence is mainly generated and modified by the droplet drag and evaporation as explained below.

For the numerical simulations of sprays, both Eulerian-Lagrangian and Eulerian-Eulerian type models have been used, even though the former have been more popular [77]-[78]. The primary jet breakup in sprays can be simulated by Eulerian-Eulerian models ([21],[22],[23] and [24]). These types of models are expected to better capture the breakup of main liquid jet, but they are not currently practical and cannot be employed for high speed evaporating sprays in realistic systems. Far enough from the nozzle, the liquid droplets are small, dispersed and far from being a continuum. They can be better represented by a collection of Lagrangian particles and Eulerian-Lagrangian models.

Dispersed-continuous phase turbulence interactions have been extensively studied ([35],[79], [80] and [81]). Most of these studies were on the modulation of turbulence by particles ([34],[82] and [83]). However, some studies also considered the turbulence generation by the dispersed phase. For example, Chen et al. [84] showed that the superposition of many laminar-like wakes randomly positioned in space and time generates turbulence in the carrier gas flow. Depending on the ratio of dispersed phase response time to the flow time scale,

known as Stokes number St , the dispersed phase particles change both the dissipation and the production of carrier fluid turbulence. To simulate the turbulence-droplet interactions, both direct numerical simulation (DNS) and large eddy simulation (LES) methods may be used [85]. DNS is extremely demanding and currently impractical for high speed sprays. LES method on the other hand has been widely applied to multiphase flows and can be a viable tool for spray simulations [85].

Earlier studies of dispersed two-phase flows were focused on the isothermal and solid particulate flows, but there have also been several studies on the evaporating droplet interactions with the gas turbulence. DNS and LES studies of [65], [86], [87] and [88] for droplet-laden homogenous shear and temporal shear layer flows, for example, showed that evaporation increases the turbulence kinetic energy and the dissipation of turbulent kinetic energy of the carrier gas. For the practical combustion systems, current spray models rely predominantly on the Reynolds-averaged Navier-Stokes (RANS) method [30]-[6]. However, because of unsteady and turbulent nature of the gas flow generated by high speed sprays and other inherently transient physical and chemical processes involved in a typical system, LES is expected to be more suitable than RANS, even though the latter remains to be useful for the design of engineering systems. LES models have been recently applied to complex combustion systems with evaporating/reacting droplets ([25], [36], [58] and [89]).

This chapter is on the detailed study of gas flow mass, momentum and energy interactions with very high speed evaporating sprays for various gas and liquid conditions. The focus is on the flow and turbulence generated by the spray in the gas and the effects that they have on the spray/droplet evolution. The gas flow turbulence is simulated by the large eddy simulation together with subgrid-scale (SGS) kinetic energy equation models that includes

the spray effects on the SGS turbulence. The effects of SGS turbulence on the droplets are also included with a stochastic subgrid model. The spray is simulated with a stochastic breakup and non-equilibrium finite rate heat and mass transfer models. Our results below show the importance and complexity of the flow and turbulence generated by the spray.

2.2 Results and Discussions

The numerical simulations are conducted for conditions close to experiments performed at Sandia National Laboratory and engine combustion network (ECN) ([69], [70], [90] and [91]). In these experiments, the fuel spray behaviour in a closed combustion chamber is studied. The characteristic size of the combustion chamber is 105 mm. The fuel injector is located in one side of the chamber, and the nozzle diameter ranges from 0.1 to 0.5 mm with the fuel injection pressures varying between 50 to 200 MPa. Also in the experiments, the temperature and density of the gas in the chamber which is mostly nitrogen is varied between 700 K to 1300 K and 3 to 60 kg/m^3 , respectively. Here, the effects of ambient gas temperature and density, and the injector pressure and nozzle diameter on the spray are studied and compared with the experiment. In comparison with the experiment, global spray parameters such as the liquid and vapour penetration lengths are considered. The liquid penetration length is the maximum extent of liquid-phase spray penetration during the injection. In the numerical simulation, the liquid penetration length is defined to be the axial location at which 97% of liquid mass exists. Initial gas phase conditions are set uniformly based on experimental conditions. The initial diameter of droplets is calculated by using the nozzle diameter and its experimentally measured area-contraction coefficient, corresponding to the mass flow rate. In the selected experiments, n-Hexadecane is the

d_{noz} (mm)	Δ (mm)	N_G	N_{PC}	N_{core}
0.900, 0.100	0.2	20,000,000	50,000-100,000	128
0.246, 0.267	0.5	3,500,000	50,000-100,000	32
0.498	1.0	1,000,000	50,000	16

Table 2.1: Computational parameters for spray turbulence interaction simulations

fuel and the injection temperature is fixed at 436K. However, for further validation of LES model, the experimental data for vapour penetration and mixing of n-dodacane fuel is also considered. The liquid n-dodacane is injected with the temperature of 363 K. The injected fuel properties are obtained and computed from data and correlations presented by Poling et al. [71]. A rectangular numerical domain is used for LES with a length of 105 mm in axial direction and 100 mm in lateral directions. For smaller nozzles, only half of chamber size in lateral directions is simulated with free-stream boundary conditions for the lateral boundaries. Table 2.1 summarizes the computational parameters for different simulations conducted in this chapter.

2.2.1 Spray Vapour Penetration and Fuel Mixing

For n-dodacane spray, designated as “Spray A” by ECN [91], there are experimental data on transient liquid and vapour penetrations as well as fuel mixing data at different axial locations. The main parameters of Spray A are listed in Table 2.2. The vapour penetration length is defined to be the maximum distance in which the fuel mass fraction reaches to 0.1 percent. Figure 2.1 shows the time variations of the liquid fuel spray and vapour phase penetration lengths for Spray A configuration as obtained by the two-phase LES model and compared with the experimental data. The results in Figure 2.1 clearly show the capability of the two-phase LES to capture the global characteristics of the spray and the evaporated

Fuel	n-dodacane
T_{fuel}	363 K
d_{noz}	90 μm
p_{inj}	150 MPa
Δt_{inj}	1.5ms
T_g	900 K
ρ_g	22.8 kg/m^3
x_{N_2}	%89.7
x_{CO_2}	%6.52
x_{H_2O}	%3.77

Table 2.2: Parameters of spray A

fuel in a highly unsteady and turbulent spray-induced gas flow. It is clear that the liquid spray quickly reaches a pseudo-steady condition while the vapour keeps on penetrating even after the liquid injection stops, hence making the spray flow essentially a transient phenomenon.

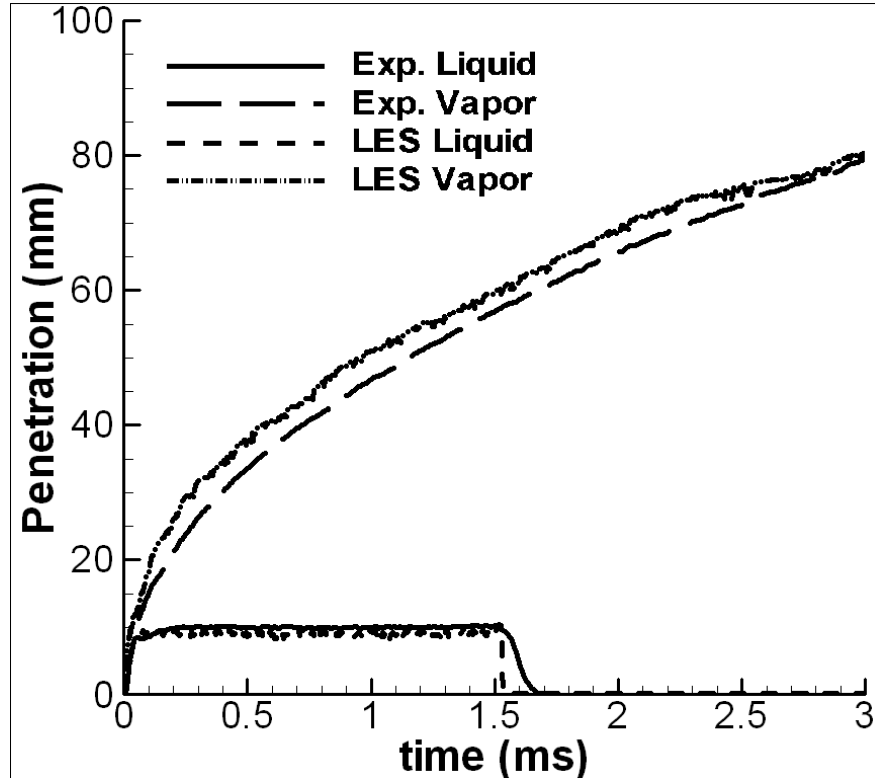
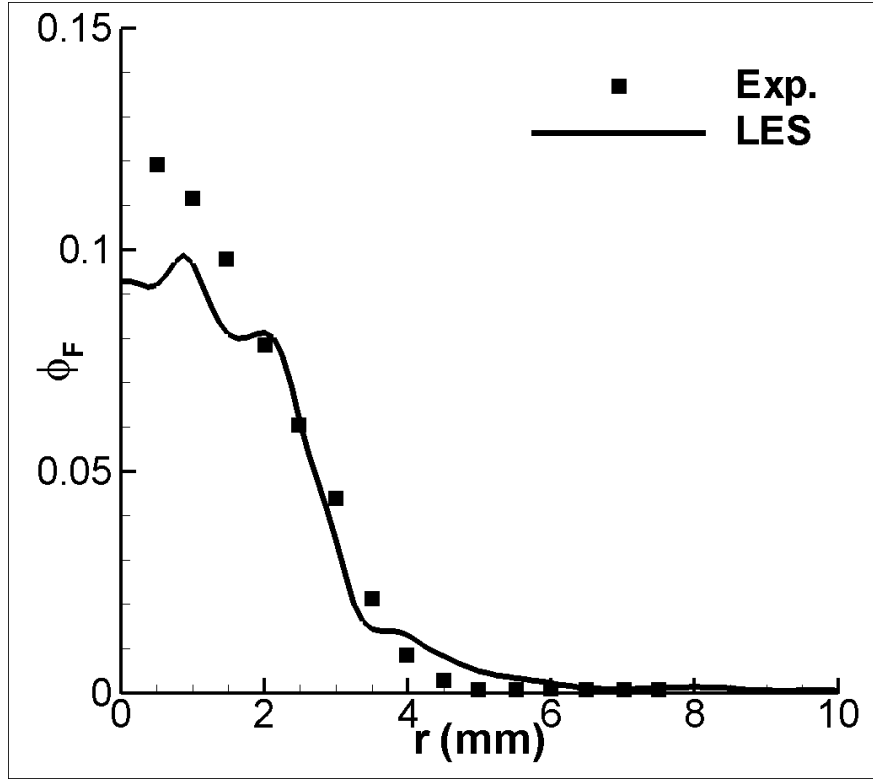


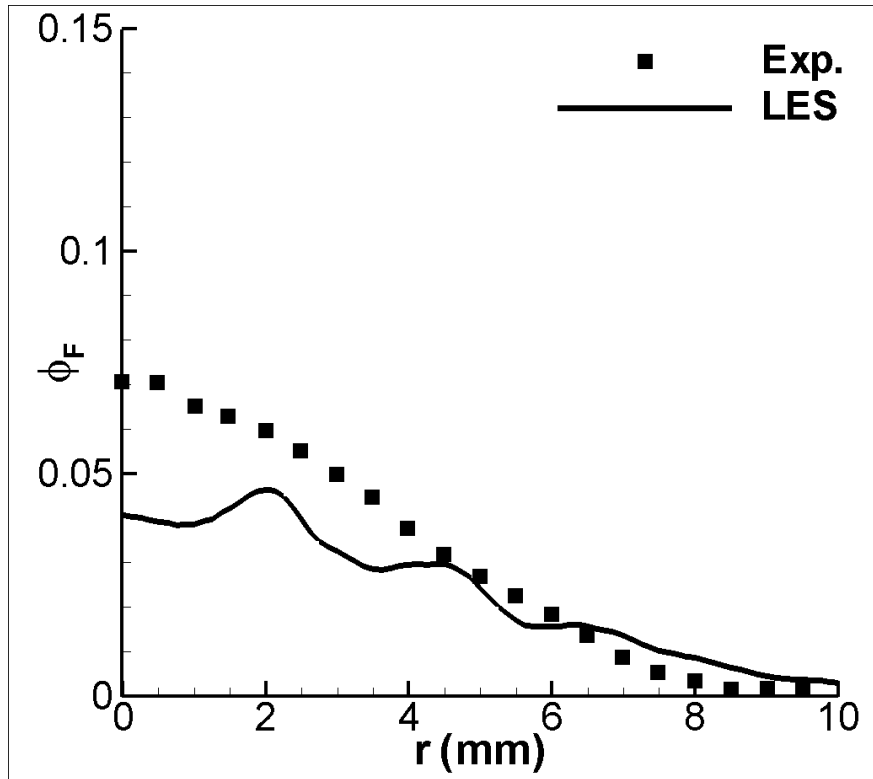
Figure 2.1: Simulated and experimental liquid and vapour penetration lengths versus time for spray A.

Figure 2.2 compares the simulated and measured radial profiles of azimuthally averaged fuel mass fraction at two axial locations at time $t=1.5$ ms after the start of injection. It should be noted that the experimental measurements involve some time averaging [91]. Overall agreement is, however, satisfactory. It is shown that at the spray axis, LES under-predicts the mean experimental values at $t=1.5$ ms since the instantaneous fuel mass fraction on this axis is oscillatory and shows the instabilities in the vapour jet.

For the rest of the chapter, the n-Hexadecane spray injected into nitrogen gas is considered for studying spray/gas flow interactions in different conditions.



(a) $x = 25\text{mm}$



(b) $x = 45\text{mm}$

Figure 2.2: Simulated and measured radial profiles of mean fuel mass fraction at two axial locations at $t=1.5\text{ ms}$ for spray A.

2.2.2 Spray-Turbulence Interactions at Different Conditions

Figure 2.3 compares the experimental values of liquid penetration length with the simulated results as a function of density for two different gas temperatures. The fuel is injected through a 0.246 mm diameter nozzle with the injection pressure of 138 MPa. The LES grid resolution was chosen to be 0.5 mm which is sufficient for capturing the essential features of the flow and turbulence in the gas. The agreement of simulated results with experimental data is fairly well for the sprays shown in Figure 2.3 and all other sprays not shown in this chapter. Once again, this indicates the accuracy of the LES results. As shown in Figure 2.3, the penetration length decreases rapidly with increasing the gas density, more so at lower gas densities. Similarly, the liquid penetration length decreases with increasing the gas temperature for the range of gas densities considered in the experiment. These are expected trends and are mainly due to enhanced drag, breakup and/or evaporation of the liquid droplets with the gas density and temperature.

Figure 2.4 shows the vorticity field of the spray induced gas flow for the two chamber gas densities of 14.8 and 30.0 kg/m^3 and gas temperature of 700K. The 3D contours in this figure clearly show the very significant and complex turbulent flow generated by the spray and droplets in the gas flow. It is also clear that more small scales are produced at lower chamber density in the aftermath of main gas jet flow breakdown to turbulence. The spray induced gas flow has a very significant subsequent effect on the dispersion, evaporation and mixing of the droplets and the evaporated fuel in the gas. These are going to be examined, and explained below together with detailed investigation of the effects of various gas and spray parameters on the spray-gas flow turbulence interactions.

Depicted in Figure 2.5 is the liquid penetration length evolution for the two gas temperatures

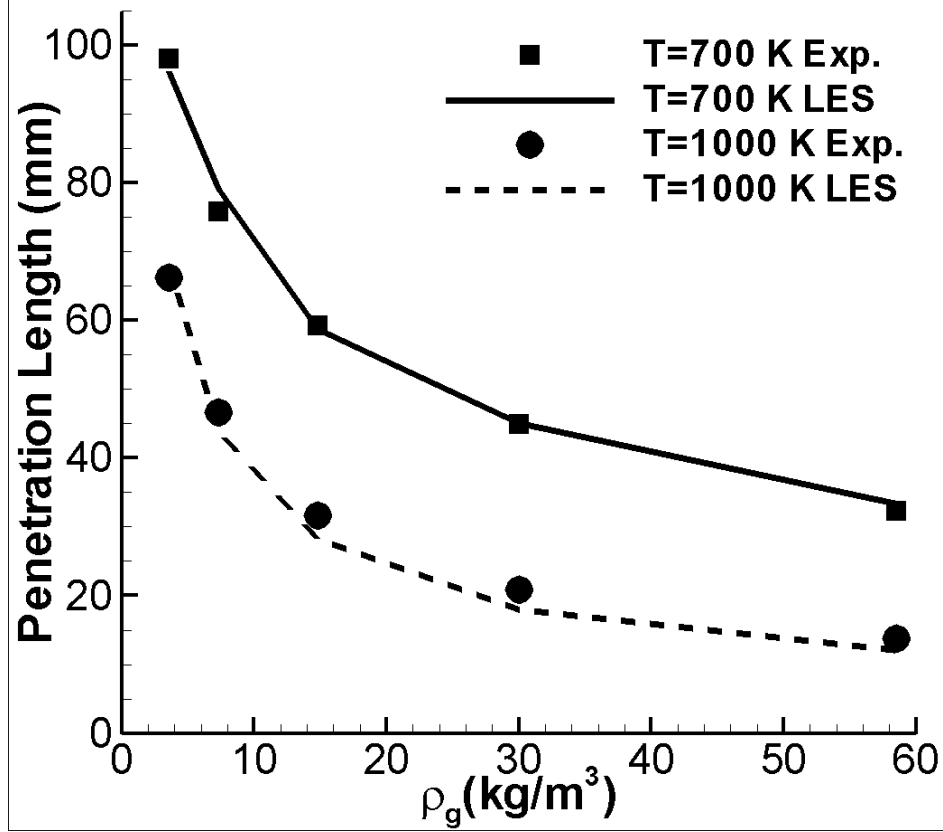
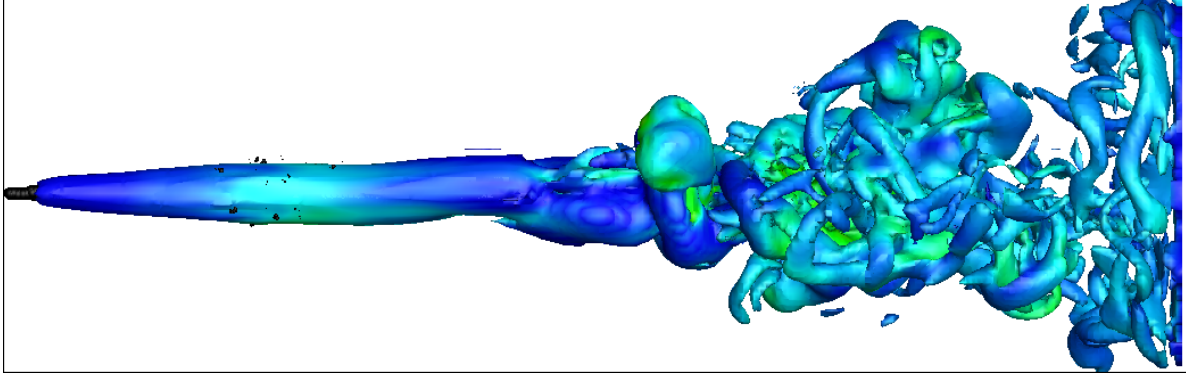
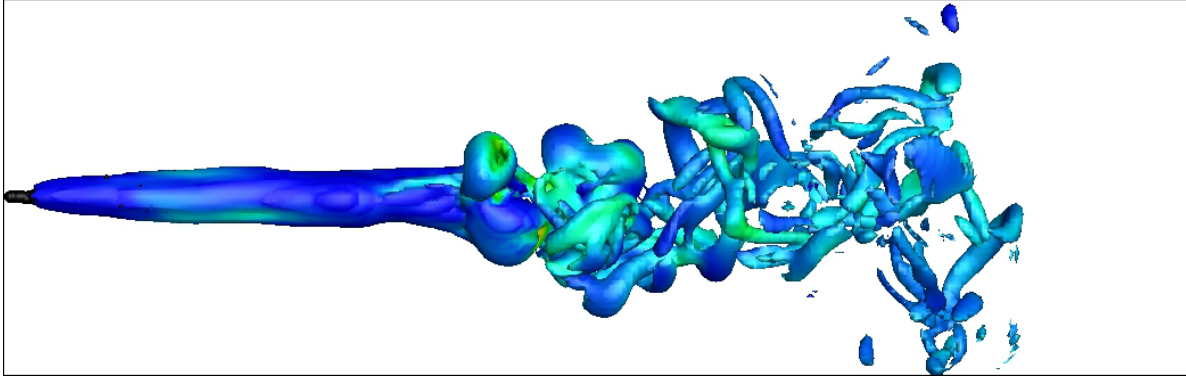


Figure 2.3: Comparison of simulated liquid Penetration with experimental values as a function of gas density for different temperatures.

at the intermediate gas density of 14.8 kg/m^3 . Figure 2.6 shows the Sature mean diameter (SMD) of spray droplets for the same gas density and temperatures as a function of distance from the injector. The maximum penetration point or the tip of spray is where the droplet fuel evaporation rate in the spray equals the fuel mass reached to that point and as shown in Figure 2.5 is fluctuating about a mean axial location in the simulated flow. The fluctuations in the spray length after it reaches to its “steady state” condition is negligible at higher ambient gas temperature of 1000 K but is very significant at lower gas temperature of 700 K. This is due to more significant effect of the induced gas flow turbulence on the spray at lower gas temperatures. At lower gas temperatures, at the tip of spray, where there is a significant number of small droplets, the spray reaches to a nearly saturated or equilibrium condition



(a) $\rho = 14.8 \text{ kg/m}^3$



(b) $\rho = 30.0 \text{ kg/m}^3$

Figure 2.4: Three-dimensional iso-level contours of the gas vorticity (magnitude) generated by the spray and droplets for different gas densities and gas temperature of 700K at $t=2.0\text{ms}$.

with the entrained ambient gas after the “transient” spray evolution period. When such a saturated condition is reached, the only means for droplets to further vaporize is to penetrate more to reach the “fresh” gas. This is made possible by the turbulence as the pseudo-steady state (but highly oscillatory) part of the liquid penetration plot for lower gas temperature of 700 K in Figure 2.5 shows. At this temperature, a considerable number of small liquid droplets survive. These droplets interact rather significantly with the gas flow turbulence. At higher gas temperatures the small droplets vaporize very rapidly in the much hotter gas. One may also note that the SMD is considerably larger for the higher gas temperature at intermediate distances from the nozzle between $x=15\text{-}30\text{mm}$. This is due to rapid evaporation

of the smaller droplets in the hot ($T=1000$ K) gas temperature in this region of the flow. For the spray injected at lower gas temperature of 700 K, the droplet SMD reaches to a constant value of around $1\mu m$ at long distances from the injector where fine droplets evaporate. This is due to the fact that a large number of fine droplets cannot evaporate any further in the cool vapour saturated induced gas jet. However as this jet goes through transition to smaller turbulent structures, the evaporated fuel is quickly convected and mixed, making it possible for the droplets to evaporate better in a less saturated environment.

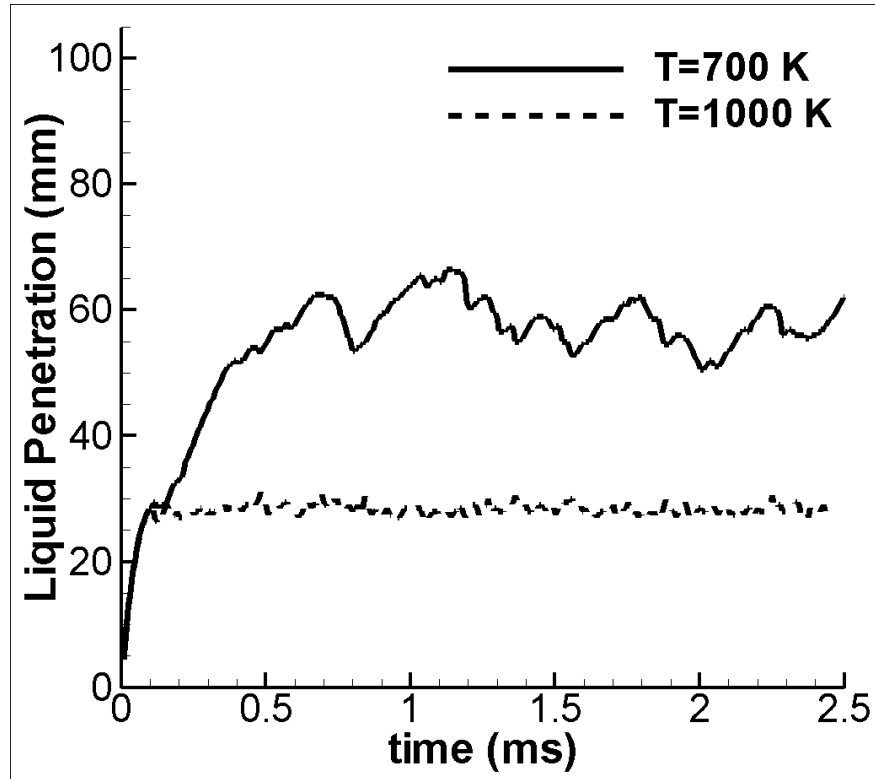


Figure 2.5: Spray penetration as a function of time at gas density of 14.8 kg/m^3 for two gas temperatures.

Figure 2.7 shows the axial gas velocity generated by the spray and droplets, and its transition to turbulence at $t=2.00$ ms. Figure 2.8 shows similar contours for the gas temperature. The induced gas velocity by the very high speed spray is indeed very significant. The oscillatory motion at the outer surface of the main gas jet near to the nozzle is shown to grow and

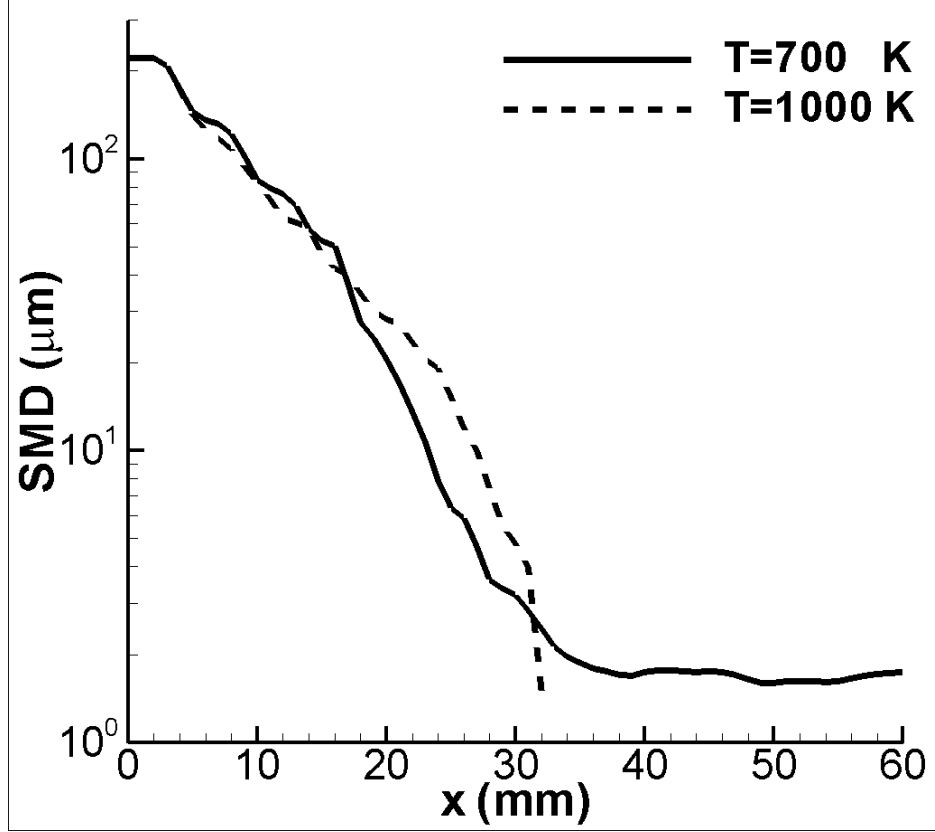


Figure 2.6: Comparison of Sature mean diameter of spray as a function of distance from injector at gas density of 14.8 kg/m^3 for two gas temperatures.

lead to smaller scale turbulent motions at downstream locations. The induced gas flow and turbulence efficiently disperses and mixes the cold dense liquid and evaporated high speed fuel with the surrounding hot lower density quiescent gas. As large drops or blobs moves in the gas, their high relative velocity creates significant dissipation which leads to heating of gas at the near injector region. As evident in Figure 2.8, the gas temperature increase by this process is very significant. Further downstream, the local gas temperature close to the spray is significantly reduced by the evaporative cooling effect of droplets. It is noteworthy to mention that the major part of this cooling is not due to latent heat of evaporation, but due to mixing of the relatively cold vaporized fuel which is at droplet surface temperature with the higher temperature gas outside the droplet boundary layer. The low temperature regions

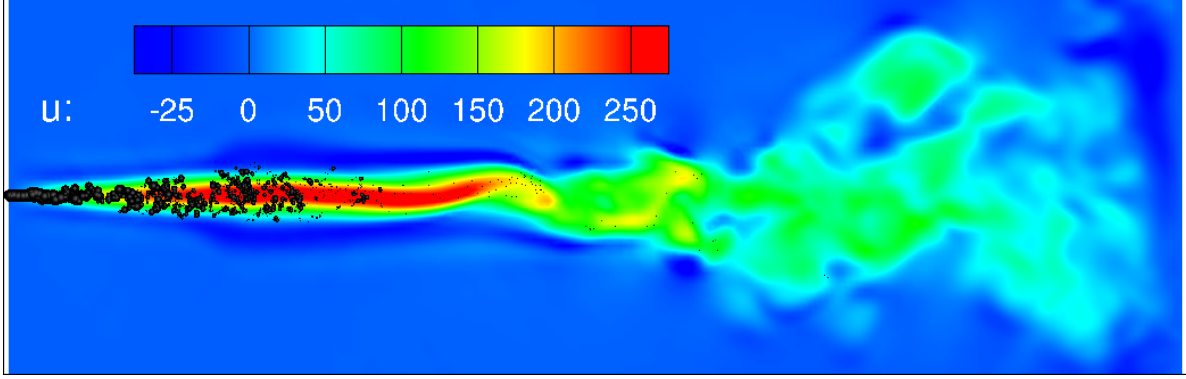


Figure 2.7: Spray induced axial gas velocity field (m/s) at gas density of 14.8 kg/m^3 and gas temperature of 700 K at $t=2.0\text{ms}$.

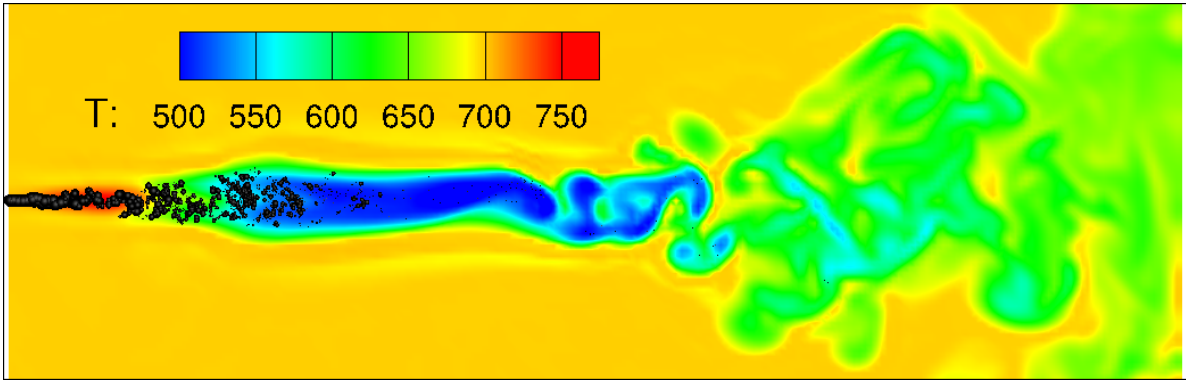


Figure 2.8: Contours of the gas temperature in the spray chamber for the gas density of 14.8 kg/m^3 and gas temperature of 700 K at $t=2.0\text{ms}$.

of the flow overlap the regions with high concentration of fuel vapour and thus hindering of further evaporation. On the other hand, small droplets survive at the tip of spray where the carrier gas is highly saturated by the fuel vapour and has significantly lower temperature. The length of spray-induced gas jet potential core, identified as the point where the main gas jet starts to “break,” is the determining factor in liquid penetration and in the prediction of the spray length at lower gas temperature of 700 K. When the main gas jet breaks to smaller turbulent structures and the dispersion and mixing increases, the regions around droplets are suddenly fed with fresh unsaturated higher energy gas and as a result the droplet evaporation quickly increases. At the same time, turbulent eddies transport and mix hotter surrounding

gas into the spray plume region. This also enhances the evaporation and shortens the liquid penetration. However, the evaporation also cools down the temperature of the surrounding gas leading to slowing down of the droplet evaporation and higher liquid penetration. As a result of these two competing mechanisms, the location of the core gas jet transition to turbulence fluctuates in time, causing a significant, high amplitude oscillations in the liquid penetration length at gas temperature of 700 K (Figure 2.5).

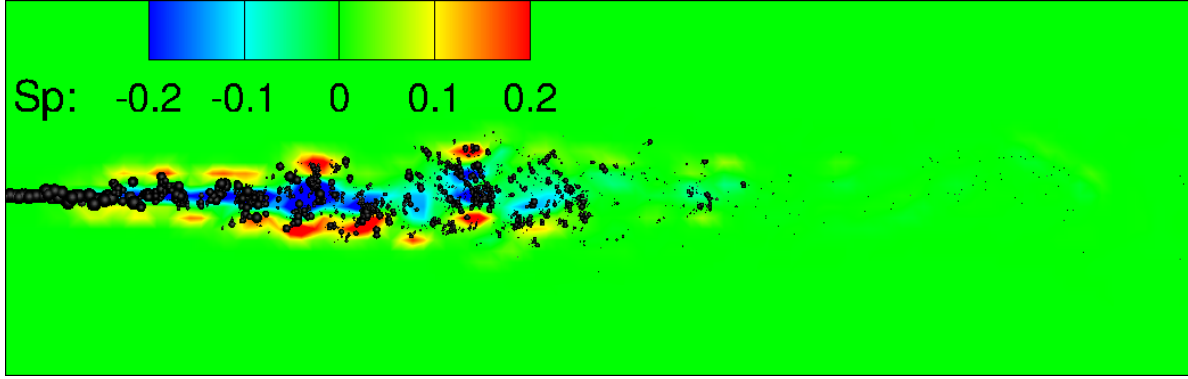
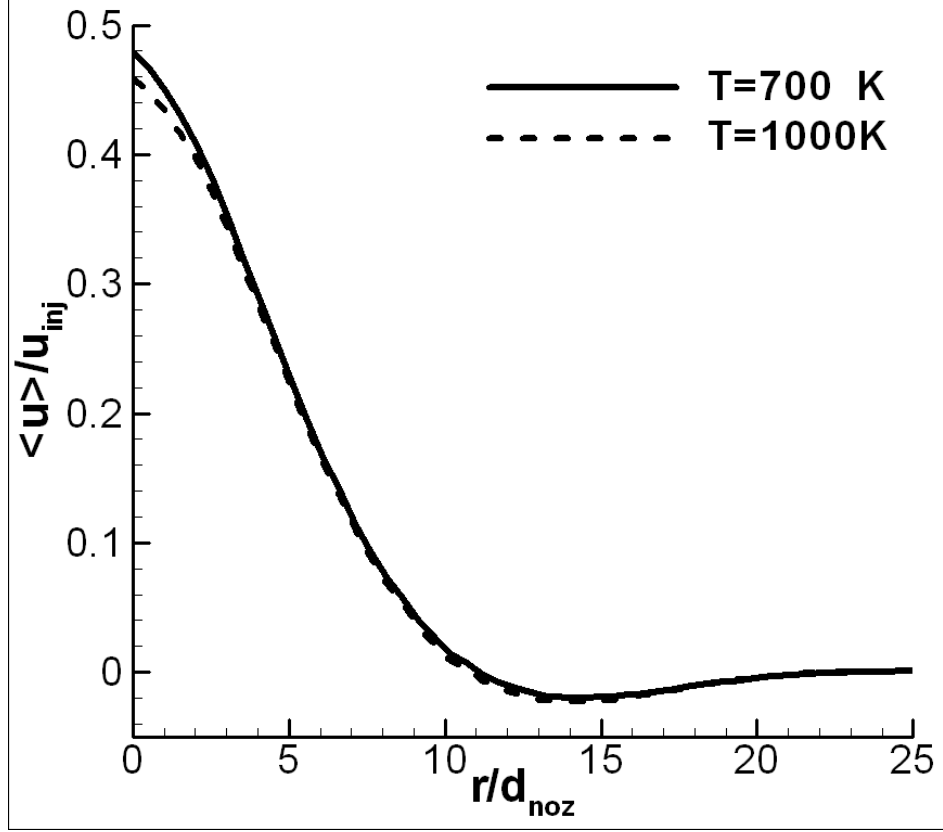


Figure 2.9: Spray source term contours in the subgrid kinetic energy equation for the gas density of 14.8 kg/m^3 and gas temperature of 700 K at $t=2.0\text{ms}$.

Figure 2.9 shows the 2D contours of the spray source term in the gas SGS kinetic energy equation for the intermediate gas density of 14.8 kg/m^3 and lower gas temperature of 700 K near to the nozzle at $t=2.00 \text{ ms}$. It is known that the liquid-gas interface can create small-scale vorticity and turbulence in the gas phase [23]; however as Figure 2.9 indicates this SGS turbulence is rather weak compared to large-scale, spray-induced gas flow and is mostly at the periphery of the spray in the near injector region or along the dense spray region. A consequence of this effect is the enhancement of the subgrid turbulence and poly-dispersity of droplets. At the spray axis, droplets dissipate turbulence due to their high speed axial velocity. In the near injector region, spray source term is the dominant term in subgrid kinetic energy equation, followed by the less pronounced dissipation term

and negligible subgrid turbulence production. Further downstream, the spray effect on the subgrid gas turbulence tends to become weaker. However, as finer droplets are produced along the axis of spray, the added mass due to evaporation have a very high kinetic energy. This further augments the induced gas momentum together with the droplet drag force and creates a high speed vapour-saturated, low-temperature gas jet with considerable density difference with the surrounding gas. The main features of the spray-induced gas jet is similar at the higher gas temperature of 1000 K, yet the gas surrounding liquid droplets has so much thermal energy that the atomized droplets evaporate quickly and their residence times are comparatively short. This indicates that the droplets disappear at shorter distances from the nozzle than the spray-induced gas jet potential core and therefore the interactions between the droplets and gas turbulence far away, as described above for $T=700$ K, are not very significant and as a result, fluctuations in liquid spray is less significant (Figure 2.5). However, the turbulence production is still higher at gas temperature of $T=1000$ K due to much higher rate of evaporation of droplets and high kinetic energy vapour introduced into the gas at this temperature.

Figure 2.10 compares the azimuthally averaged mean axial velocity and the variance of axial velocity fluctuations for the two gas temperatures of $T=700$ K and 1000 K at the normalized distance of $x = 15d_{noz}\sqrt{\rho_l/\rho_g}$ from the injector at $t=2.00$ ms. As observed in this figure, while the mean velocities are nearly the same, the perturbations in the gas jet are rather larger for the spray injected into hotter gas. It might be noted that although the overall or total liquid evaporation is similar for sprays injected into different gas temperatures as mean vapour concentrations and induced gas velocities are almost identical, the local evaporation rate is higher at higher gas temperature. This causes higher velocity fluctuations in the gas



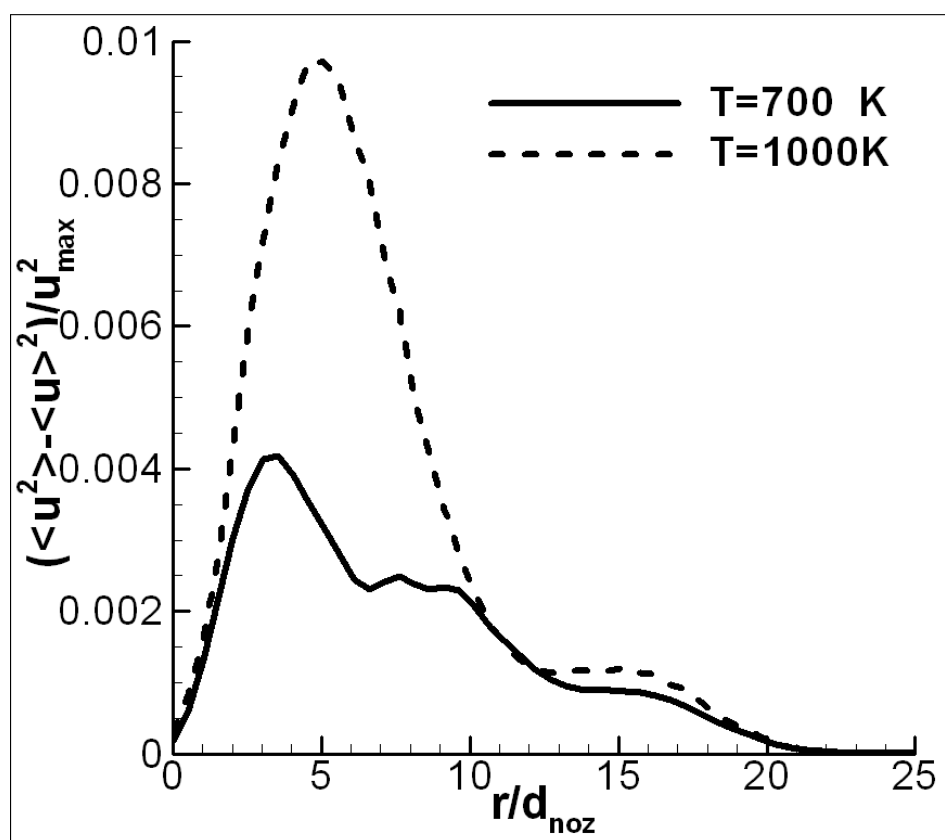
(a)

Figure 2.10: Effect of gas temperature on (a) azimuthally averaged induced gas velocity and (b) its fluctuating velocity variance at non-dimensional distance of $x=15$ from the injector for gas density of 14.8 kg/m^3 .

jet. As a result of higher velocity fluctuations in the gas, the gas jet becomes turbulent at a shorter distance from the nozzle in the case with higher initial gas temperature of $T=1000 \text{ K}$. However, even though the velocity fluctuations are significantly higher for the higher gas temperature at the shorter distance of $x=15$ from the injector, they grow much less when the fuel is sprayed into hotter gas and become closer or even smaller than those for the lower gas temperature at $x=40$ and 50 . This is shown in Figure 2.11, where the turbulent velocity fluctuations at normalized locations of $x/d_{noz} \sqrt{\rho_l/\rho_g} = 40$ and 50 for the two gas temperatures are compared. As the gas jet becomes turbulent at a shorter distance from the injector at higher gas temperature of $T=1000 \text{ K}$, the turbulence production and dissipation

Figure 2.10: (cont'd)

(b)



reduces the mean induced gas kinetic energy and therefore the growth rate of turbulence is reduced more after it reaches to its peak. In contrast, the induced turbulent gas jet has a longer potential core and higher kinetic energy at lower gas temperature of $T=700$ K. Therefore, the growth rate of turbulence is higher further downstream of the main gas jet core compared to that seen for higher gas temperature.

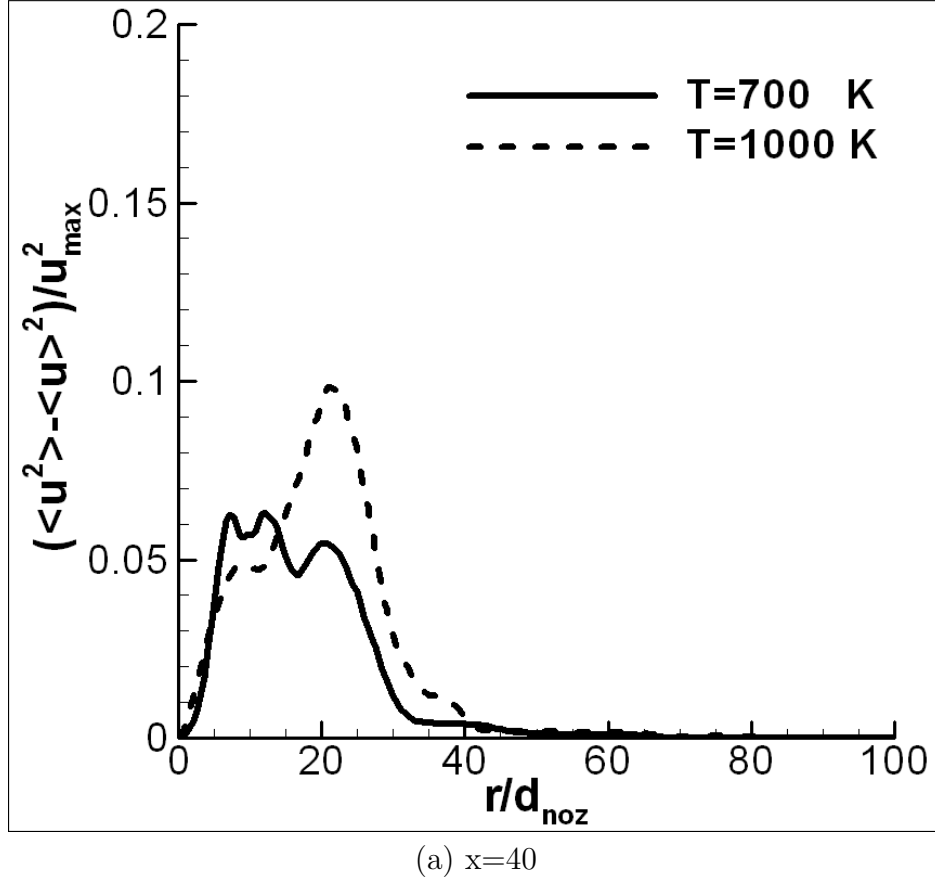
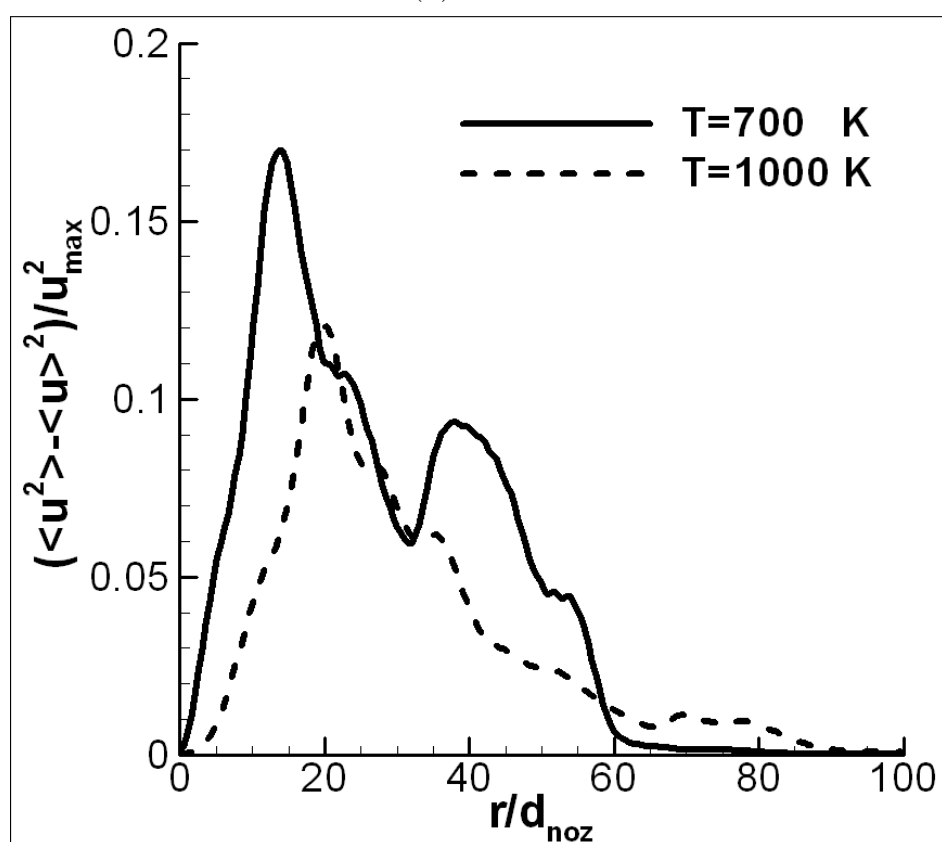


Figure 2.11: Effect of gas temperature on axial velocity fluctuations at different non-dimensional distances from the injector for the gas density of 14.8 kg/m^3 .

The spray induced gas flow and turbulence is also a function of the gas density; overall the spray generates stronger flow in a less dense gas but the effect on the gas turbulence is somewhat complex. Figure 2.12 compares the azimuthally-averaged induced gas velocity and its fluctuations for the two gas densities of 14.8 and 30 kg/m^3 and gas temperature

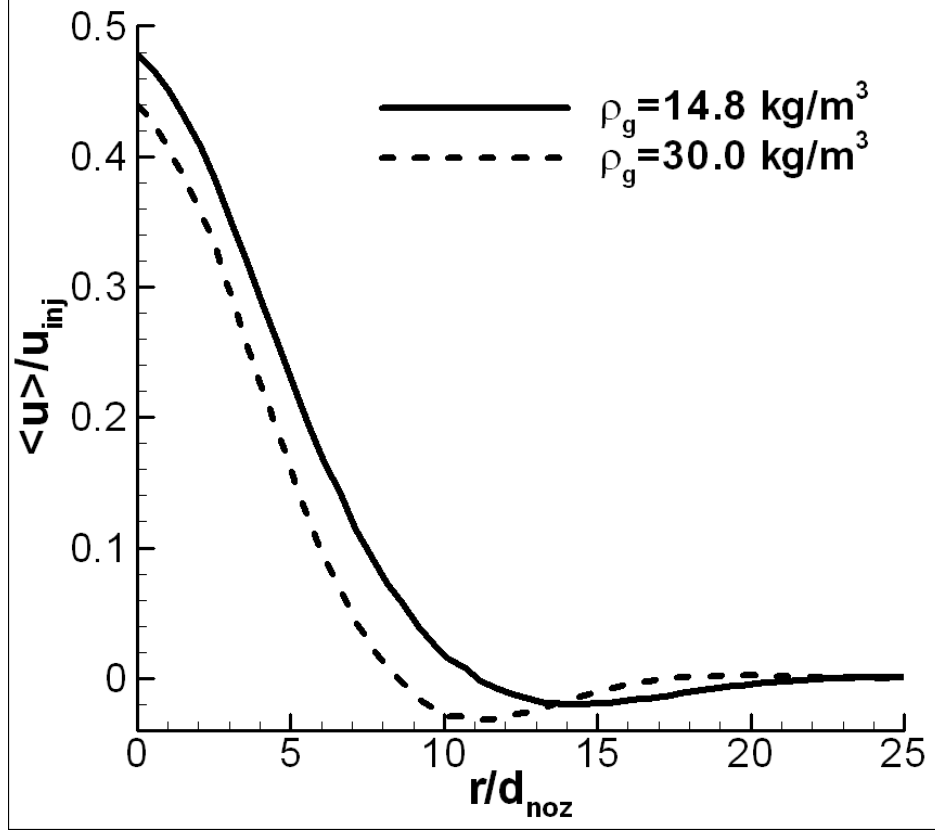
Figure 2.11: (cont'd)

(b) $x=50$



of 700 K at a distance of $x/d_{noz}\sqrt{\rho_l/\rho_g}=15$ from the injector at $t=2.00$ ms. It is obvious that the induced gas jet is narrower in the denser gas. The more pronounced negative mean axial velocity in this case implies augmented recirculation zones at the periphery of the spray and gas jet flow. While the mean induced gas velocity is lower for higher gas density, the fluctuations in gas velocity are actually more significant for this case. The effect of ambient gas density on the spray-induced gas flow/turbulence is better understood and explained by looking at the evaporation of liquid in different gas densities. Figure 2.13 shows the radial profiles of the mean evaporated fuel mass fraction and the evaporation rate parameter for the two gas densities of 14.8 and 30.0 kg/m^3 . Evidently, the evaporation rate is lower in the denser gas close to the spray axis but it becomes higher at a larger radial distance due to relatively lower vapour concentration in this region of the flow which in turn is due to the augmented recirculation in the gas flow. Radial profiles of the evaporation rate parameter together with those of the axial velocity fluctuations show that despite the lower local evaporation rate and lower mean axial velocity, the velocity fluctuations are higher in the denser gas. On the other hand, Figure 2.14, which shows the radial variations of the variance of gas density, indicates that the higher velocity fluctuations in the denser gas is a result of higher density fluctuations caused by the evaporation and momentum transfer. This pushes the induced gas jet to become turbulent at a shorter distance from the nozzle such that the corresponding liquid penetration length, which correlates with the induced gas jet, to become shorter for the denser gas at the lower gas temperature of 700 K, as observed in the experiments.

To further investigate the gas density effect on the spray induced gas turbulence far from the nozzle, the turbulent velocity fluctuations for the two gas densities are compared in Figure



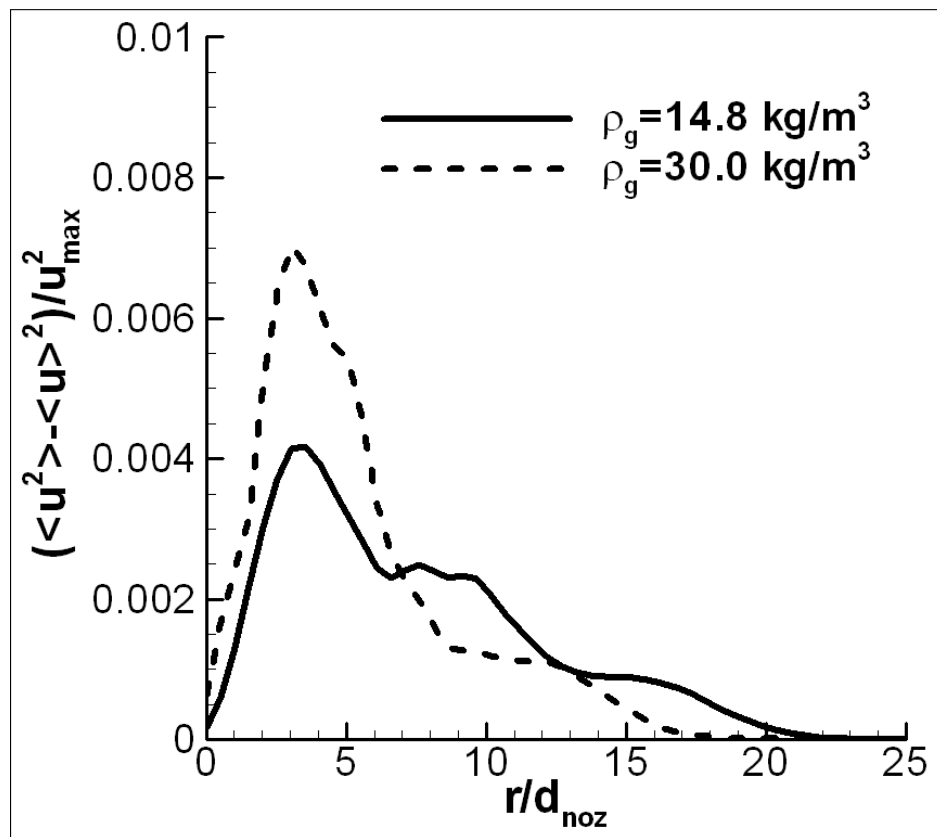
(a)

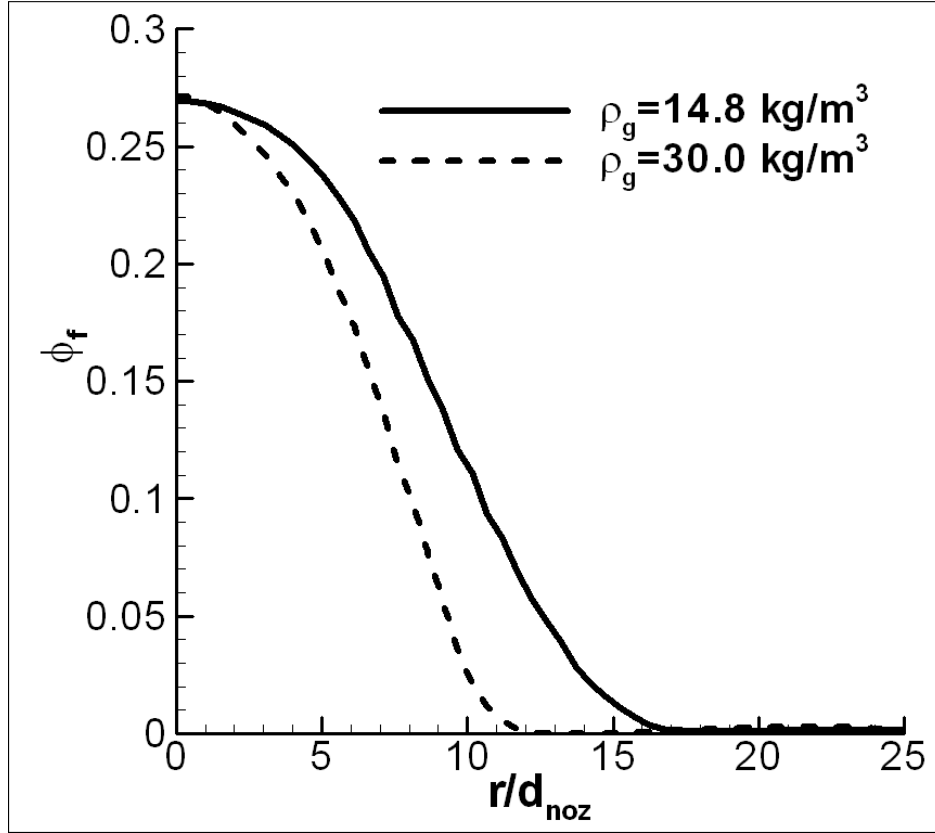
Figure 2.12: Effect of gas density on (a) azimuthally averaged induced gas velocity and (b) its fluctuations at non-dimensional distance of 15 from injector at temperature of 700 K.

2.15 at distances of $x/d_{noz}\sqrt{\rho_l/\rho_g} = 40$ and 50 from the injector. As demonstrated in this figure, the gas flow in the denser environment has a higher turbulence level as it becomes turbulent much faster, but also decays faster at downstream locations because it is made of more small scale motions and has more turbulent kinetic energy dissipation. This is clearly shown in Figure 2.4, where the vorticity iso-levels of the spray induced flow for the two chamber densities of 14.8 and 30 kg/m^3 are compared.

Figure 2.12: (cont'd)

(b)



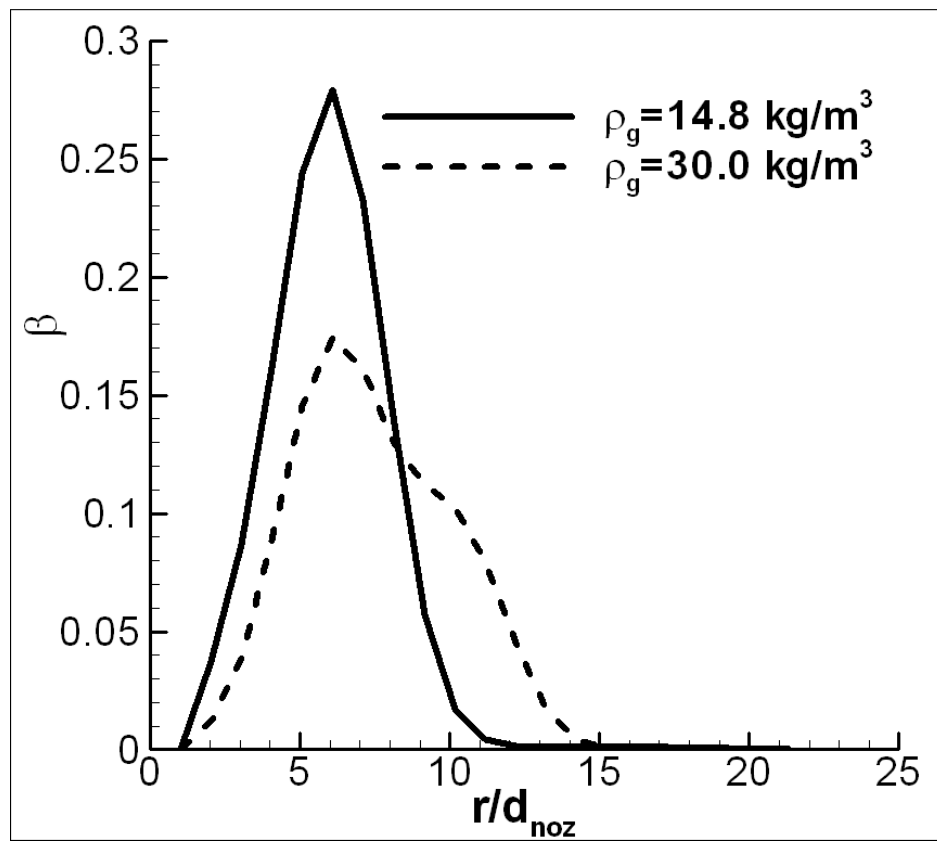


(a)

Figure 2.13: Effect of gas density on radial profiles of (a) azimuthally averaged vapour fuel mass fraction and (b) non-dimensional evaporation rate at non-dimensional distance of 15 from injector at gas temperature of 700 K.

Figure 2.13: (cont'd)

(b)



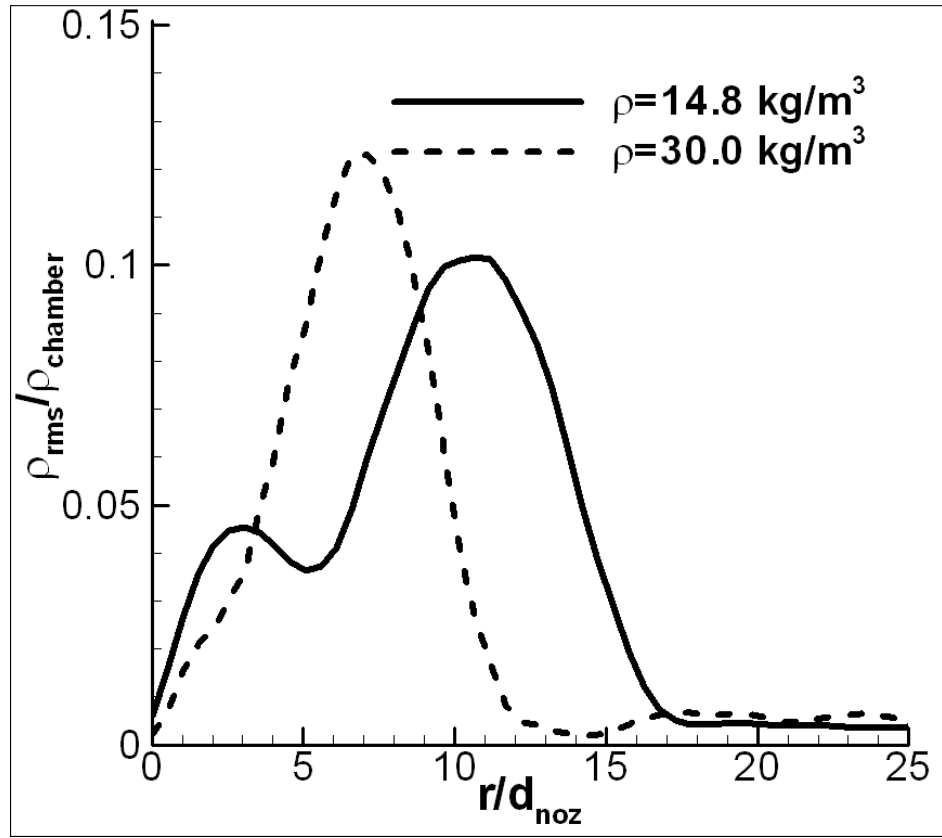
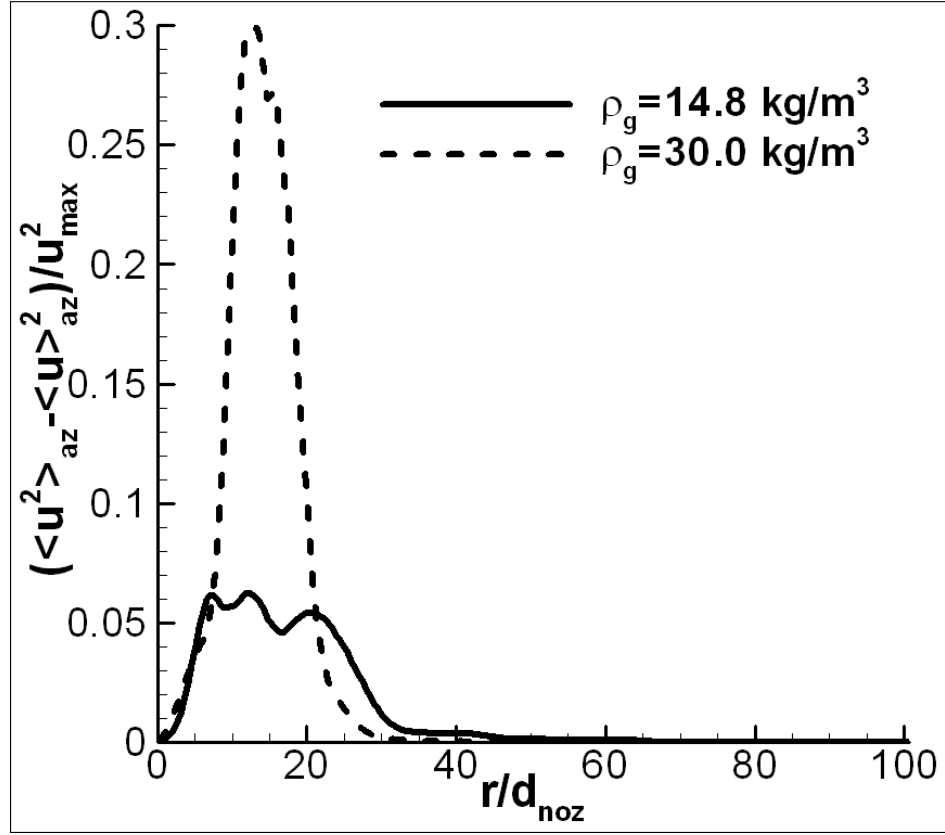


Figure 2.14: Effect of chamber gas density on radial profiles of density fluctuations at non-dimensional distance of 15 from injector at gas temperature of 700 K.

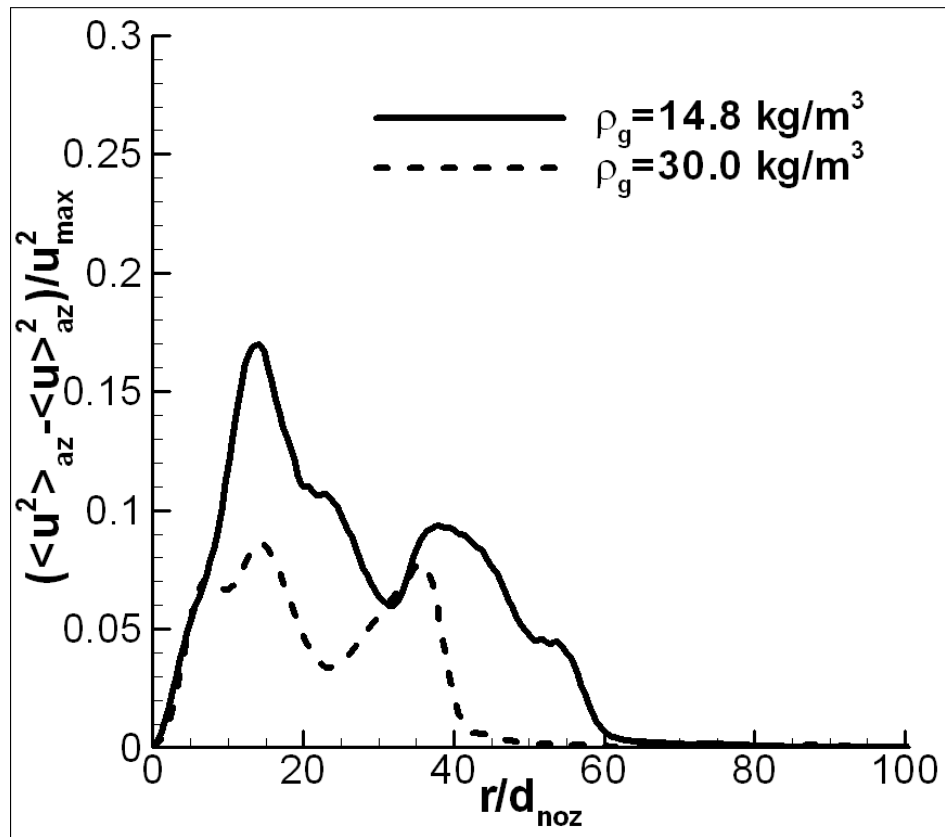


(a) $x=40$

Figure 2.15: Effect of gas density on axial velocity fluctuations at two non-dimensional distances from injector.

Figure 2.15: (cont'd)

(b) $x=50$



2.2.3 Spray Behaviour for Different Nozzles

Figure 2.16 shows the comparison of liquid penetration lengths predicted by LES with the experimental data for nozzles with different sizes at various gas densities and temperatures. The LES grid resolution was chosen to be 0.2 mm for the nozzle diameter of 0.1 mm, and 0.5 mm for the nozzle diameters of 0.246 and 0.267 mm, and 1.0 mm for the nozzle diameter of 0.498 mm. It can be seen that the simulated results agree fairly well with the experimental values at all conditions. This further confirms the overall accuracy of LES results presented in this work. While the general trend is well-captured by LES, the predictions become less accurate and the liquid penetration is under-predicted at $T=1000$ K and over-predicted at $T=1300$ K by the LES. This is mainly due to supercritical condition for some of the droplets and lack of a reliable supercritical submodel in the present LES calculations. The supercritical effect on the evaporation is more pronounced for larger nozzles and higher liquid mass flow rate as the overall drop size, breakup and evaporation rate are dependent on the nozzle size. The higher liquid mass flow rate in larger nozzle simulations increases the penetration length, almost linearly. With the simple model used for the dense spray region, it has been shown that the total entrained gas to the spray increases linearly with the nozzle diameter, while the injected mass depends on the square of the nozzle diameter [70], [92].

Figure 2.17 shows the azimuthally averaged induced gas velocity and its fluctuations at the non-dimensional distance of $x/d_{noz} \sqrt{\rho_l/\rho_g}=15$ from the injector for the two nozzle diameters of 0.100 and 0.246 mm. The chamber gas density and temperature are 14.8 kg/m^3 and 1000 K, respectively. While the mean gas flow velocities for the two different nozzles nearly collapse, when properly normalized, the variance or intensity of the velocity fluctuations in

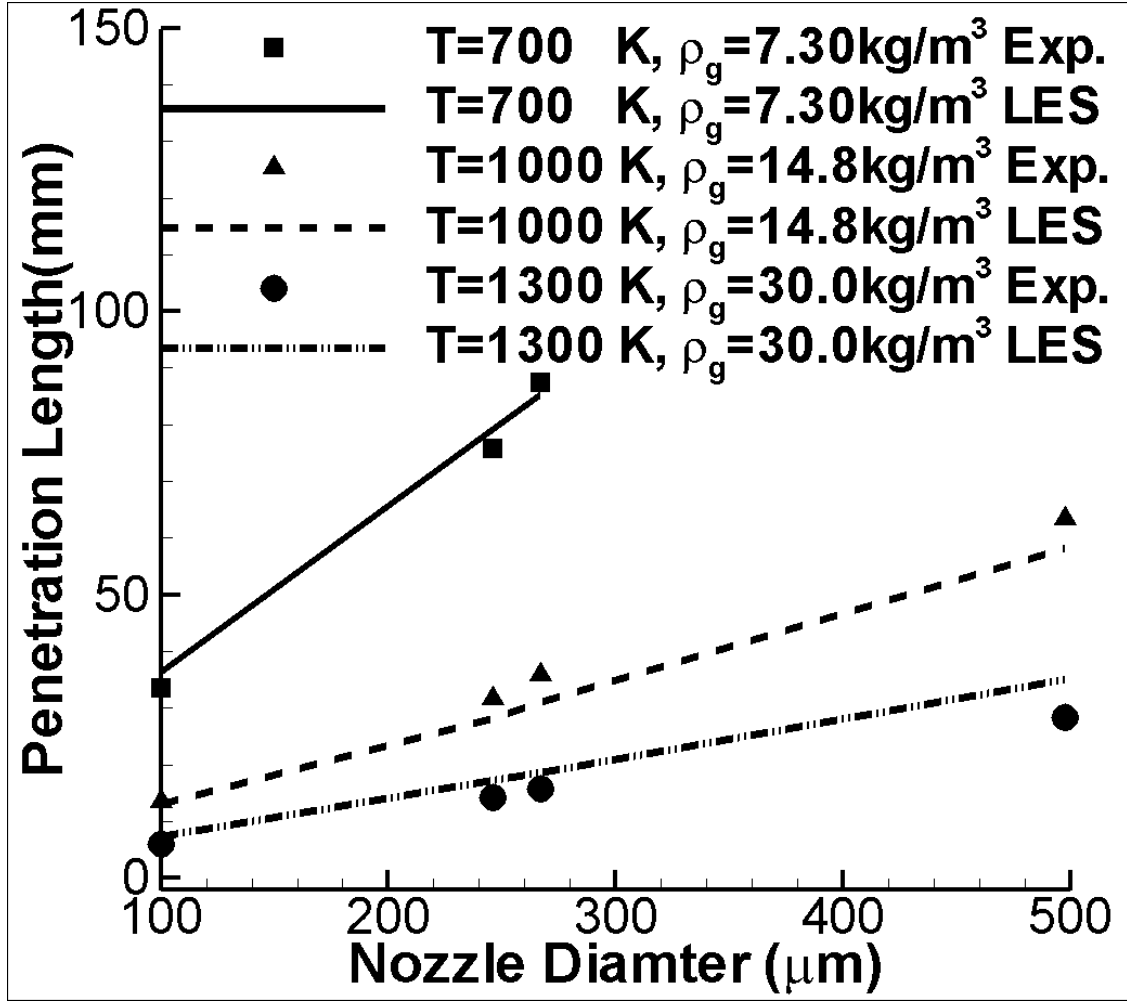
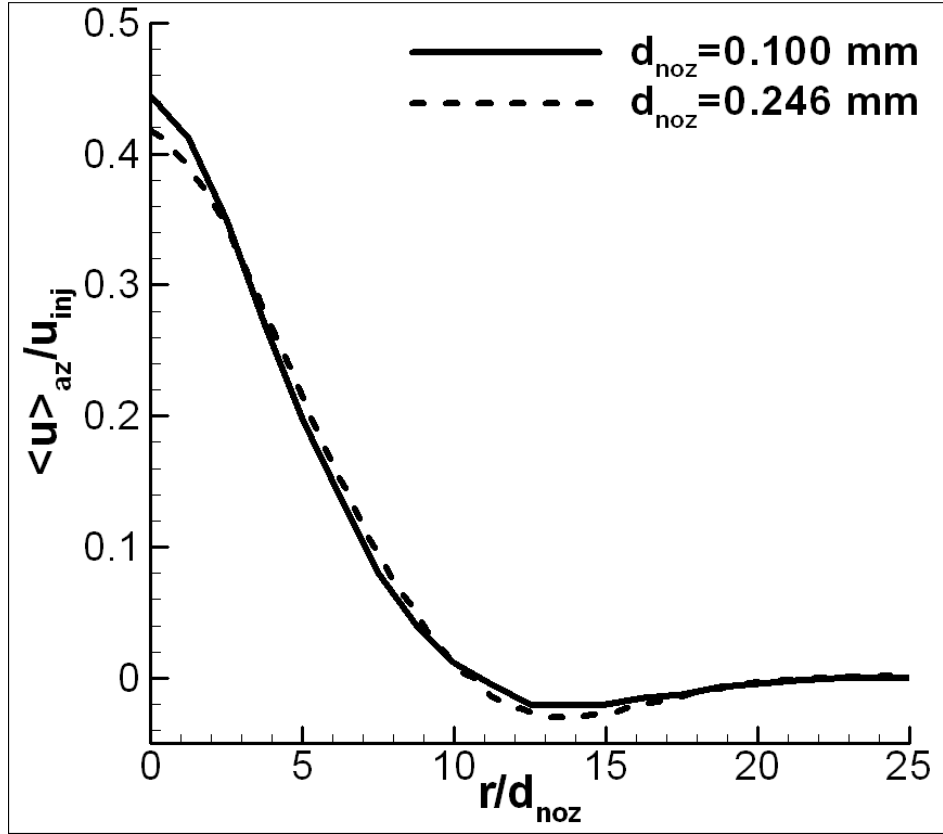


Figure 2.16: Effect of nozzle diameter on liquid penetration at different ambient conditions.

the flow induced by the larger nozzle spray is much more significant. Figure 2.18 shows that the evaporation rate of small droplets (which are responsible for most of evaporation in the spray) are also higher in the case with larger nozzle. When scaled based on the nozzle diameter, the radial profile of normalized mean gas velocity does not change with the change in nozzle diameter, arguably because the details of spray and droplet field does not seem to have a very significant effect on the mean gas flow. Accordingly, the mean evaporated vapour fuel concentrations are also nearly the same when are normalized in a similar fashion. On the other hand, the higher rate of evaporation for the larger nozzle induces more perturbations in



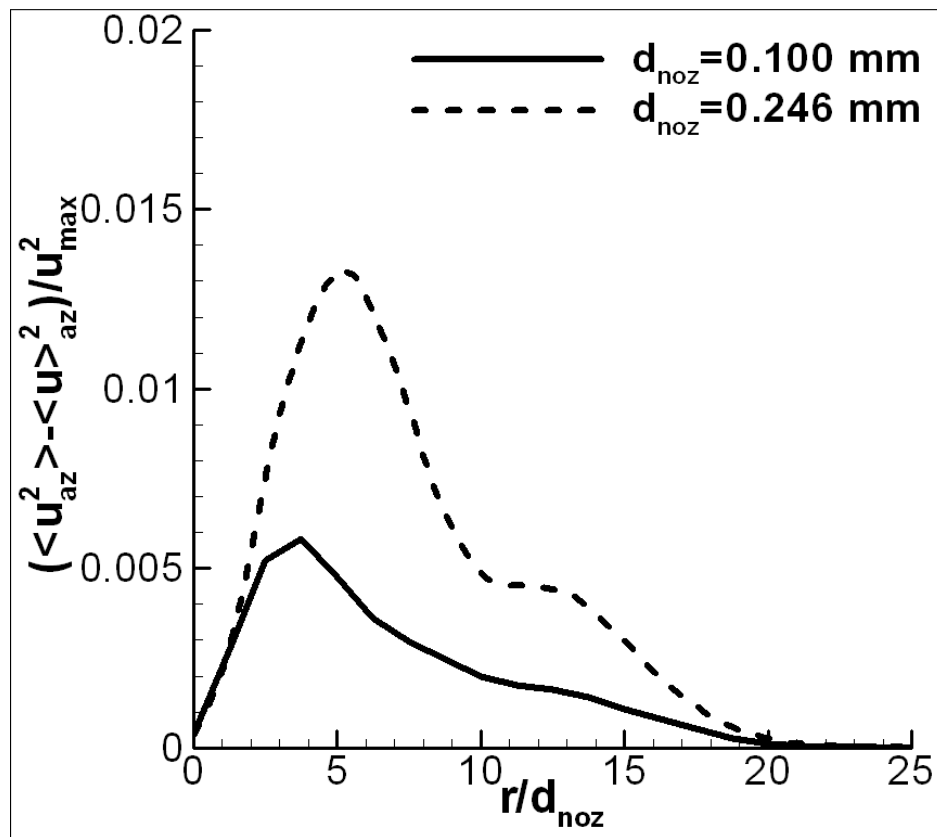
(a)

Figure 2.17: Effect of nozzle diameter on the (a) induced gas velocity, and (b) its fluctuations at non-dimensional distance of 15.

the gas velocity and lead to more significant turbulence. The higher evaporation rate of small droplets in the larger nozzle is attributed to higher gas entrainment and lesser dissipation of the velocity and vapour gas fluctuations.

Figure 2.17: (cont'd)

(b)



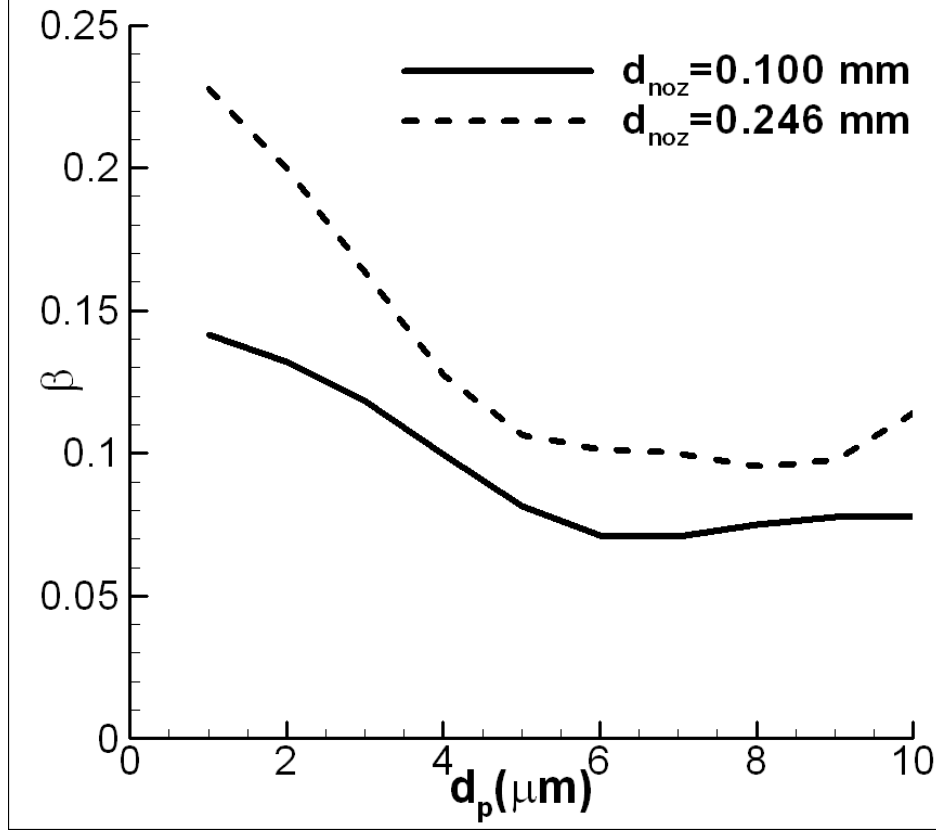


Figure 2.18: Effect of nozzle diameter on the evaporation rate of small droplets.

2.2.4 Spray Behaviour for Various Injection Pressures

Figure 2.19 shows the LES and experimental values of the spray length or liquid penetration for different injection pressures and various gas temperatures and densities. Overall the LES results are in good agreement with the experimental data. The slight discrepancy in results at the lower gas temperature of 700 K and lower gas density of 7.3 kg/m^3 could be due to uncertainties in the injected liquid fuel conditions. The injector nozzle diameter is 100 microns. The characteristics of the flow in the nozzle play a crucial role in the way the injection liquid pressure affects the spray. More specifically, there is a considerable level of uncertainty in the velocity discharge coefficients for different liquid injection pressures as for most cases the actual values are interpolated from the values given for the two injection

pressures of 72 and 138 MPa. The insensitivity of the liquid penetration length to the injection pressure in Figure 2.19 indicates that the change in fuel flow rate due to change in injection pressure must cause exactly the same change in the overall fuel evaporation rate and even though the increase in injection pressure accelerates the atomization as well as the evaporation, the time required for the injected fuel to break and evaporate remain to be nearly proportional to the injection pressure.

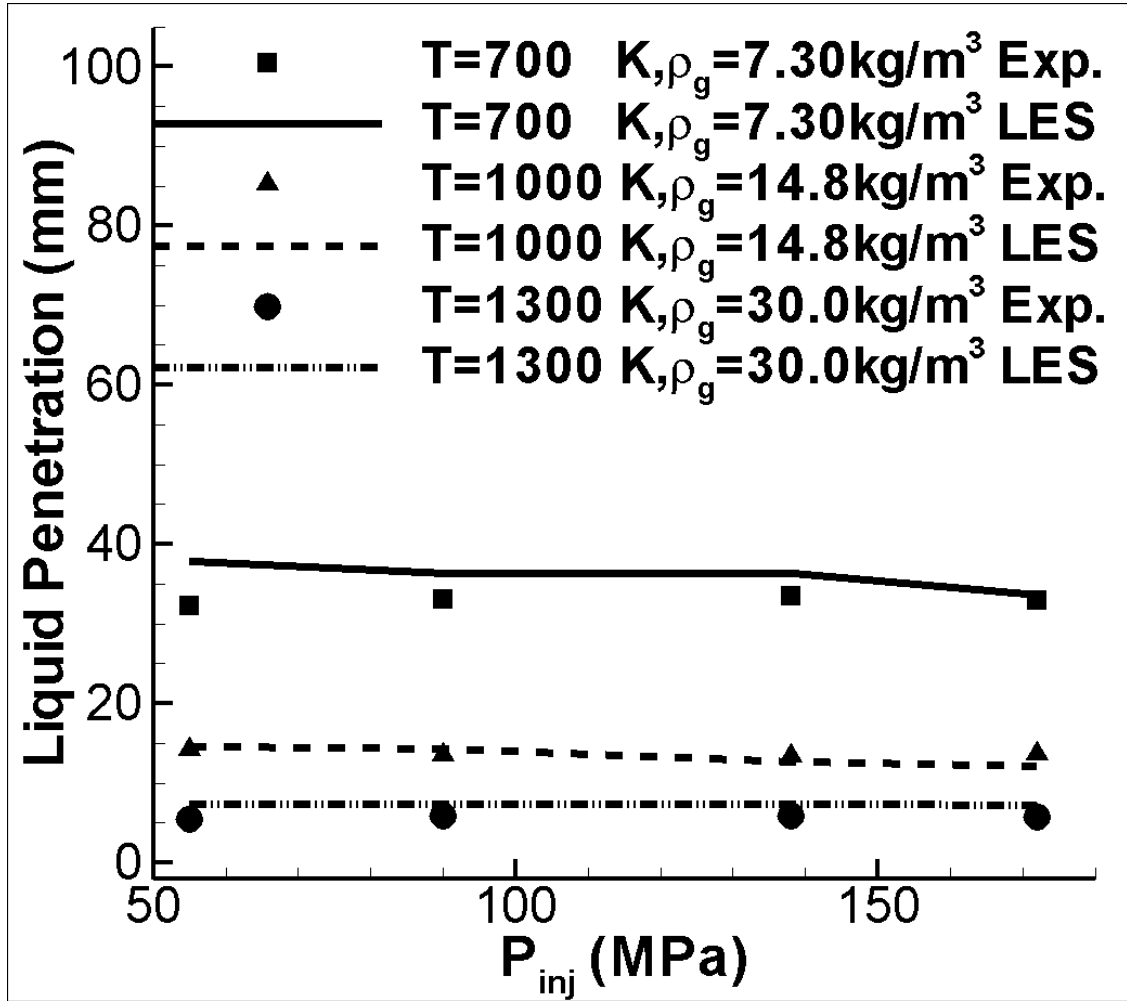


Figure 2.19: Effect of the liquid injection pressure on spray penetration.

Figure 2.20 shows the mass averaged gas to liquid relative velocity of the spray droplets along the axis of spray for different injection pressures at the lower gas temperature of

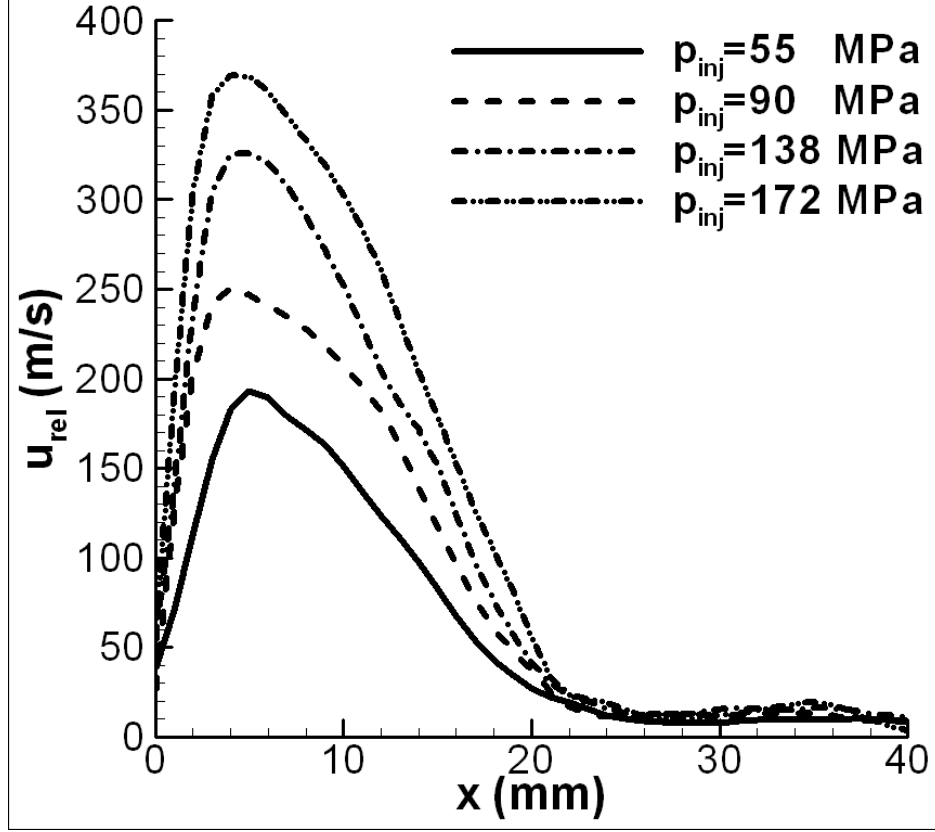


Figure 2.20: Effect of injection pressure on mass averaged relative velocity profile of spray for $\rho = 7.3 \text{ kg/m}^3$ and $T=700 \text{ K}$.

700 K. As expected, the relative velocity is higher along the spray axis for higher injection pressures. Higher relative velocity enhances both the breakup and the evaporation of the liquid. However, injection pressure does not change the SMD profile of the spray significantly as shown in Figure 2.21. Kamimoto et. al. [93] experimentally studied the effect of injection pressure on spray and showed that with an increase in injection pressure, SMD decreases for non-evaporating sprays. This tendency is conspicuous in the range of low injection pressures and SMD change with the injection pressure will be insignificant at sufficiently high injection pressures. Accordingly, in the evaporating sprays injected with high pressures in this work, the effect of injection pressure on the spray is not very significant. At higher injection pressures, finer droplets are produced along the spray axis. But these fine droplets have very

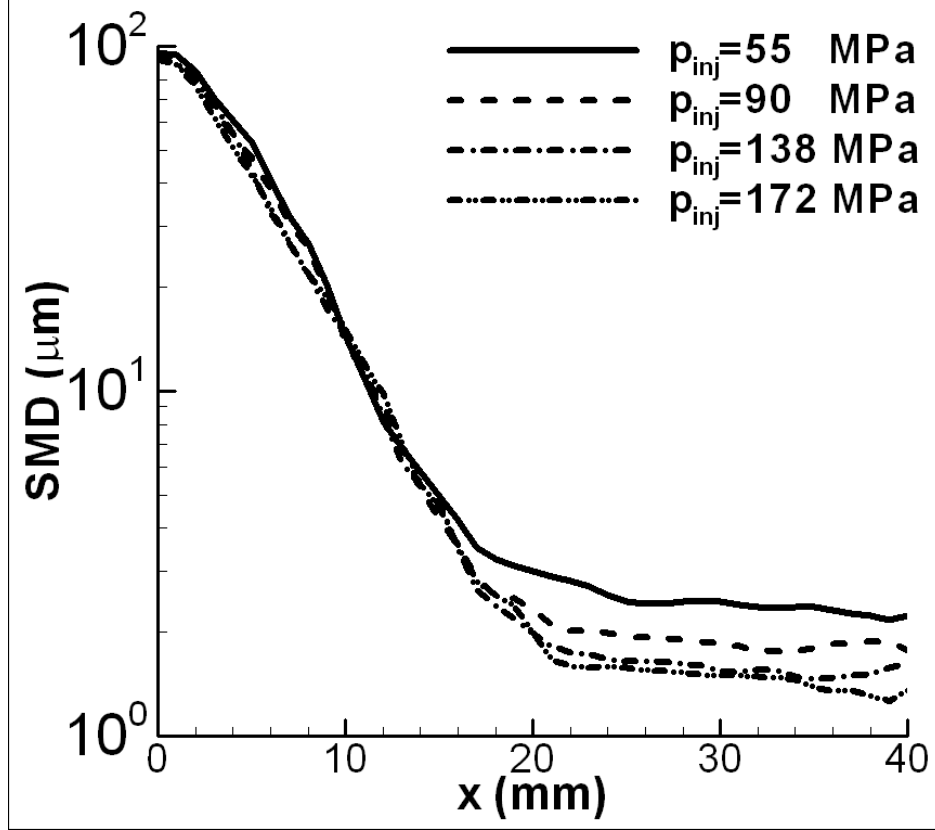
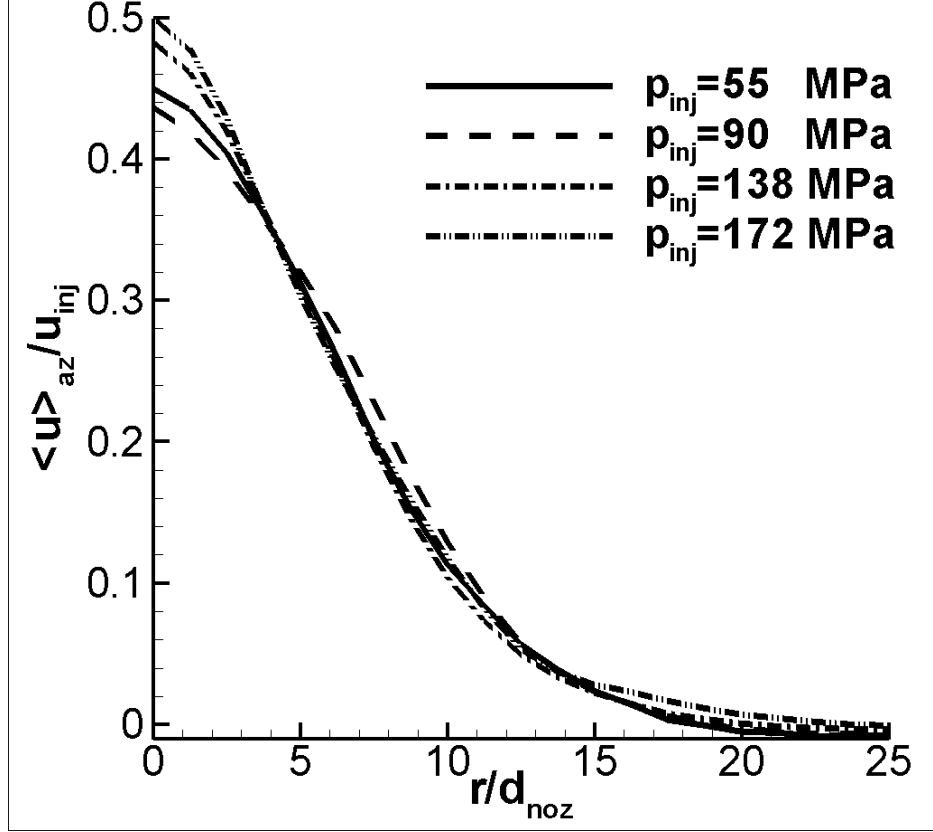


Figure 2.21: Effect of injection pressure on SMD profile of spray for $\rho = 7.3 \text{ kg/m}^3$ and $T = 700 \text{ K}$.

high relative velocities, thus evaporate fast enough so that the net SMD remains to be the same and invariant with respect to the injection pressure. It might be noted however that at the very tip of the spray, the size of surviving droplets is slightly smaller at higher injection pressures.

Figure 2.22 shows the azimuthally averaged axial velocity and its fluctuations for different injection pressures at the non-dimensional axial distance of 20 from the injector. The azimuthally averaged vapour mass fraction and evaporation rate parameter for small droplet are shown in Figure 2.23. Sprays with higher injection pressures generate higher gas velocity as well, but when the mean induced gas velocity is scaled with the corresponding injection velocity, the gas velocity profiles become almost identical. It is interesting to note that



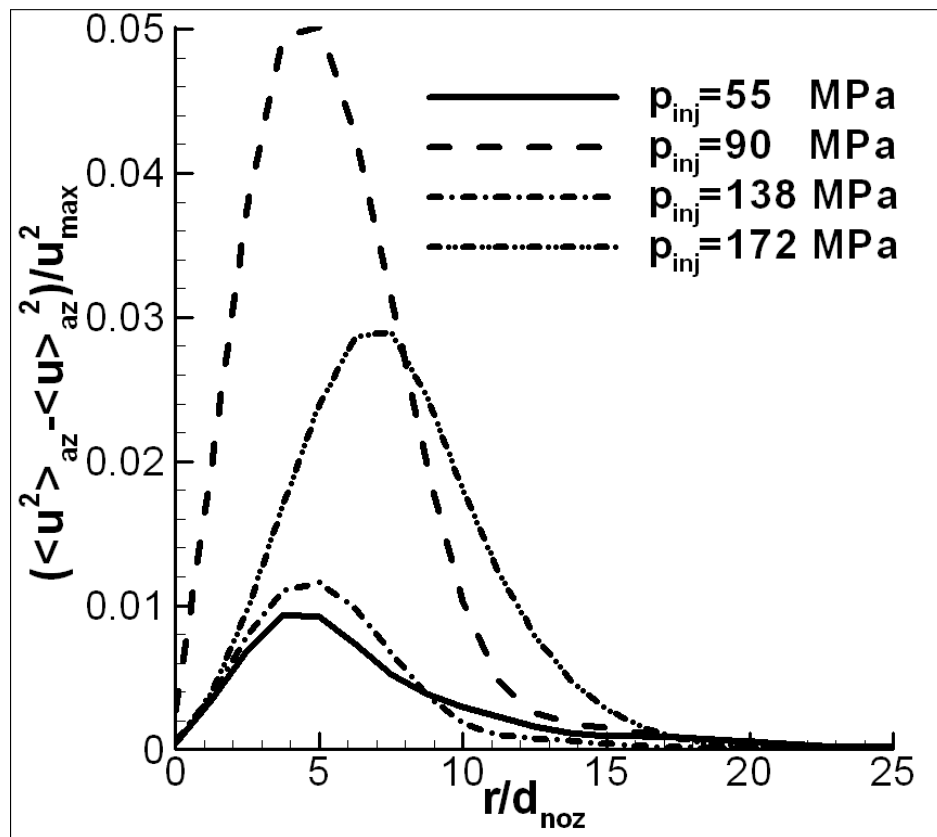
(a)

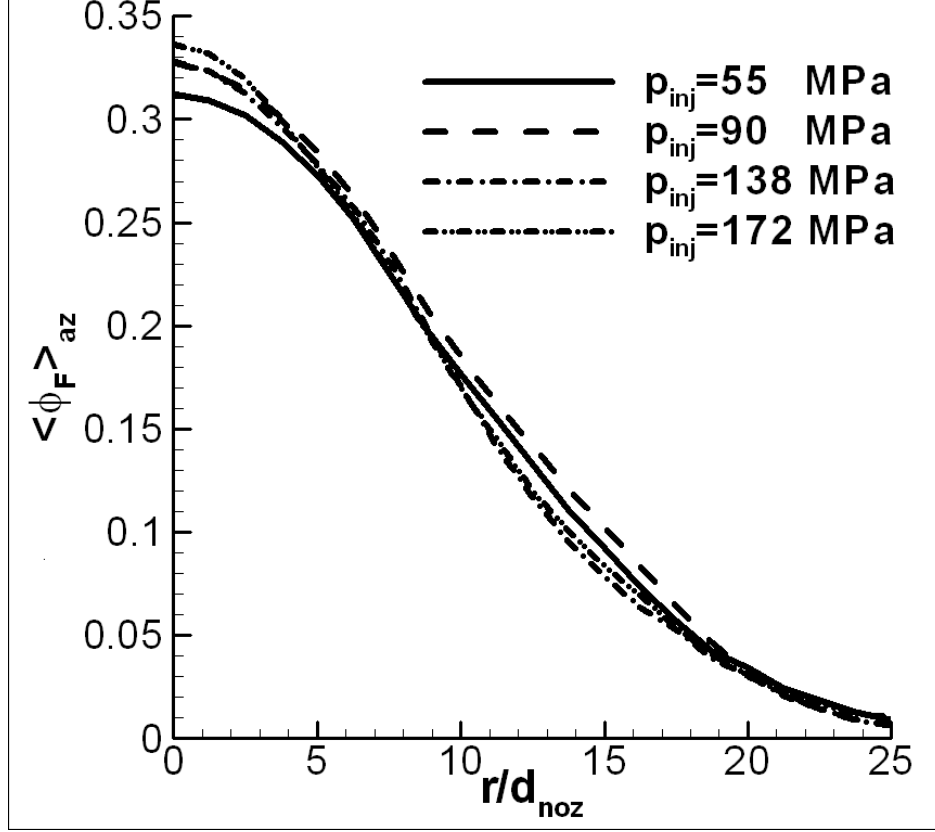
Figure 2.22: Effect of injection pressure on (a) induced gas velocity and (b) its fluctuations at $x=20$ for $\rho = 7.3 \text{ kg/m}^3$ and $T=700 \text{ K}$.

while the overall or average evaporation is almost the same as the nearly identical vapour mass fraction results suggest, the magnitude of velocity fluctuations in the vapour saturated gas is changing non-linearly with the injection pressure. Obviously, the change in velocity fluctuation magnitude is directly proportional to the local rate of evaporation parameter. The change in local evaporation rate is due to convection of the evaporated fuel by the spray induced gas flow and turbulence. An increase in injection pressure causes higher relative velocity which enhances the evaporation, and as a result the gas velocity fluctuations. Meanwhile, the higher induced gas velocity more efficiently convects the evaporated fuel away from the spray and droplets, allowing higher evaporation rate to be achieved. With

Figure 2.22: (cont'd)

(b)





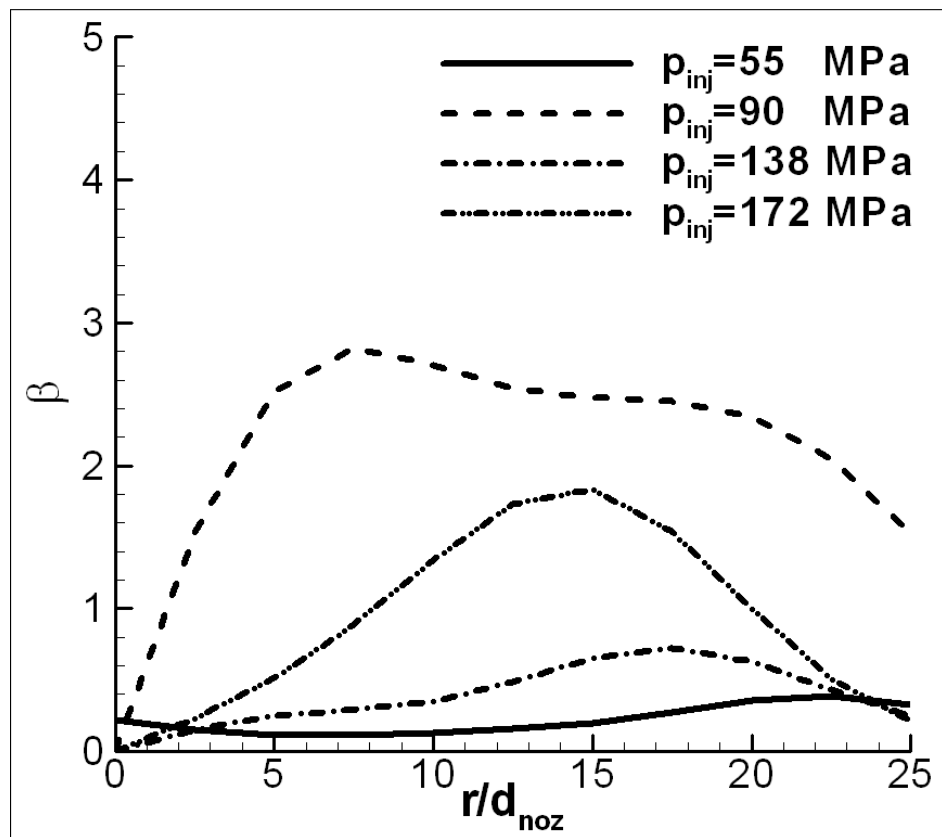
(a)

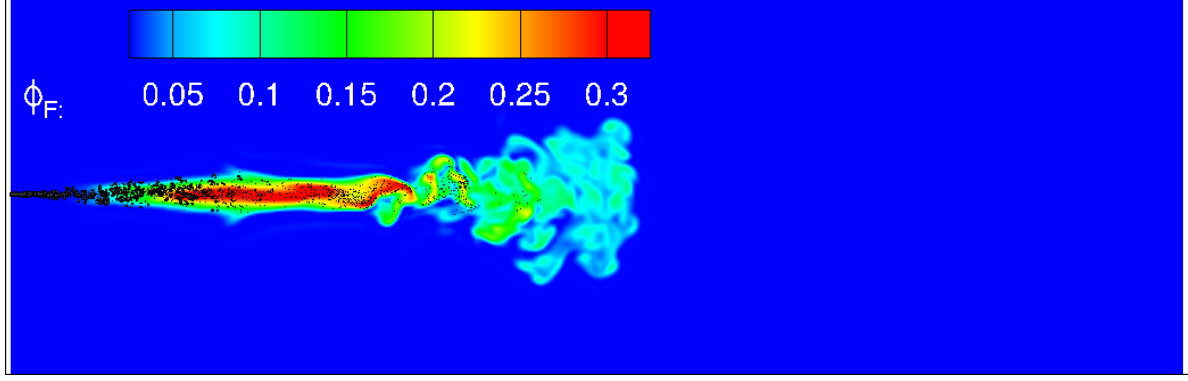
Figure 2.23: Effect of injection pressure on the radial profiles of (a) the azimuthally averaged vapour fuel mass fractions and (b) the mass averaged non-dimensional evaporation rate at non-dimensional distance of 20 from the injector and gas density and temperature of 7.3 kg/m^3 and 700 K, respectively.

further increase in the injection pressure, the gas phase will be saturated to such an extent that the local evaporation rate starts to decrease. Consequently, the gas velocity fluctuations start to subside too. However, with even more increase in the injection pressure the induced gas velocity and vapour convection becomes so significant that the local evaporation rate increases again. This local behaviour is due to the fact that momentum transfer happens not only through evaporation, but also by means of droplet drag force. While the rate of liquid evaporation is fluctuating along the spray axis with the increase in injection pressure; the induced gas velocity constantly increases. Higher induced gas velocity for higher in-

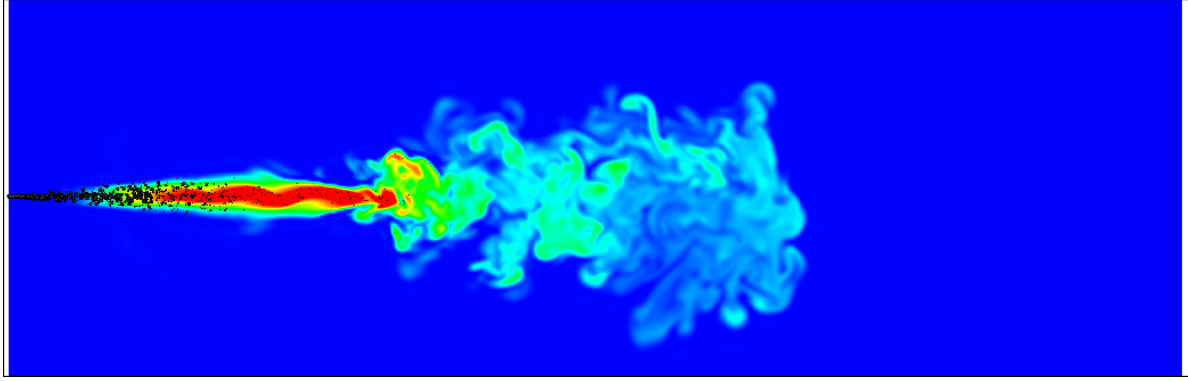
Figure 2.23: (cont'd)

(b)





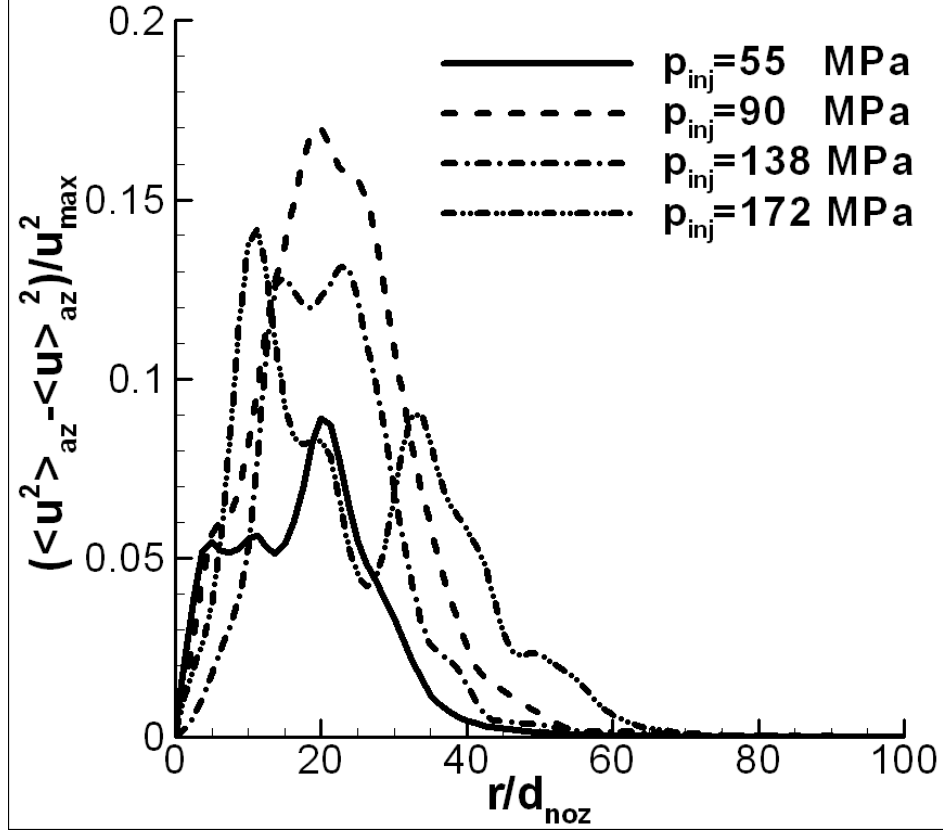
(a) $p_{inj} = 55 MPa$



(b) $p_{inj} = 172 MPa$

Figure 2.24: Evaporated vapour fuel contours for two injection pressures at $t=1.0$ ms for $T=700$ K, $\rho = 7.3 kg/m^3$.

jection pressures causes more vapour penetration, while the liquid penetration remains the same. This is evident in Figure 2.24, where the contours of evaporated fuel concentration for two injection pressures of 55 and 172 MPa are compared at $t=1.0$ ms. As suggested by the results in this figure and consistent with the observation that the liquid penetration does not change so much with the injection pressure, the overall evaporation profile of the spray does not change with the injection pressure. The fluctuations in the gas jet grow accordingly so that the mean length of the potential core of high speed, low temperature, vapour-saturated, gas jet remains nearly unchanged with the change in injection pressure. Figure 2.25 compares the fluctuations of the axial velocity at distances of 40 and 50 from injector. Apparently, after the gas jet becomes turbulent, the variance or turbulent intensity



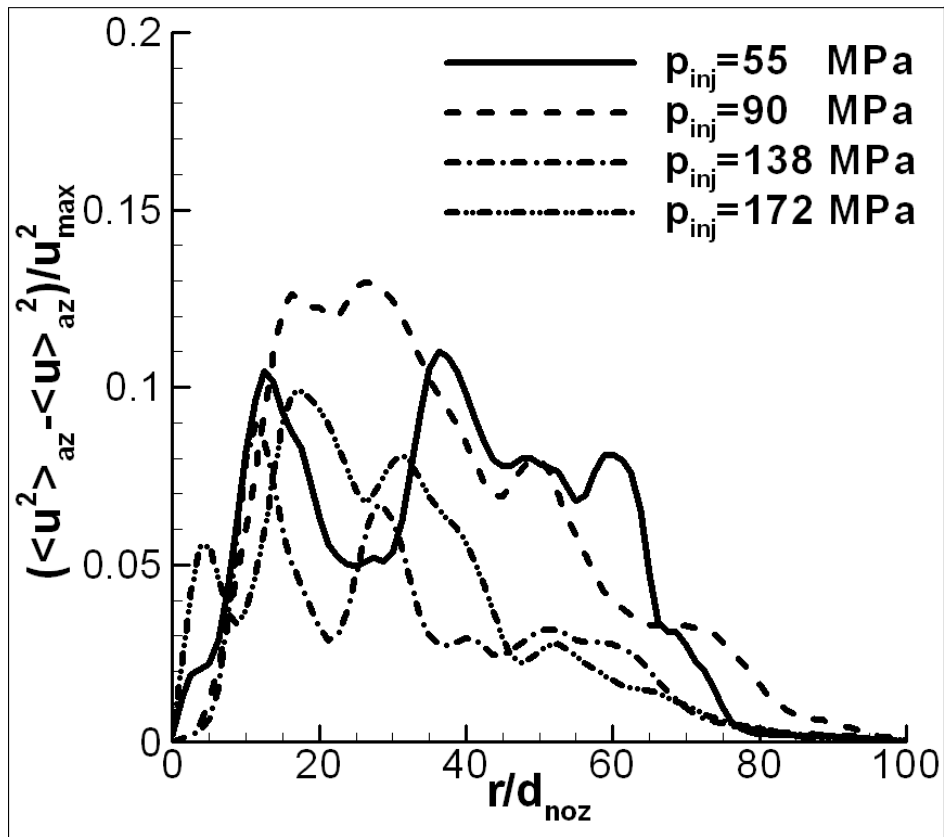
(a) $x=40$

Figure 2.25: Effect of injection pressure on the spray induced axial gas velocity fluctuations at two non-dimensional distances from the injector.

of the axial velocity follows the same trend as that of velocity oscillations in the potential core of the jet. With almost the same mean gas potential core length, the higher fluctuations in the gas jet enhance the turbulence production, dissipation and mixing.

Figure 2.25: (cont'd)

(b) $x=50$



2.3 Summary and Conclusions

Large eddy simulations of high speed evaporating sprays with significant spray-induced gas flow turbulence are simulated with a hybrid Eulerian-Lagrangian mathematical/computational methodology. The spray, modelled with Lagrangian droplet, stochastic breakup and non-equilibrium heat and mass transfer models, are fully coupled with the Eulerian gas phase flow and turbulence through series of mass, momentum and energy coupling terms in the resolved and subgrid-scale gas equations. The spray is issued into a quiescent heated chamber at different gas conditions. A wide range of chamber gas temperatures and densities as well as spray injection pressures and nozzle diameters are considered. The predicted results with the hybrid LES/Spray model are shown to compare well with the experimental data for all tested spray and gas conditions that indicates the reliability of the model. The interactions of high speed evaporating spray with the spray induced gas flow and turbulence with spray is studied by examining several global and local flow and spray variables. It is shown that spray induces more turbulence at higher gas chamber temperatures due to higher local evaporation rate. More turbulence is also generated by the spray for the denser chamber gas because of higher velocity and density fluctuations caused by the momentum transfer and evaporation. Furthermore, spray is shown to generate stronger turbulence with a larger nozzle as a result of higher evaporation rate caused by higher gas entrainment. Our results indicate that although the increase in injection pressure enhances local evaporation rates of droplets, the mean normalized gas flow remains unchanged and the liquid penetration is almost constant for the range of high injection pressures considered due to competing factors of evaporation and vapour convection. While the injection pressure does not affect the liquid penetration, the vapour penetrates more and mixes much better at higher injection pressures

due to higher induced gas velocity and turbulence.

Chapter 3

Large Eddy Simulation of Turbulent Spray Combustion

3.1 Introduction

Turbulent spray combustion is complicated by multi-scale and multi-time interactions of the liquid with gas flow, finite-rate evaporation and multi-step reactions. There is a limited understanding of turbulence-spray-combustion interactions and the auto-ignition and flame stabilization of reacting sprays ([94],[95] and [96]) due to challenges in experimental measurements and computational modelling. High fidelity affordable computational models are certainly needed which can at least describe the most important interactions among spray, turbulence and combustion. Direct numerical simulation (DNS) of spray combustion with complex chemistry models is well beyond the current computational power. Only very recently, three dimensional DNS of relatively simple dilute two-phase homogeneous turbulent combustion with reduced kinetics mechanism has been reported [97]. Due to significant spatial and temporal variations in flow variables and the presence of large-scale coherent vortical structures and other inherently transient physical and chemical processes involved in turbulent spray combustion, large-eddy simulation (LES) models are expected to be much

more suitable than Reynolds-averaged Navier-Stokes (RANS) models for this problem, even though the latter remains to be a useful tool for the design of engineering systems. LES has been widely used for single-phase reacting flows ([98],[99] and [101]). However, its use for turbulent spray simulations is limited to few studies using low speed sprays or relatively simple kinetics ([36],[58], [101],[102] and [103]). In particular, simulations of reacting sprays have proven to be very difficult, mainly because of challenges in modelling of subgrid-scale (SGS) turbulence-spray-combustion interactions. The ignition of sprays show strong dependence on the chemical kinetics [104], making the choice of chemical kinetics model also important.

The traditional approach to the spray simulation is to solve the gas-phase equations by a grid-based Eulerian method and to compute the spray by a particle-based Lagrangian method. In this approach, submodels are required to account for the various physical processes taking place at “small” time and length scales in both Eulerian and Lagrangian fields. Provided that the SGS particle motion and scalar fluxes are correctly modelled, the accuracy of simulations is still dependent on the models used for the liquid evaporation, micro-mixing and highly non-linear chemical reactions ([6] and [101]). Transported probability density function (PDF) methods have proven to be particularly effective in accounting for turbulence-chemistry interactions [101]. Filtered mass density function (FMDF) is a promising model for LES of turbulent reacting flows which is developed based on the solution of single-point SGS PDF of energy and species mass fractions [105]. In this approach, the joint statistics of turbulent variables at subgrid level are obtained by solving the transport equation for the FMDF. The main advantage of FMDF is that the single-point statistics like reaction terms appear in a closed form in its formulation. This allows simulations of various types of reactions (slow,

fast, premixed, non-premixed, etc.) with different chemical kinetic models ([57],[99], [106], [107], [108],[109] and [110]). Li et al. [111] presented the newly developed two-phase FMDF model for simulation of two-phase reacting flows. They validated the results of this model with DNS data in a spatially developing droplet-laden reactive mixing layer.

Depending on the type of flow and flame, the reaction time and length scales can be comparable or far different than those of the turbulence and the spray. This has led to the development of reaction mechanisms at various levels of details and comprehensiveness [112]. For some of the hydrocarbon fuels such as n-heptane [113], complex (skeletal or reduced) kinetics models are available beyond simple global mechanisms ([114], [115] and [116]). For problems like turbulent spray combustion, complex reaction models are normally needed. However, the computational cost of making the chemistry calculations with complex kinetics is often prohibitive and efficient implementation of chemistry is a necessity for an affordable computation.

There are different ways for efficient implementation of chemical reaction in computational models such as LES/FMDF. Among the methods proposed, one can refer to the storage/retrieval algorithms [117] including structured look-up tabulation [118], repro-modeling [119], artificial neural networks (ANN) [120]-[121], in situ adaptive tabulation (ISAT) [122]-[123], piecewise reusable implementation of solution mapping (PRISM) [124], and high dimension model representations (HDMR) [125]. A prominent method is the in situ adaptive tabulation or ISAT, a storage and retrieval methodology which has been widely adopted especially with PDF methods. ISAT algorithm gives the highest speed-up for statistically stationary flows such as non-premixed piloted jet flames [126], where a speed-up factor of 100-1000 is achieved. However, it has also been applied to the calculation of transient pro-

cesses such as combustion in internal combustion (IC) engines [127] where a speed up factor of 10 is reported. The original ISAT algorithm by Pope [122] has been improved [123] and is extended for parallel PDF calculations [128] and improved efficiency and scalability [129].

The Engine Combustion Network [91] provides an open forum for experimental and computational studies and collaborations on turbulent spray combustion. One of the configurations of the ECN is a constant volume turbulent spray combustion chamber that has the thermochemical conditions that are representative of those in modern direct injection (DI) compression ignition engines ([69], [130] and [131]). Measurements have shown that the turbulent spray flame is often lifted off from the injector tip. From a practical viewpoint, the interest in flame liftoff in diesel sprays arises because of its correlation with soot concentration in the spray [95]. In the DI systems, the spray is injected with a very high velocity into a low speed ambient gas and therefore is a significant source of generating the gas flow turbulence. As the liquid fuel has to go through breakup, droplet formation, and evaporation before reaction, all parts of the spray evolution is important to the combustion. The rate of evaporation, alone is dependent on details of breakup and droplet size distribution but is also affected by the local gas temperature and vapour concentrations which are controlled by the spray induced turbulent flow and turbulent mixing ([69] and [90]). Most of the numerical studies of the ECN sprays have been focused on unsteady RANS with different turbulent-combustion models, very recently with the PDF method ([104]-[132]).

In this chapter, the LES and spray model is coupled with the two-phase FMDF for simulations of high speed evaporating and reacting sprays with complex chemical kinetics mechanisms. The main goals are to first establish the reliability and accuracy of the LES/FMDF

methodology for turbulent spray combustion simulations and then use the model for detailed study of spray-turbulence-combustion interactions in several high speed sprays. The numerical data provide a wealth of information on these interactions for very different spray and gas flow conditions. The developed computational method for the solution of two-phase LES/FMDF has one Eulerian and two Lagrangian solvers. The compressible LES equations are solved by high-order finite difference methods via a grid-based Eulerian flow solver. The FMDF is obtained by solution of its transport equation with an efficient Lagrangian stochastic Monte Carlo method, with spray effects included ([105], [111]). The spray is simulated with a non-equilibrium Lagrangian particle method together with a stochastic droplet breakup model which allows full two-way mass, momentum, and energy coupling between phases. The chemistry is based on finite rate compact skeletal kinetics together with ISAT and chemistry load balancing for parallel processing. Details of the mathematical and computational approach for the two-phase FMDF and combustion chemistry calculation are described in the next section below, followed by the results obtained with the LES/FMDF and conclusions.

3.2 Two-Phase Filtered Mass Density Function

The scalar FMDF is a joint probability density function of the scalars (species mass fractions and energy) at the subgrid-level which was originally developed by Jaber et al. [105] for single-phase reacting flows and has proven to be very reliable and accurate for these flows.

$$F_L(\Psi; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \xi(\Psi, \Phi(\mathbf{x}', t)) G(\mathbf{x}' - \mathbf{x}) d\mathbf{x}', \quad (3.1)$$

where G denotes the filter function, Ψ is the scalar vector in the sample space and ξ is the fine grained density [133], defined based on a series of delta functions. The scalar vector includes species mass fractions and specific sensible enthalpy.

The FMDF transport equation is obtained by inserting the instantaneous unfiltered scalar equation into the time derivative of the fine grained density and filtering that. Li et al. [111] extended the original FMDF to two phase flows. Banaeizadeh et al. [134] included the compressibility effects due to total pressure variations. For a compressible two-phase reacting system with small liquid volume fractions, the FMDF equation can be written in the following form:

$$\begin{aligned} \frac{\partial F_L}{\partial t} + \frac{\partial}{\partial x_i} [\langle u_i(\mathbf{x}, t) \rangle_L F_L] = & - \frac{\partial}{\partial x_i} [\langle \langle u_i(\mathbf{x}, t) | \Psi \rangle_l - \langle u_i \rangle_L \rangle F_L] + \frac{\partial}{\partial \psi_\alpha} [\langle \frac{1}{\rho(\Psi)} \frac{\partial J_i^\alpha}{\partial x_i} | \Psi \rangle_l F_L] \\ & - \frac{\partial}{\partial \psi_\alpha} (\dot{S}_\alpha(\Psi) F_L) - \frac{\partial}{\partial \psi_\alpha} [\langle S_\alpha^{comp} | \Psi \rangle_l F_L] \\ & - \frac{\partial}{\partial \psi_\alpha} [\frac{\langle \dot{S}_\alpha^{sp} | \Psi \rangle F_L}{\rho(\Psi)}] + \frac{\partial}{\partial \psi_\alpha} [\frac{\langle \dot{S}_{Mass}^{sp} | \Psi \rangle F_L}{\rho(\Psi)}] + \frac{\langle \dot{S}_{Mass}^{sp} \rangle F_L}{\rho(\Psi)}. \end{aligned} \quad (3.2)$$

It is noted here that in the FMDF equation reaction terms are all closed but in conventional LES methods they are not closed and have to be modelled. Hence, the filtered heat of reaction and rate of species production in equations 1.36 and 1.37 are obtained from the FMDF. The first term in the right hand side (RHS) of equation 3.2 represents the SGS convection which is modelled with a gradient type closure:

$$(\langle u_i(\mathbf{x}, t) | \Psi \rangle_l - \langle u_i \rangle_L) F_L = -\Gamma_t \frac{\partial (F_L / \langle \rho \rangle_l)}{\partial x_i}, \quad (3.3)$$

where $\Gamma_t = \mu_t / Pr_t$ or $\Gamma_t = \mu_t / Sc_t$ is the turbulent diffusivity. The term due to molecular

diffusion is decomposed into two parts of molecular transport and the SGS dissipation. The SGS dissipation is modelled with the linear mean-square estimation (LMSE) [135]-[136] or the interaction by exchange with the mean (IEM) model [137]:

$$\frac{\partial}{\partial \psi_\alpha} [\langle \frac{1}{\rho(\Phi)} \frac{\partial J_i^\alpha}{\partial x_i} | \Psi \rangle_l F_L] = \frac{\partial}{\partial x_i} [\Gamma \frac{\partial}{\partial x_i} (\frac{F_L}{\langle \rho \rangle_l})] + \frac{\partial}{\partial \psi_\alpha} [\Omega_m (\psi_\alpha - \langle \phi_\alpha \rangle_L) F_L], \quad (3.4)$$

where the molecular diffusivity is $\Gamma = \mu/Pr$ or $\Gamma = \mu/Sc$ and the SGS mixing frequency is $\Omega_m = \frac{1}{2} c_\phi (\Gamma + \Gamma_t) / (\Delta^2 \langle \rho \rangle_l)$.

The compressible source term due to pressure variation in the scalar FMDF is obtained by taking into account the total derivative of filtered pressure for mixture enthalpy as [134]:

$$\langle \dot{S}_\alpha^{comp} | \Psi \rangle_l = \frac{1}{\langle \rho \rangle_l} (\frac{\partial \langle p \rangle_l}{\partial t} + \langle u_i \rangle_L \frac{\partial \langle p \rangle_l}{\partial x_i}), \alpha = N_s + 1. \quad (3.5)$$

The last three terms on the RHS of equation 3.2 represent the spray/droplet effects on FMDF. They involve particle source/sink terms affecting the gas composition and density. The modelled FMDF transport equation is closed and may be solved to get the scalar FMDF and consequently all single-point statistical information concerning reactive species and temperature at various times and locations, including the first moment or filtered variables. Also, by integrating the FMDF equation in PDF or composition space, one can recover the transport equations for the first, second and all the other SGS scalar moments. This indicates a mathematical consistency between the FMDF and the conventional LES methods which solve the moment equations directly.

The most convenient means of solving the FMDF transport equation is via the Lagrangian Monte Carlo (MC) procedure [138]. With the Lagrangian procedure, the FMDF is repre-

sented by an ensemble of computational “stochastic elements” (or “Monte Carlo particles”). These notional particles evolve via a “stochastic process,” described by a set of stochastic differential equations (SDEs) ([51],[139]). PDFs of the stochastic processes are governed by the Fokker-Planck equation. A comparison between the Fokker-Planck equation and the FMDF equation under consideration identifies the parameters of the stochastic equation [105]. A unique feature of this procedure is that the large-scale, subgrid-scale, and molecular mixing processes, the chemical reaction and the two-phase terms can be separately incorporated and evaluated, offering a systematic way to compute and interpret these processes in the LES/FMDF calculations. The simplest means of simulating the spatial transport in this equation is via the Euler-Maruyamma approximation. Higher order numerical schemes are available, but one must be cautious in using them for LES since the diffusion term in stochastic equation depends on the stochastic process. The numerical scheme must preserve the Ito-Gikhman nature of the process. The Euler-Maruyamma approximation provides sufficient accuracy for the flows studied here.

In the solution procedure, each MC particle is transported in the “physical space” by the combined actions of large scale convection and diffusion (molecular and subgrid).

$$dX_i^+ = [\langle u_i \rangle_L + \frac{1}{\langle \rho \rangle_l} \frac{\partial(\Gamma + \Gamma_t)}{\partial x_i}]dt + \sqrt{\frac{2(\Gamma + \Gamma_t)}{\langle \rho \rangle_l}} dW_i, \quad (3.6)$$

In addition, transport in the “composition space” occurs due to SGS/molecular mixing, chemical reaction, pressure variation and droplet heat and mass transfer.

$$d\phi_\alpha^+ = -\Omega_m(\phi_\alpha^+ - \langle \phi_\alpha \rangle_L) + \dot{S}_\alpha(\phi^+)dt + \langle \dot{S}_\alpha^{comp} \rangle_l dt + [\frac{\langle \dot{S}_\alpha^{sp} \rangle_l - \phi_\alpha^+ \langle \dot{S}_{Mass}^{sp} \rangle_l}{\langle \rho \rangle_l}]dt. \quad (3.7)$$

Compared to RANS for which the choice of mixing model makes a significant difference, most of mixing models in LES yield similar results [99]. In the present work, the mixing of evaporated fuel is included via two-phase terms in the FMDF equation and standard subgrid scalar mixing coefficient $c_\phi = 2.0$ is used.

In this work, the spray terms in the FMDF equation are weighted averaged from FD grid points to the MC particle locations. To manage the number of MC particles and to reduce the computational cost, a procedure involving the use of non-uniform weights is considered. The variable weighting for particles allows the particle number density to stay above a certain minimum value regardless of density variations. It has been shown that the sum of weights within the ensemble averaging domain is related to the filtered fluid density as

$$\langle \rho \rangle_l \approx \frac{\Delta m}{\Delta V} \sum_{n \in \Delta V} w^{(n)}, \quad (3.8)$$

where ΔV is the volume of the domain and Δm is the mass of a MC particle with unit weight. For the spray simulation, particle weights should be modified due to added mass to the carrier gas from the evaporating droplets. The MC particle weight then is adjusted as

$$dw^{(n)} = \frac{\Delta V}{\Delta m} \langle \dot{S}_{Mass}^{sp} \rangle_l dt. \quad (3.9)$$

In the present hybrid methodology, the filtered scalar values like temperature may be calculated from both FD grids and MC particles. This provides the unique opportunity for the assessment of LES-FD and FMDF-MC parts of the LES/FMDF method. Mathematically, LES-FD and FMDF-MC results are identical. Consistency of MC and FD data implies numerical accuracy of both. For establishing the consistency between FD and MC methods in

reacting flows, the chemical source terms in the FD equations which are closed in the FMDF formulation are calculated from the MC particles.

3.2.1 Combustion Chemistry and in situ Adaptive Tabulation

As mentioned before, the chemical kinetics model plays a crucial role in LES of spray auto-ignition, combustion and extinction and should include the essential features of the fuel-air chemistry. In this work, the skeletal mechanism of Liu et al. [115] is used which has been extensively tested for high pressure non-premixed flames, conditions similar to those considered in our spray combustion simulations. This mechanism has 44 species and 185 reactions, counting forward and backward reactions individually. The evolution of the scalar field due to reaction is carried out on MC particles with a fractional step method according to the following equation.

$$d\phi_{\alpha}^{+} = \dot{S}_{\alpha}(\phi^{+})dt. \quad (3.10)$$

ISAT uses the ordinary differential equation (ODE) solver DDASAC [140] to integrate equation 3.10 and stores the relevant information in a binary tree, with each termination node (or leaf) representing a record of the tabulation point of a specific composition, the reaction mapping in time Δt and the mapping gradient matrix. Using this matrix, for a given query composition close to a tabulated composition point, a linear approximation to the mapping is obtained under a controlled tolerance. An ellipsoid of accuracy (EOA) is used to approximate the region of accuracy. An EOA is a hyperellipsoid in composition space, representing the connected region in composition space containing a tree leaf. For a given query, ISAT traverses the tree until a leaf representing a point close to the query is reached. The following events are invoked to obtain an approximation to the corresponding reaction

mapping by the following steps ([122], [123] and [128]): (1) Retrieve: if the query falls within the ellipsoid of accuracy of the leaf, a linear approximation is returned. (2) Grow: otherwise, a function evaluation is performed to determine the reaction mapping. The error in linear approximation at the leaf is calculated and if the error is within the tolerance, the EOA of the leaf node is grown to include the query point. (3) Add: if the computed error is greater than the tolerance and the table is not full, then a new leaf is added. (4) Discarded evaluation: if the table is full, then the reaction mapping is evaluated and no further action is performed regarding the ISAT table. For transient flows such as spray combustion, it is better in some cases to replace new evaluations with old ones as the flow is developing. This procedure is implemented for the simulations conducted in this chapter.

In large scale parallel LES/FMDF computations; there is a need to distribute the chemistry workload among the cores to reduce the overall computational time. Lu et al. [128] and Hiremath et al. [129] developed different distribution strategies for ISAT to balance the combustion chemistry workload on different computational cores. In the parallel calculations, each processor maintains its own ISAT table. However, during the reaction calculation, particles on one processor may be distributed to one or more other processors and be resolved by ISAT tables there. Among the distribution strategies tested by Hiremath et al., the so called partitioned uniform random distribution (P-URAN) has the highest efficiency and scalability which is adopted here as well. This strategy works in two stages: in stage 1 (for a specified duration of time for which the ISAT table is being built-up), all particles on a core are resolved using the local ISAT table; then in stage 2 (for the remainder of the time steps), the participating cores are partitioned into smaller groups and within each partition, the URAN strategy is used to uniformly distribute the chemistry workload. The

URAN strategy aims at achieving statistically ideal load balancing by evenly distributing the chemistry workload among various cores.

3.3 Results and Discussions

For the selected experiments considered in this chapter, the fuel is normal heptane which is injected with the temperature of 373 K from a 100 micron nozzle with the injection pressure of 150 MPa. This spray is designated “Spray H” by Sandia National laboratory researchers [141]. The main parameters of spray H are listed in Table 3.1. The effect of injection pressure and nozzle size on the spray induced gas turbulence has been considered in the previous chapter mainly for n-Hexadecane. In the present work, the focus is on temperature and oxygen concentration effect on combustng sprays. The rectangular computational domain used in the simulations covers the entire axial length of the chamber, but in other directions it extends only to half of the chamber length for computational efficiency. Free stream boundary conditions are applied along these directions. Table 3.2 summarizes the main computational parameters of the simulations. The LES grid size is 0.2 mm which is uniform in axial direction and tends to stretch in other directions for %40 of their lengths reaching to 0.95 mm at free stream boundaries. In contrast to conventional spray models, there are no adjustable

Fuel	n-heptane
T_{fuel}	363 K
d_{noz}	100 μm
p_{inj}	150 MPa
Δt_{inj}	4 ms
T_g	800-1200 K
ρ_g	14.8 kg/m^3

Table 3.1: Parameters of spray H

N_{core}	624
N_{PC}	50,000
N_G	20,000,000
N_{MC}	120,000,000
Δ (mm)	0.2
d_{noz} (mm)	0.90
simulated time duration	3-4 ms
average runtime	10 days

Table 3.2: Computational parameters for LES of turbulent spray combustion

O_2	N_2	CO_2	H_2O
21	69.33	6.11	3.56
15	75.15	6.22	3.63
12	78.07	6.28	3.65
10	80.00	6.33	3.67
8	81.95	6.36	3.69
0.0	89.71	6.52	3.77

Table 3.3: Molar percentages of chamber constituents for different initial oxygen concentrations.

coefficients in our spray model. However, for initial size of liquid injection and injection velocity, the experimentally measured area contraction and nozzle discharge coefficients are used [26]. It has been shown that the spray model is not sensitive to grid size and the coefficients of k_{sgs} equation for high ambient gas temperatures with respect to evaporative properties of the fuel (chapter 1). However, the grid size is chosen to be the smallest that can be used with the specific nozzle size to capture the maximum achievable turbulent scales in the spray generated flow. The computational domain is massively partitioned in all three dimensions for efficient parallel calculations using 624 cores. The code is highly optimized for efficient and non-blocking parallel processing and communications for all the three fields of the solver. The first stage of P-URAN for chemistry load balancing is generally set to the first 24 hours as the initial stage of simulation is dealing with breakup and evaporation rather than reaction. This is generally prior to ignition time. The simulation is initialized

using stagnant chamber conditions based on temperature, density and composition. The chamber ambient density and temperature for the base case are 14.8 kg/m^3 and 1000 K. Table 3.3 summarizes initial chamber composition for different oxygen concentrations. The oxygen molar percentage for the base case corresponds to % 21 in Table 3.3.

3.3.1 Vapour Mixing in Non-Reacting Sprays

For the non-reacting n-heptane spray, experimental data for temporal evolution of liquid and vapour penetration lengths as well as fuel mass fraction distributions are available. The computed liquid and vapour penetrations are defined as the distance from the nozzle exit to the axial location where the liquid volume fraction and vapour mass fraction drop to % 0.1 of their initial values [141]. The ambient density and temperature are 14.8 kg/m^3 and 1000 K with zero oxygen concentration. The simulated liquid and vapour penetrations are compared with the experimental data in Figure 3.1. During the transient period, the fuel liquid and vapour penetration lengths are both over-predicted by the numerical model. This can be attributed to liquid jet model used for the dense and early development part of the spray. After this period, the results agree well with the experimental data. Additionally, the vapour penetration lengths computed from LES-FD and FMDF-MC parts of the LES/FMDF solver also agree very well with each other. Comparison of fuel vapour distributions obtained by LES-FD and FMDF-MC are made in Figure 3.2 through contour and scatter plots of the vapour mass fraction at $t=2.00 \text{ ms}$. It is clear that the Eulerian and Lagrangian parts are very much consistent and therefore numerically accurate. The scatter in Figure 3.2c at low vapour mass fraction values could be attributed to over-shoots in the Eulerian FD solver at the tip of fuel vapour jet, where the flow is highly turbulent and fluctuating. The high speed

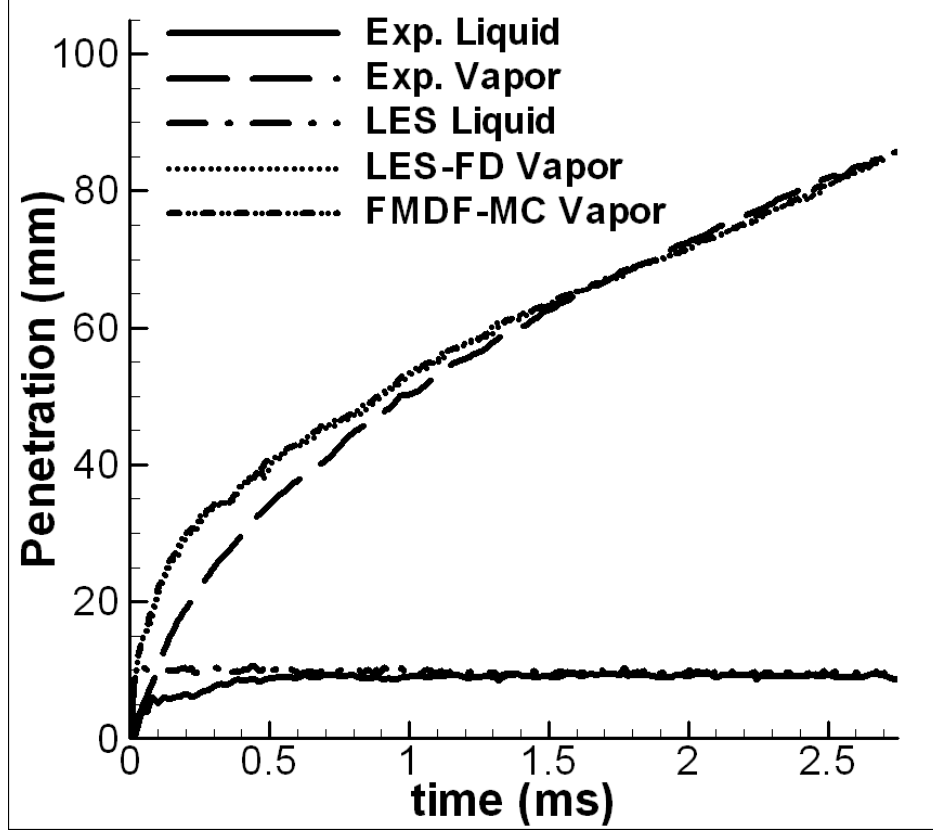
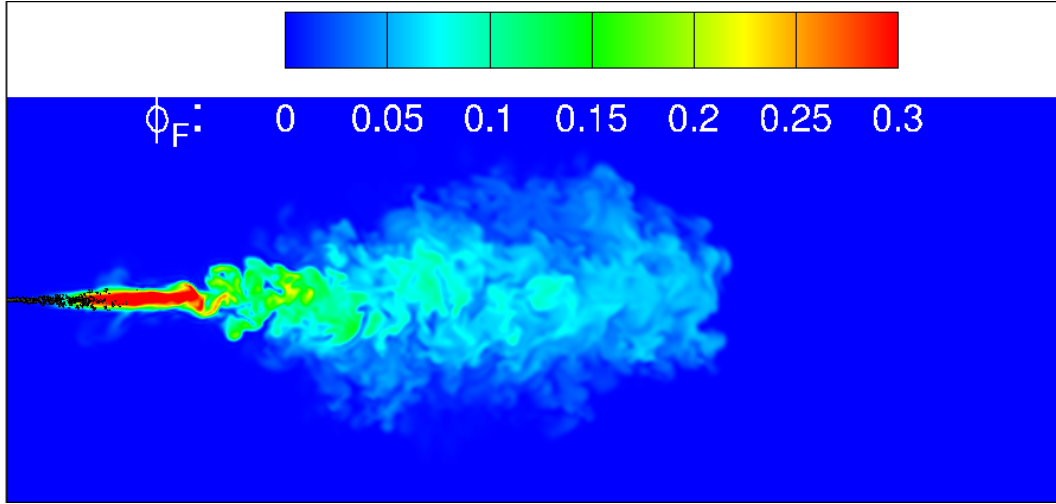


Figure 3.1: Variation of simulated and measured liquid and vapour penetration lengths in time for $T=1000$ K, $\rho = 14.8 \text{ kg/m}^3$ (base case) and %0.0 O_2 concentration.

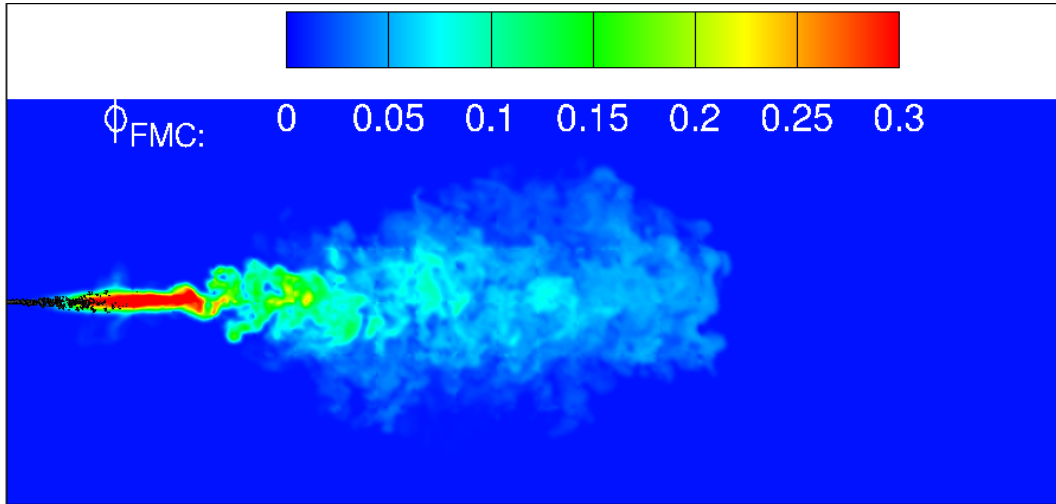
spray vaporization generates a highly unstable jet in the gas which is breaking into turbulent structures downstream of the liquid length. The species mass fractions used in the solver are obtained from the FMDF part which is non-diffusive and free from overshoot/undershoot errors usually seen in high order FD simulations with limited grid resolution.

Comparisons of the simulated and measured radial profiles of azimuthally averaged fuel mass fraction at different axial locations and its corresponding variance at $x=40$ mm are shown in Figure 3.3. It is indicated that the computed fuel mass fractions from LES-FD and FMDF-MC are consistent and agree fairly well with the measured values. It should be noted that the variance calculated from the experimental data has high level of statistical uncertainty, the same order as the fuel fraction variance itself [142]. Therefore, only a qualitative comparison

can be made. Nevertheless, we observe that the LES/FMDF profiles are narrower and have higher central peak values in comparison to experiment for axial locations close to the nozzle. This can be attributed to the localized spray source terms which are computed at FD grid points with finite-size volumetric averaging of the droplet information. Further downstream, the simulated values are slightly lower than the experimental data. This is expected as the narrow jet upstream becomes unstable and grows with a rate slightly more than the experiment.



(a)

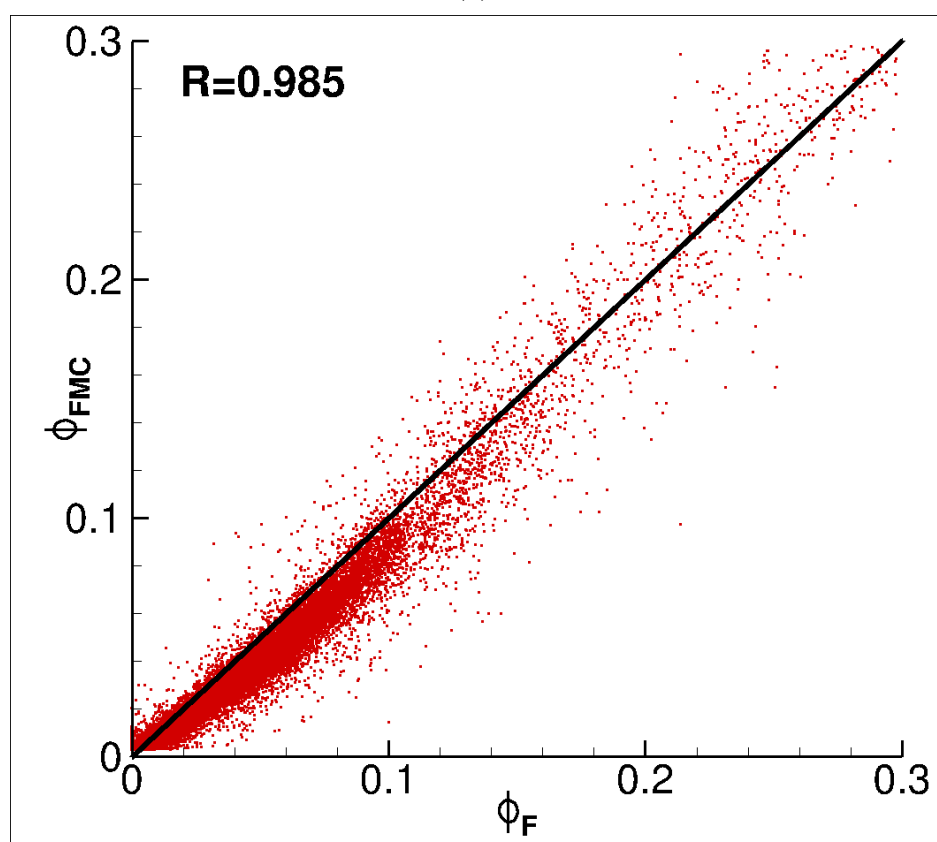


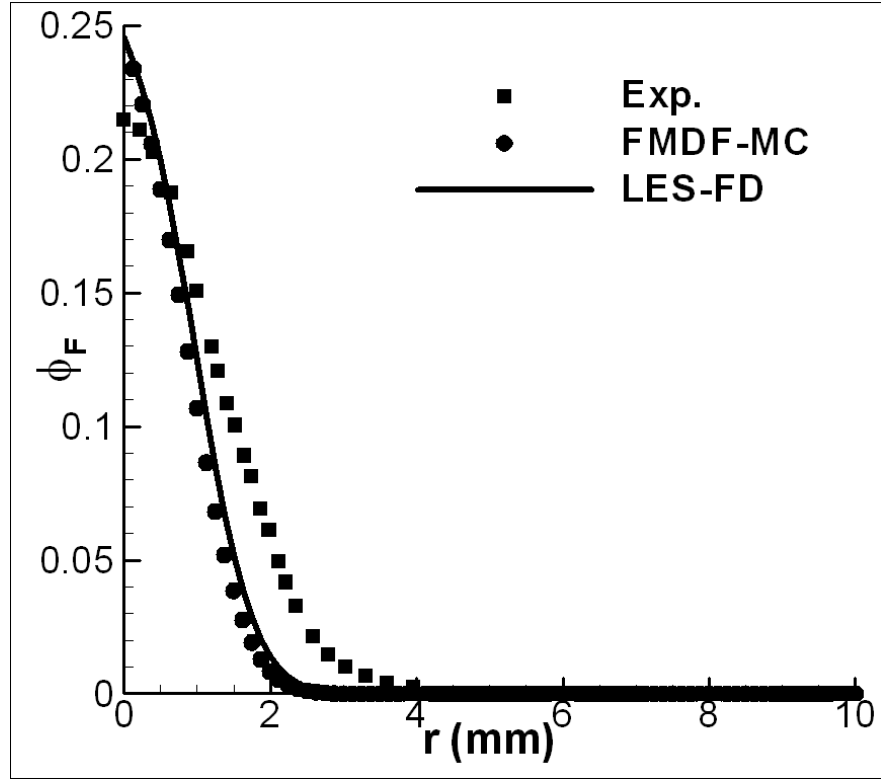
(b)

Figure 3.2: Fuel vapour mass fraction fields in the non-reacting spray at $T=1000$ K, $\rho = 14.8 kg/m^3$. (a) contours from LES-FD data, (b) contours from FMDF-MC data, (c) scatter comparison of vapour mass fraction obtained from LES-FD and FMDF-MC data.

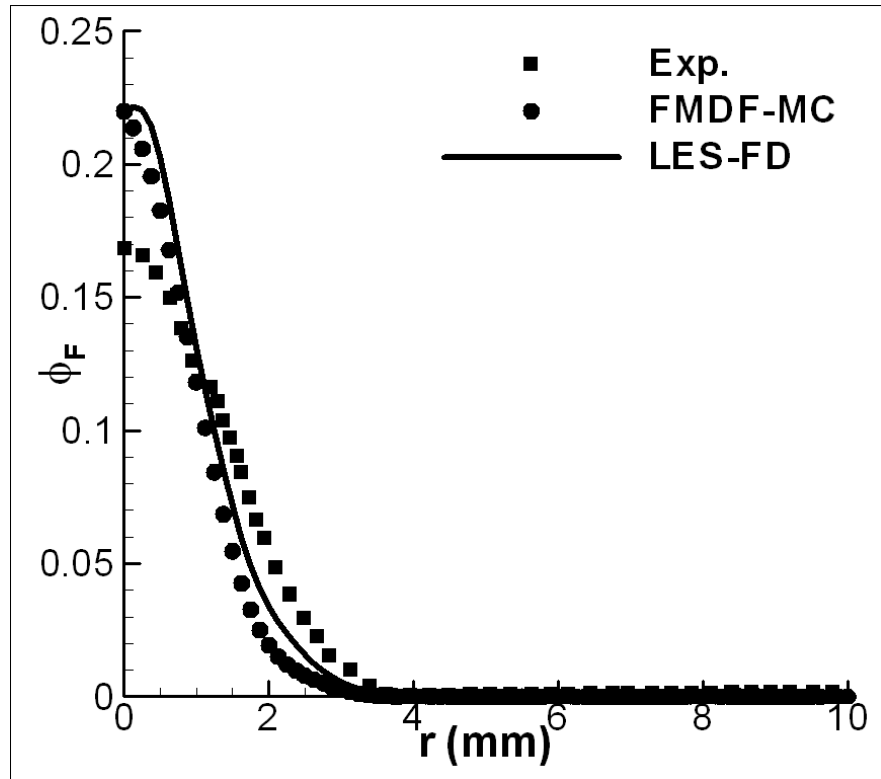
Figure 3.2: (cont'd)

(c)





(a) $x=17\text{mm}$

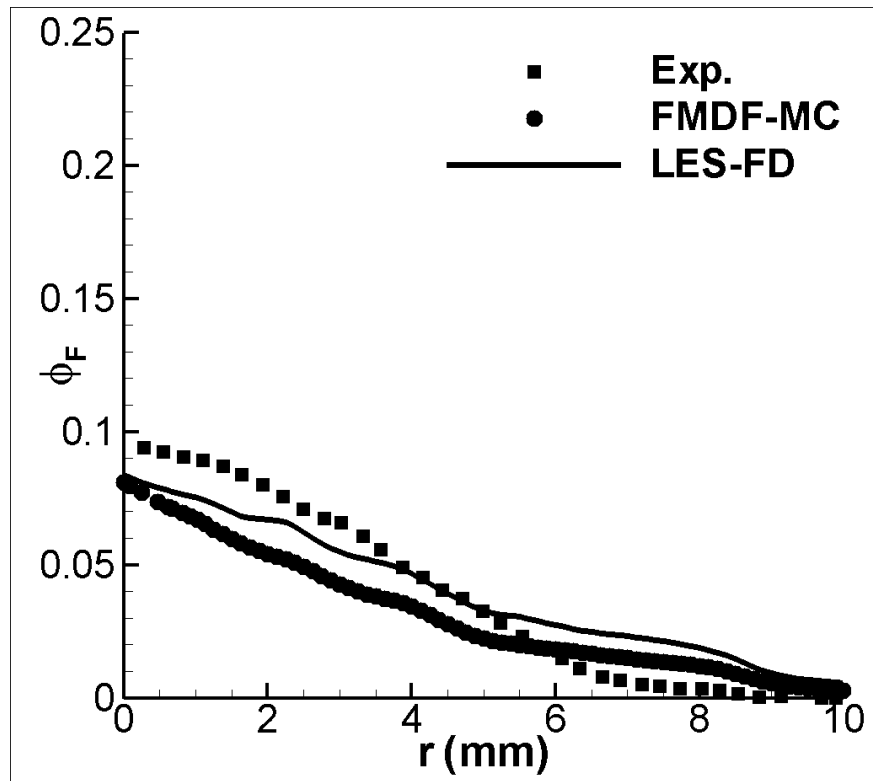


(b) $x=20\text{mm}$

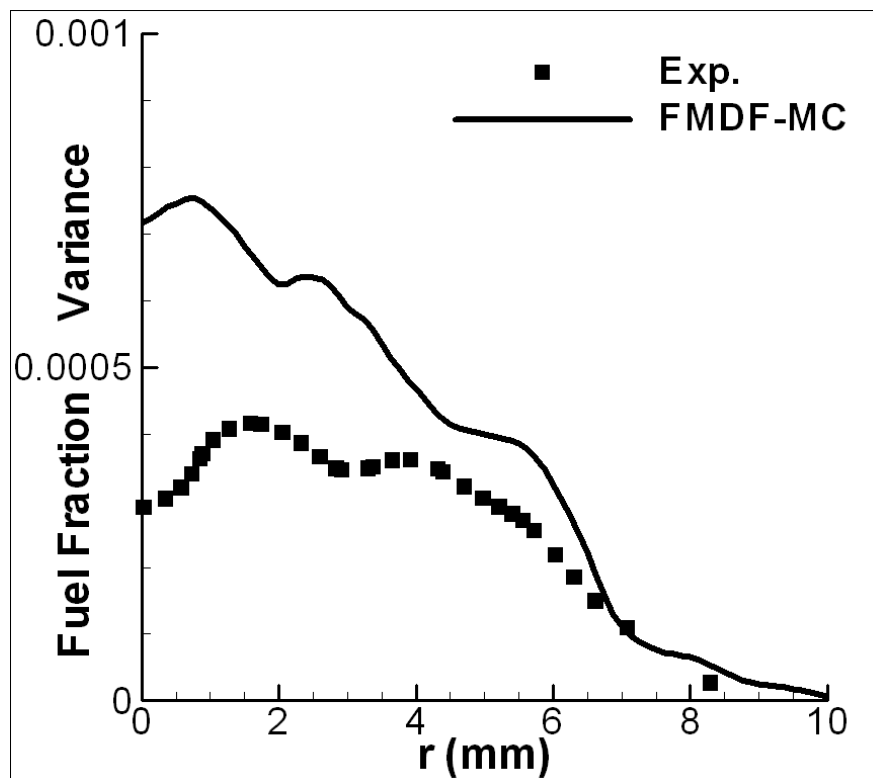
Figure 3.3: Radial profiles of simulated and measured fuel mass fraction and its variance at different axial locations for non-reacting evaporating spray.

Figure 3.3: (cont'd)

(c) $x=40\text{mm}$



(d) variance $x=40\text{mm}$



3.3.2 Reacting Sprays

The available experimental quantities for the reacting sprays are the ignition delay and the quasi-steady liftoff length. Variation of these global quantities with the ambient gas conditions is important and could further assess the global accuracy of the LES/FMDF/Spray model in comparison to experiments. The definitions for computational ignition delay and liftoff length have been the subject of discussions at the ECN workshops [91]. In particular, several different ignition criteria have been employed to identify the spray ignition in experiments as well as theoretical and numerical studies ([91],[94]). However, it is generally agreed that the ignition delay results are not sensitive to the exact definition in contrast to liftoff data [141]. Here, following Bhattacharjee and Haworth [132] and the ECN recommendations [141], the ignition delay is defined to be the time from the start of combustion to the time when the maximum temperature in the domain exceeds the initial temperature by 400 K. The liftoff length is defined to be the axial distance from the injector at which the computed OH mass fraction reaches to %2 of its maximum value for that operating condition.

3.3.2.1 Ignition Delay and Auto-Ignition

Figure 3.4 shows comparison of the simulated and measured ignition delay times as a function of the gas oxygen concentration for the ambient gas temperature of 1000 K and as a function of ambient gas temperature for the initial O_2 concentration of %21 in the chamber. Evidently, the numerical results are in good overall agreement with the experimental data. Note that the ignition can be identified as the initiation of rapid exothermic reactions or the appearance of a flame in a combustible mixture. However, the ignition delay considered in the spray experiments comprises of a physical delay and a chemical delay. The physical delay deals with

the spray breakup, evaporation and vapour mixing times and the chemical delay involves generation of a radical pool and heat release reactions. The physical delay prediction can be assessed by non-reacting spray mixing as conducted in the previous section. The chemical delay depends both on the chemical kinetics model as well as the turbulence-chemistry interactions. It has been shown that even with the same reaction mechanism, results are dependent on the consideration of turbulence chemistry interaction (TCI) which can be captured by PDF methods in RANS ([104],[132]) and is dealt with in the present simulations by the FMDF.

It is indicated in Figure 3.4 that the hybrid two-phase LES/FMDF captures very well the variation of ignition delay with the O_2 concentration in the initial gas. From a practical point of view, reductions in the ambient gas oxygen concentration occur in an engine when exhaust gas recirculation (EGR) is used to reduce the emission of nitrogen oxides [131]. Expectedly, ignition delay increases with the decrease in O_2 concentration. The simulated results, however, diverge from the experiments for lower initial gas temperatures. At lower temperatures, ignition is a two stage process. The first stage or the cool flame ignition stage involves the fuel oxidation at a slow rate. This is followed by the second stage of ignition with a normal rate. As the chemistry is relatively slow at lower gas temperatures and chemical and turbulent time scales are commensurate, the solution will be more dependent on the chemical kinetics model and its ability to capture the cool flame phenomena appropriately. The overpredicting trend of the simulated results compared to the experiments is suggested to be mostly related to the chemical kinetics modeling. The performance of different kinetic models at the lower temperature of $T=800$ K can be assessed by comparing the results obtained with a detailed mechanism for a simple system such as perfectly stirred reactor (PSR) at the

same pressure of 3.34 MPa as that of the chamber. The detailed mechanism, developed by the Lawrence Livermore national laboratory (LLNL), has proven to be a reliable mechanism ([143] and [144]). We have compared the results obtained with this mechanism for the PSR with several other reduced and skeletal mechanisms. The considered mechanisms are: (1) reduced mechanism by LLNL with 160 species and 770 reversible reactions [114], (2) skeletal mechanism with 88 species and 387 reversible reactions [116], and (3) skeletal mechanism with 44 species and 112 reversible reactions [115]. Smaller reduced mechanisms such as the 29 species mechanism of Patel et al. [145] do not perform as well as those above and are not considered. The PSR simulation with detailed chemistry is performed using commercial CHEMKINTM, while other simulations are performed using ISAT and DDASAC solver. It is clear from Figure 3.5 that none of reduced and skeletal mechanisms can fully capture the low temperature trend in detailed mechanism, although the predictions of comprehensive reduced mechanism of LLNL are closer to the detailed solutions. The 44 species mechanism gives the highest delay for the PSR and as the loss of heat and radicals from the ignition kernels in the actual spray flow has a delaying effect on the ignition, more delay will be observed in spray combustion simulation when this mechanism is used. The conclusion is that the change in chemical kinetics model to those tested would not significantly improve the spray combustion results unless a comprehensive mechanism is used. We would like to mention here that although the transient low temperature PSR results are different for different mechanisms, the overall agreement for all tested mechanisms is reasonably good.

There can be different type or modes of ignition in liquid-fuel combustion systems depending on the relative importance of evaporation time scales and convective and molecular diffusion time scales in the surrounding gas [146]. Three modes of ignition are identified: (1) individual

droplet ignition, (2) group ignition around droplets, and (3) spray ignition or global ignition. For high speed evaporating sprays, such as those considered in diesel engines, the spray ignition mode dominates and the ignition occurs mainly away from the liquid spray. This is due to the fact that the evaporating spray generates a high momentum, cold, vapour-saturated jet in which the ignition cannot occur. Figures 3.6 and 3.7 show the evolution of flame and the overall view of the auto-ignition as captured by OH levels and temperature field for the base case. It is clear that as the induced fuel vapour jet is breaking into smaller eddies and highly turbulent downstream of the liquid spray, mixing of cold fuel vapour and hot oxidizer gas becomes so significant that auto-ignition starts. Evidence of localized ignition kernels in spray combustion is provided by Sato et al. [147], who indicated that the ignition occurs in the stagnation region of the fuel vapour tip. On the other hand, Edwards et al. [148] concluded that the formation and shedding of eddies along the induced vapour-saturated gas jet provide a suitable environment for local mixing and chemical reactions away from the main high-momentum fuel vapour saturated jet. These eddies serve as a medium in which the chemistry and flow time scales can be balanced, leading to the auto-ignition. Consistent with experimental observations, Figures 3.6 and 3.7 show that the ignition kernels, i.e. localized regions of high reactivity and heat release are created at the vapour tip in turbulent eddies, followed by establishment of the flame which propagates downstream.

Pickett et al. [149] found out that prior to auto-ignition, a “cool flame” is established upstream or near the same axial location as the quasi-steady liftoff length is stabilized later, well after auto-ignition. The “pre-liftoff” region for high ambient gas temperatures ($T > 1000K$) is generally low speed recirculation zones around the periphery of the intact spray induced

gas jet flow. Mixing in this region occurs with a much slower rate compared to that in turbulent region further downstream and therefore a highly reactive flame cannot be maintained for intermediate ambient gas temperature of $T=1000$ K. The experimentally observed “cool flame” prior to auto-ignition is qualitatively shown in Figure 3.8 by comparison of gas temperature and the OH concentration contours obtained by LES/FMDF at earlier time of $t=0.30$ ms. It is noted that the pre-ignition OH concentrations in the pre-liftoff region are much smaller than those in the auto-ignition kernels just before ignition. To show the significance of the chemical ignition delay and the reaction model in spray combustion, LES/FMDF results obtained with a fast global chemistry model are also considered in this chapter. With a simple global reaction mechanism[150], there is virtually no chemical ignition delay and the only observed delay is due to physical delays by evaporation and mixing. Because of absence of OH radical in the global mechanism, the appearance of high temperature regions in the flow is inferred as the ignition. Figure 3.9 shows that with a global mechanism, the low speed recirculation zones on the periphery of the vapour jet are the ignition spots. Simulations with more detailed chemistry, however, delays the auto-ignition and moves it away from the spray where the mixing by spray/evaporation induced turbulence is very significant.

Auto-ignition can also be studied by maps or scatter plots of temperature, equivalence ratio, or mixture fraction. Such illustration is often used to illustrate the combustion type or regime ([97], [132] and [151]). The equivalence ratio ε is computed from the mixture fraction Ξ based on the elemental carbon and hydrogen mass fractions as:

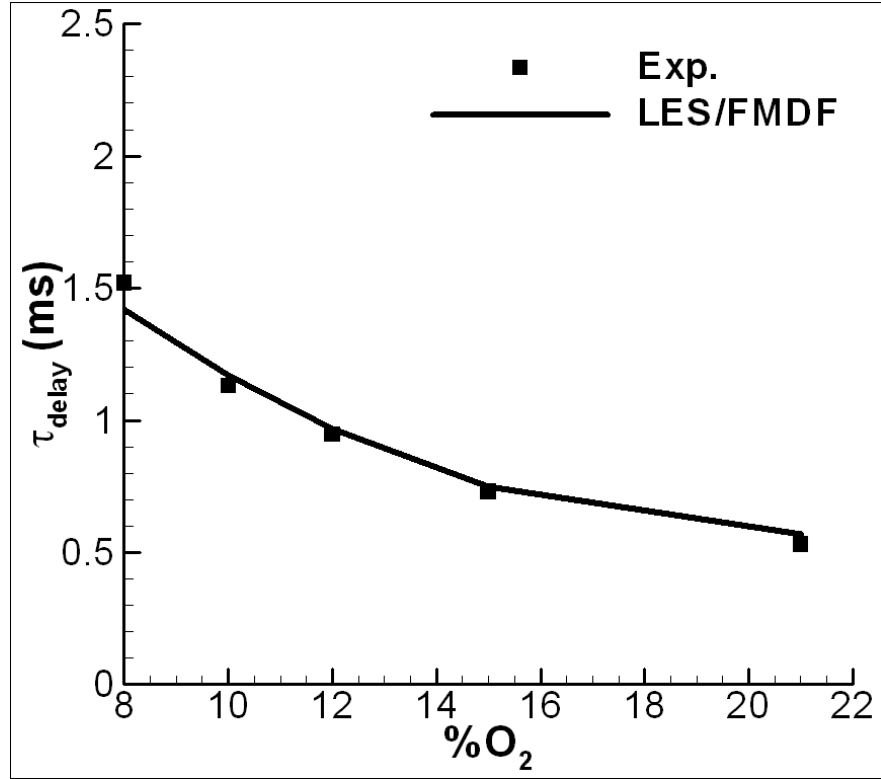
$$\Xi = \sum_{\alpha=1}^{N_s} (MW_C n_{C,\alpha} + MW_H n_{H,\alpha}) \frac{\phi_\alpha}{MW_\alpha},$$

$$\varepsilon = \frac{\Xi - \Xi_a}{1 - \Xi} \left(\frac{A}{F} \right)_{st},$$

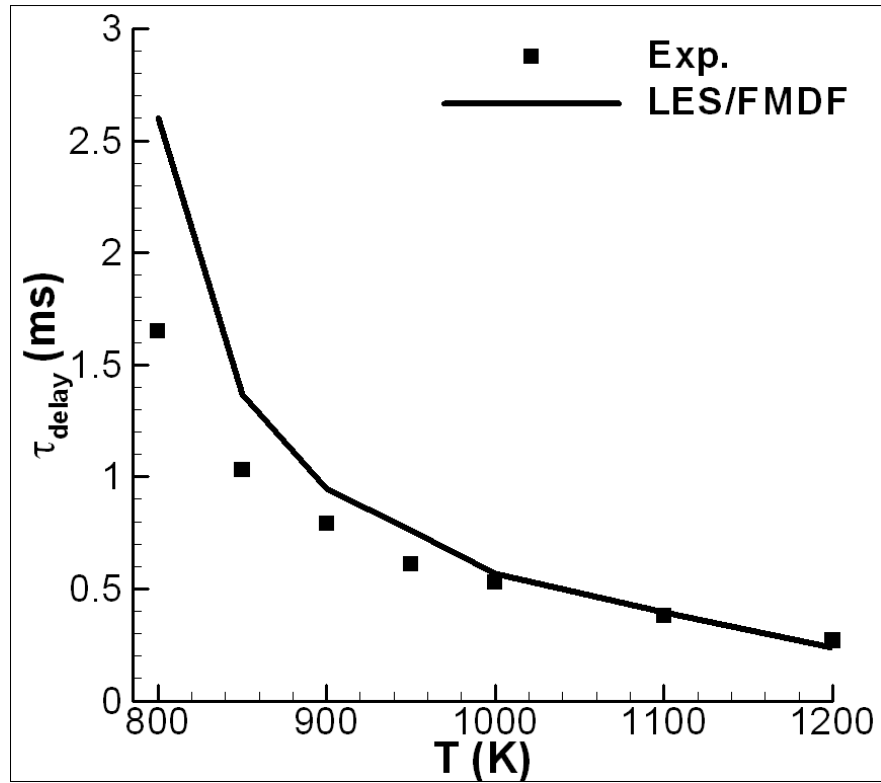
where $\left(\frac{A}{F} \right)_{st}$ is the stoichiometric ratio of ambient gas to fuel and Ξ_a is the ambient mix-

ture fraction. For a typical quasi-steady diesel combustion system ([151],[152],[153]), one can distinguish different regions in the spray combustion on the $\varepsilon - T$ map: ambient gas corresponds to low T and low ε ; the near injector vapour saturated jet has low T and high ε ; the lower rate mixing regions have low T and variable ε ; and two different flame zones of rich premixed core in the flame interior and the outer diffusion flame sheath between the products of premixed core and the ambient gas/vapour jet have high T and high ε ; and high T and low ε , respectively. Figure 3.10 shows the $\varepsilon - T$ scatter plots at different times for the base case. Prior to ignition, before time $\tau_{delay} = 0.57ms$, the temperature of MC particles with equivalence ratios ranging approximately between 1.5 to 1.8 begin to rise by ignition time. The temperature first reaches to 2000 K for the higher equivalence ratios of around 1.8 and then rises moderately for equivalence ratios of 1.4 and lower. This shows that the ignition first occurs at the fuel-rich zones with equivalence ratios below 1.8. These zones correspond to turbulent eddies at the tip of vapour jet, where the mixing and chemical time scales reach a balance. However after the ignition, the high temperature (burned) gas quickly spreads to other zones with lower equivalence ratios. By $t=0.65$ ms, MC particles with $\varepsilon = 1$ reach to temperature of 2000 K and gradually the flame front establishes around the outer diffusion layer of the turbulent jet with the ambient gas, where the equivalence ratio is unity or lower. The regions with intermediate temperature and equivalence ratios correspond to turbulent eddies in which the fuel from the vapour jet is being mixed with the outer high temperature flow regions. From $t=0.70$ ms onward, the outer diffusion flame on the fuel vapour and ambient gas sides begins to establish and by $t=1.00$ ms the quasi-steady flame structure is nearly constructed. Figure 3.11 shows the evolution of OH mass fraction versus equivalence ratio during ignition. Evidently, the OH mass fractions evolve around the stoichiometric (unity) equivalence ratio, even though the auto-ignition occurs on the fuel

rich and high equivalence ratio side. This is expected as OH is the footprint of the reaction zone or flame front rather than the auto-ignition zone [96].



(a)



(b)

Figure 3.4: Simulated and measured ignition delays (a) versus oxygen molar percentage for $T=1000$ K and (b) versus chamber temperature for %21 of O_2 concentrations.

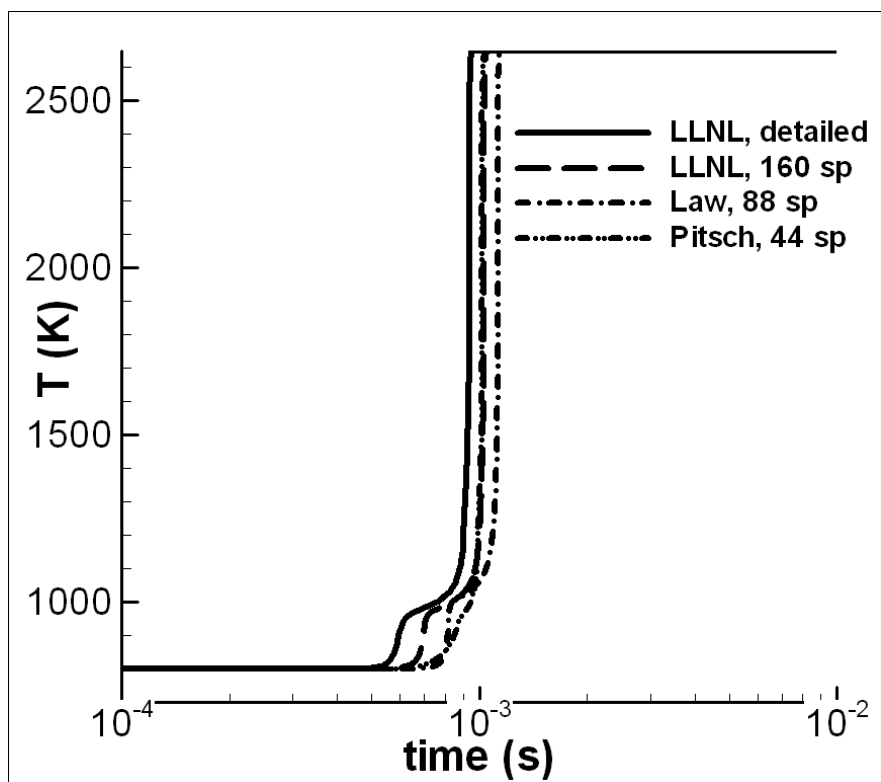


Figure 3.5: Comparison of kinetic models for low temperature combustion of n-heptane in a high pressure perfectly stirred reactor at $T=800$ K and $P=3.34$ MPa.

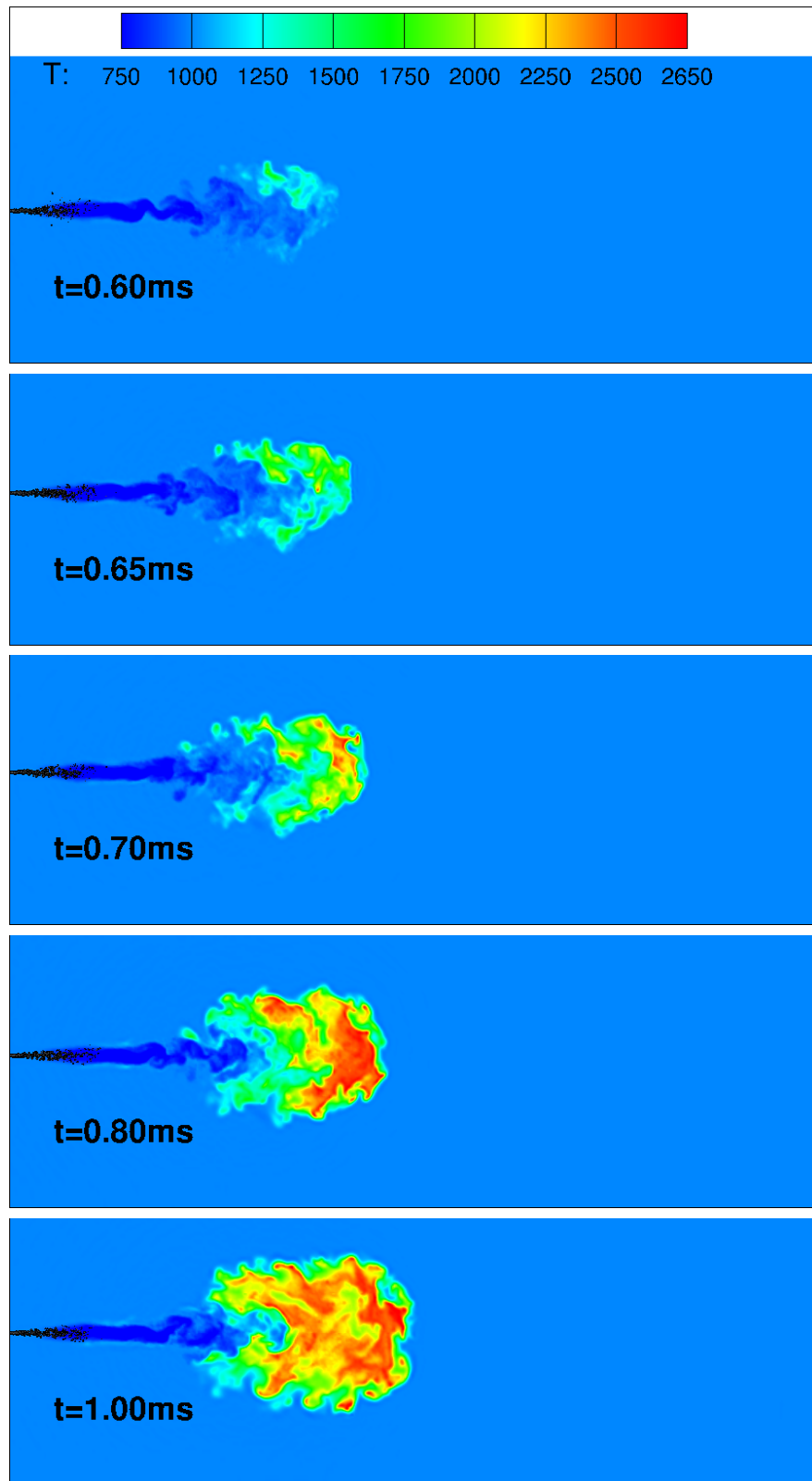


Figure 3.6: Contours of temperature in the reacting spray (base case) at different times.

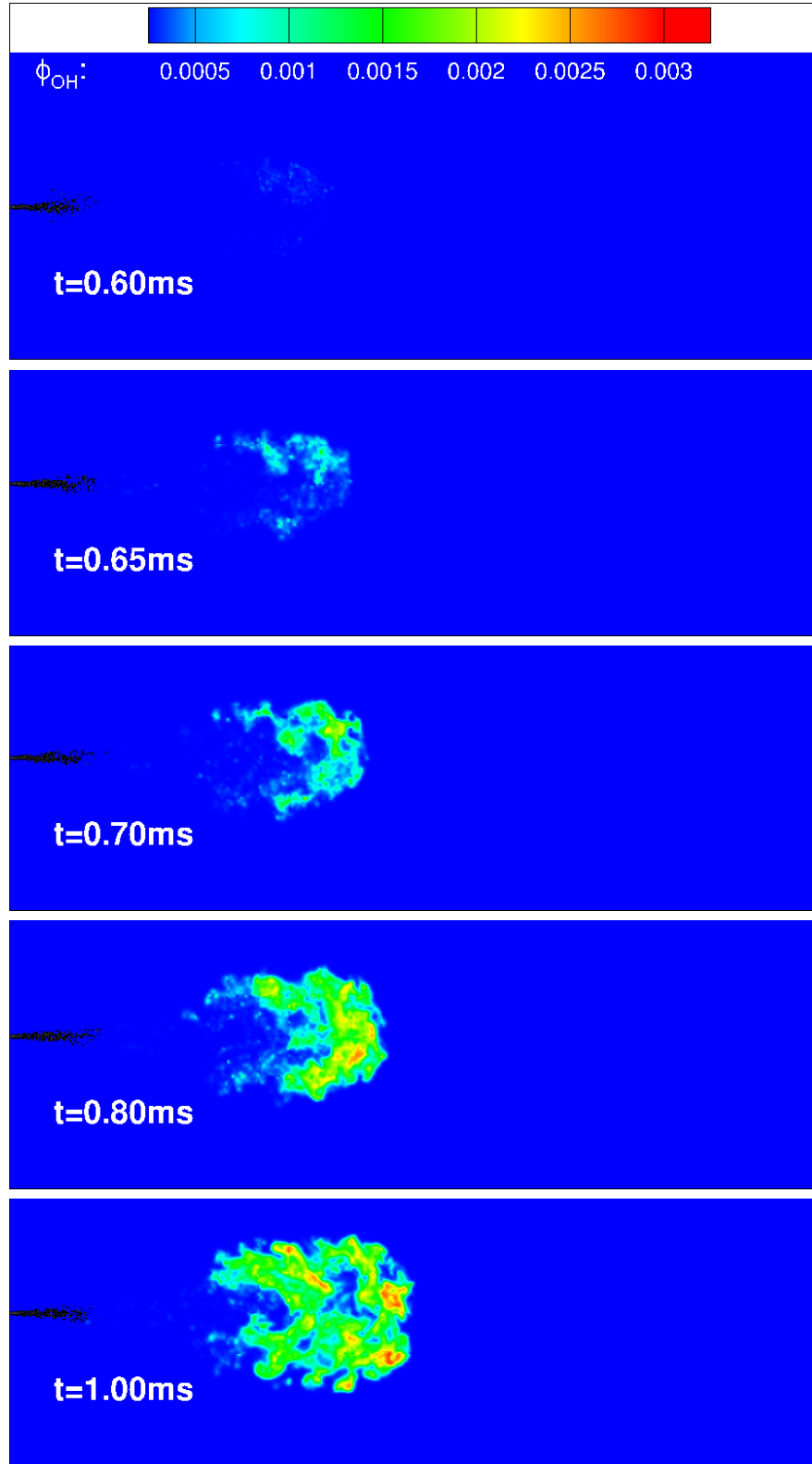
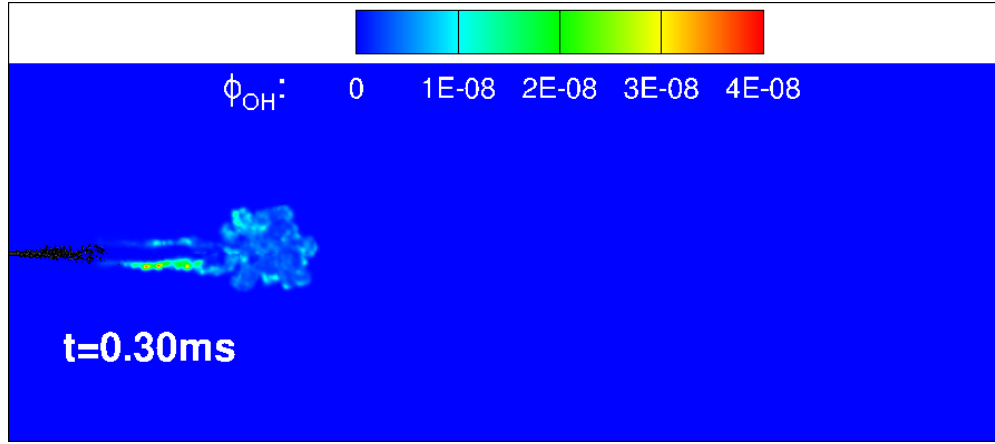
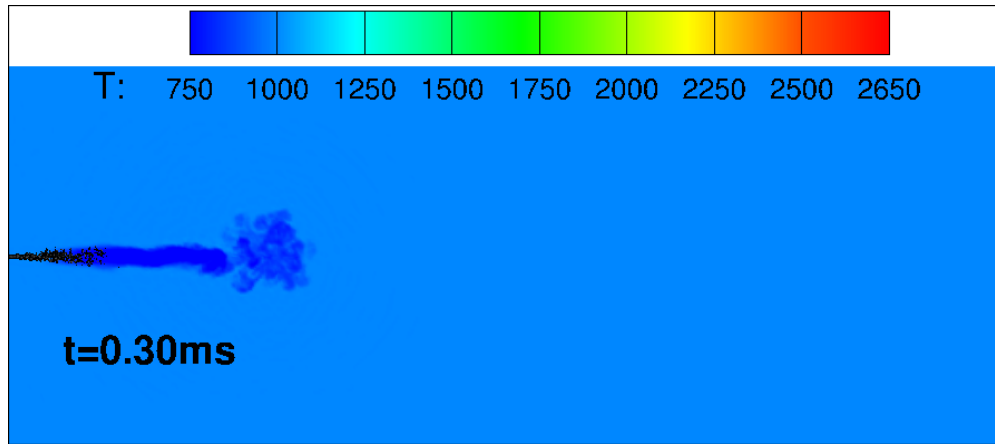


Figure 3.7: Contours of OH radical mass fraction in the reacting spray (base case) at different times.



(a)



(b)

Figure 3.8: Visualization of “cool flame” at the liftoff region prior to auto-ignition by (a) OH mass fraction and (b) temperature contours, at $t=0.30$ ms.

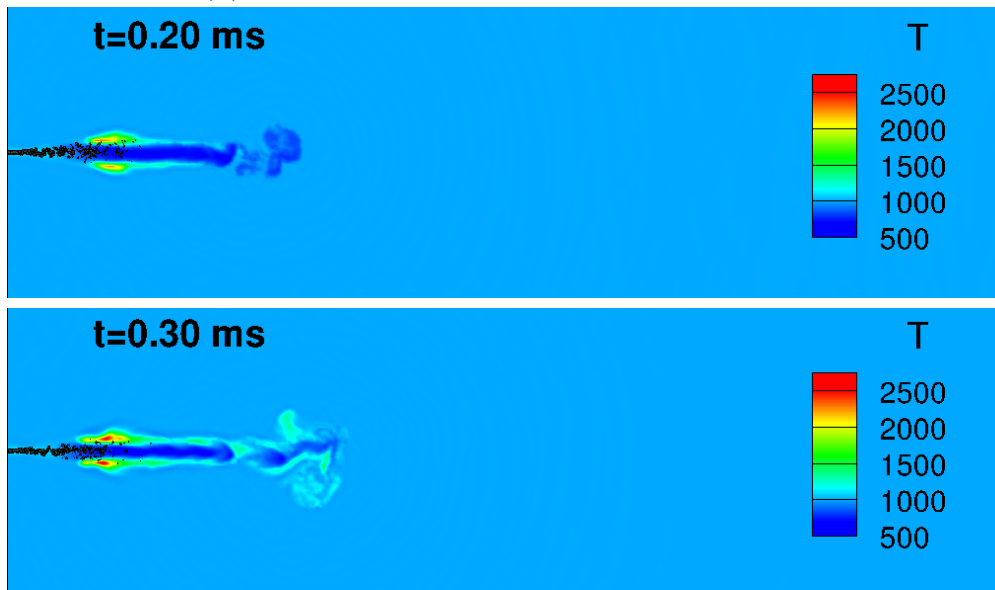
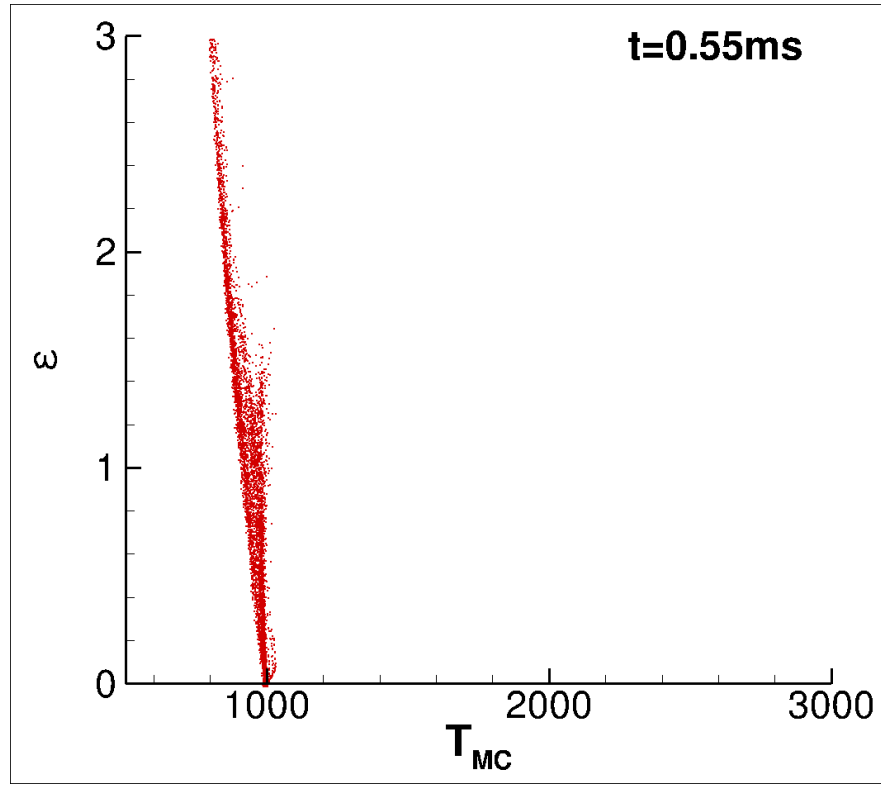
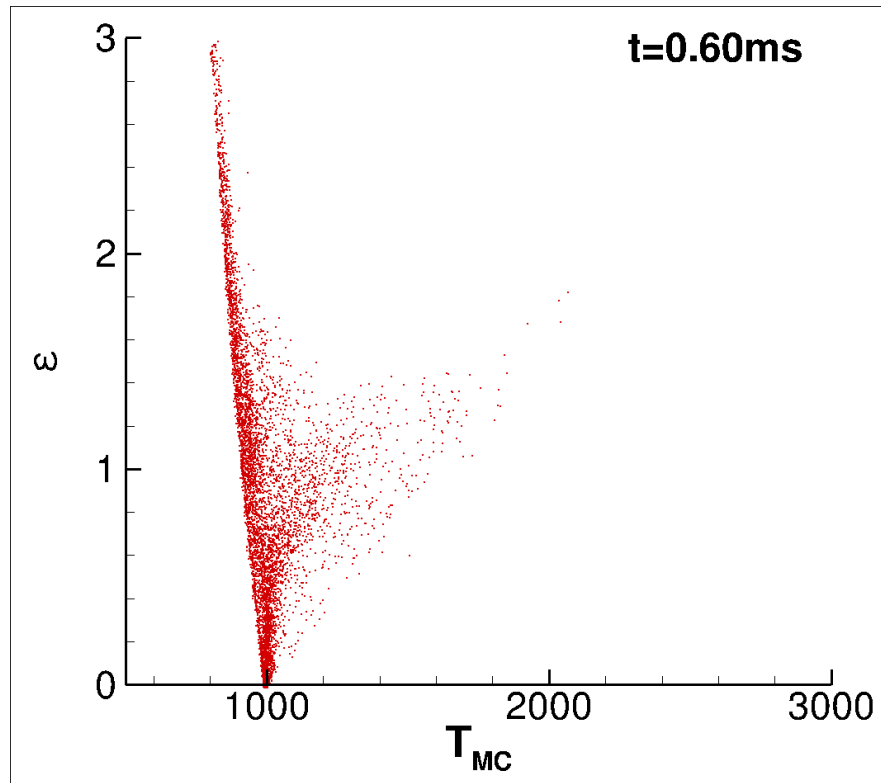


Figure 3.9: Temperature contours at the onset of ignition, obtained by a global reaction model.



(a) $t=0.55\text{ ms}$

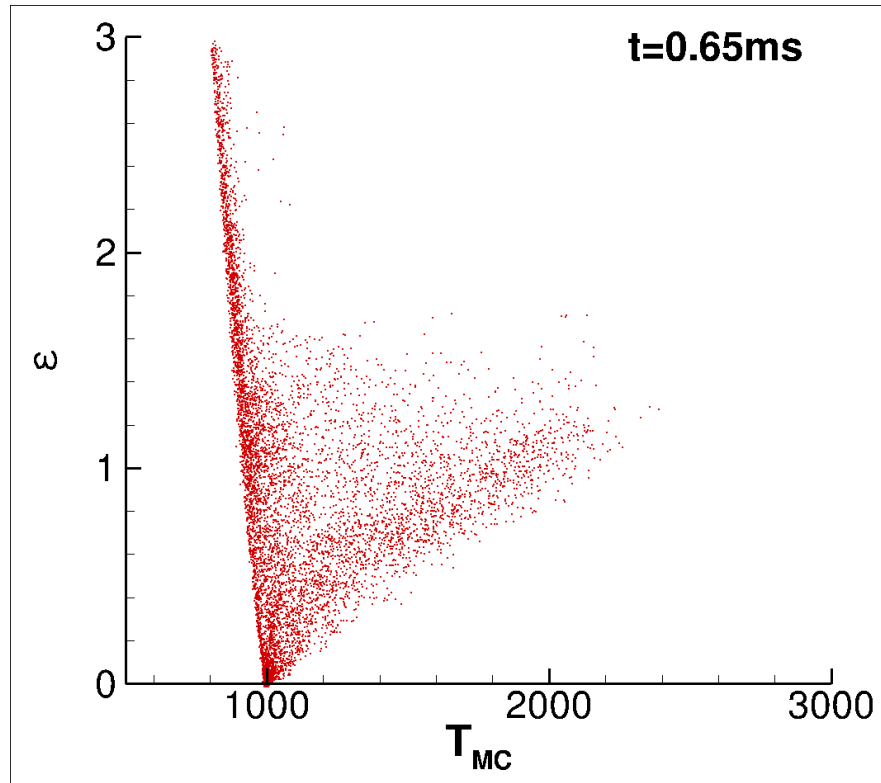


(b) $t=0.60\text{ ms}$

Figure 3.10: Evolution of equivalence ratio versus temperature map in the reacting spray during auto-ignition.

Figure 3.10: (cont'd)

(c) $t=0.65$ ms



(d) $t=0.70$ ms

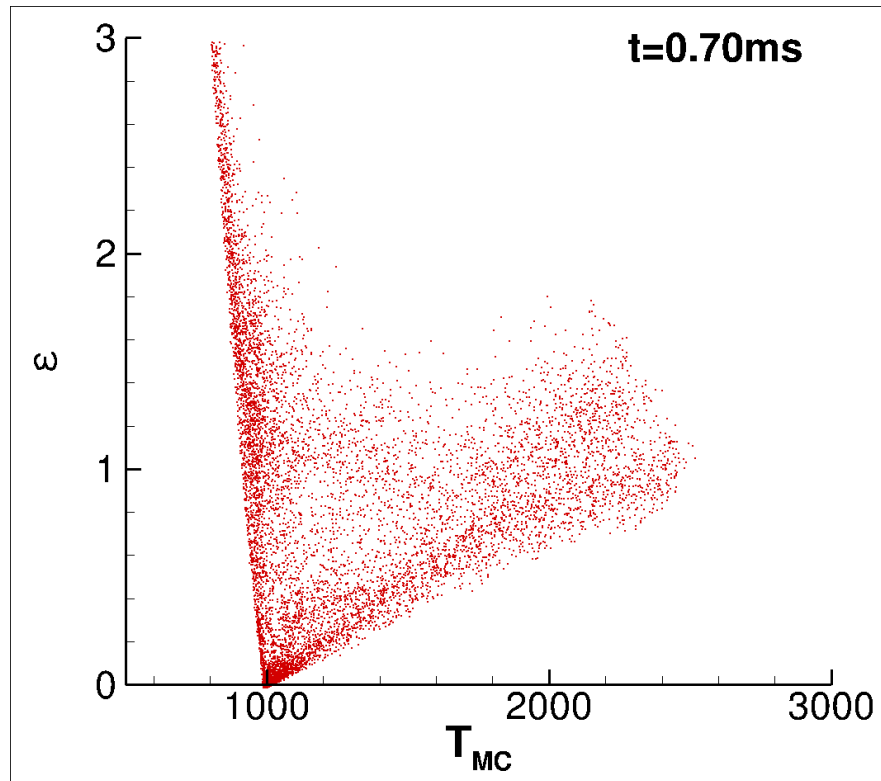
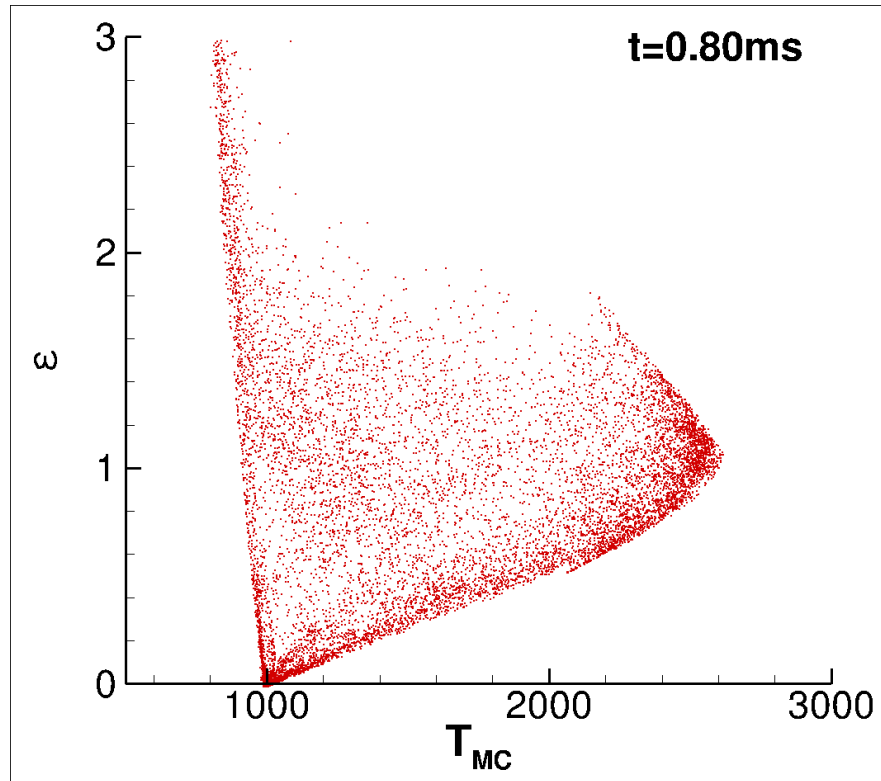
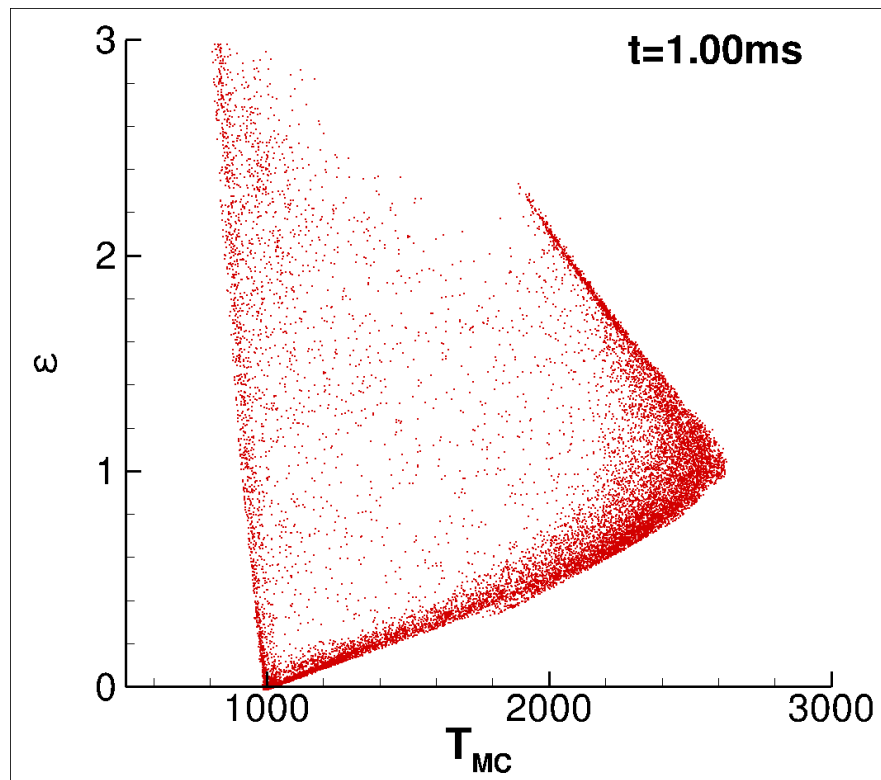


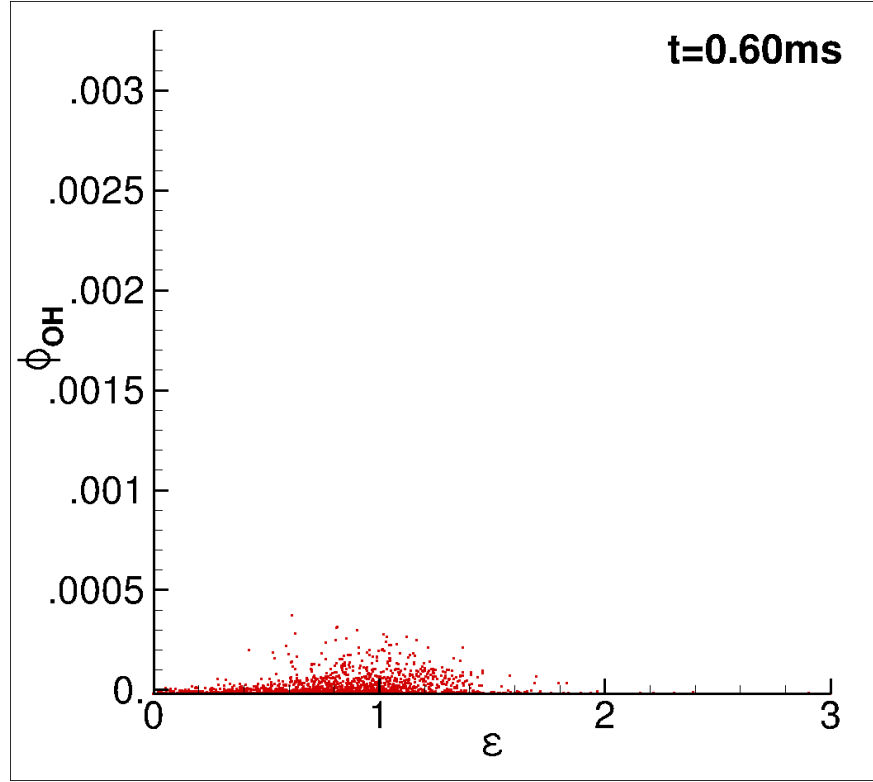
Figure 3.10: (cont'd)

(e) $t=0.80$ ms

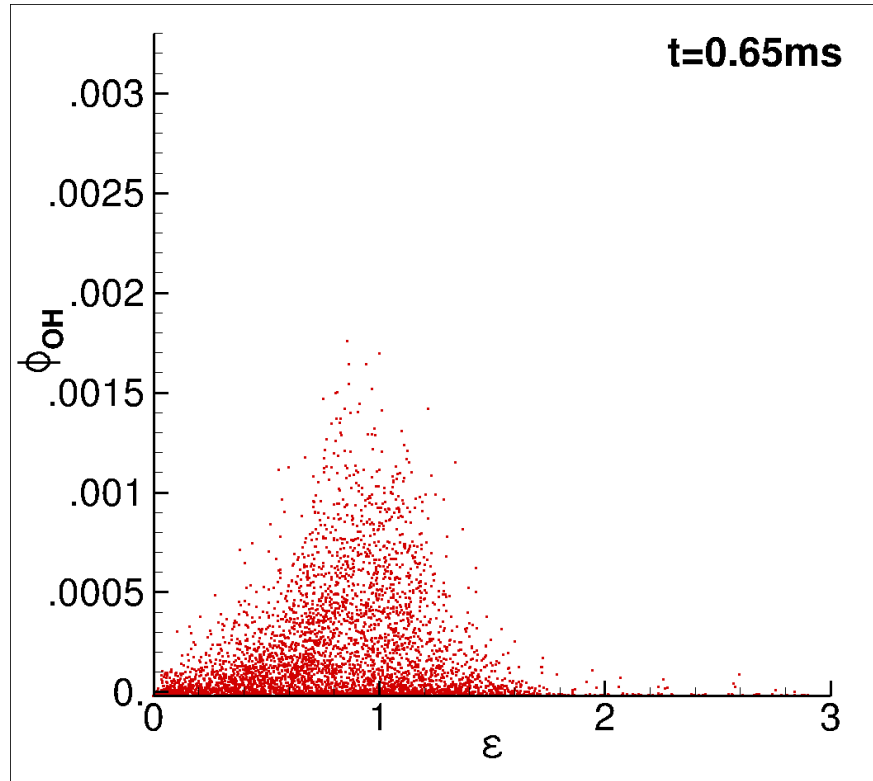


(f) $t=1.00$ ms





(a) $t=0.55\text{ ms}$

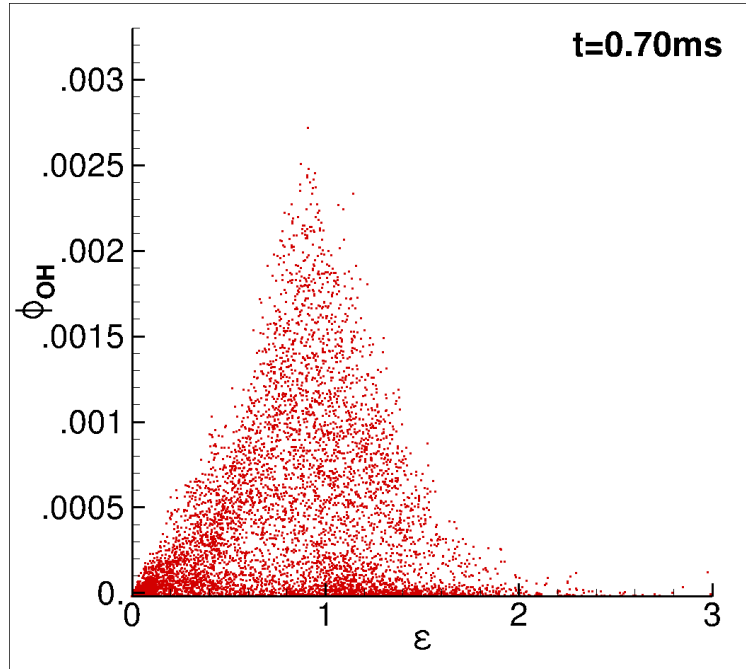


(b) $t=0.60\text{ ms}$

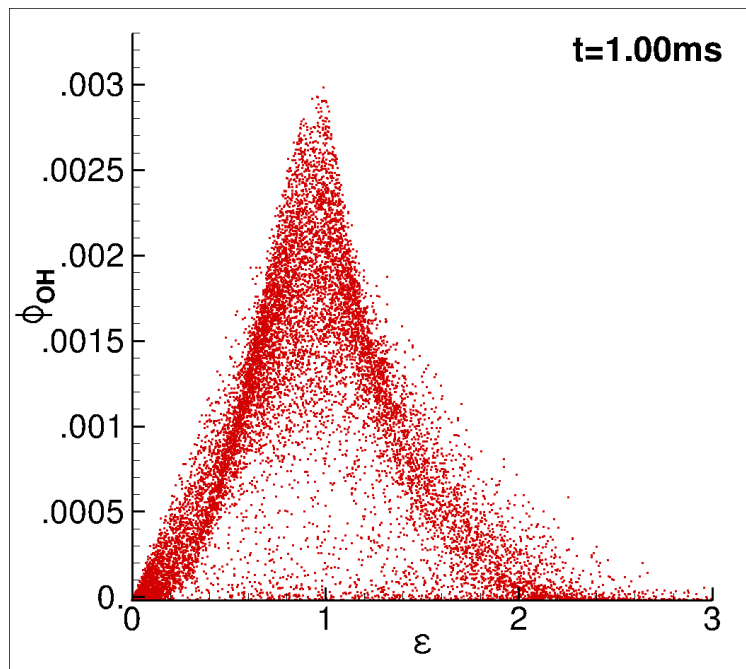
Figure 3.11: Evolution of OH mass fraction versus equivalence ratio map in the reacting spray, simulated by LES/FMDF/Spray model with skeletal mechanism during auto-ignition.

Figure 3.11: (cont'd)

(c) $t=0.65$ ms



(d) $t=0.70$ ms



3.3.2.2 Flame Liftoff

Figure 3.12 shows the lifted turbulent flame visualization for the base case at $t=2.0$ ms as visualized by instantaneous iso-surfaces of OH mass fractions. For the base case, the liftoff region corresponds to the most upstream region of the flow filled by eddies shed from the spray-induced vapour jet, although it occasionally extends upstream to the recirculation zones on the periphery of the vapour jet. For lower gas temperatures and lower oxygen concentrations, the liftoff length increases and the flames move further downstream to the turbulent plume zone. On the other hand, the liftoff length decreases and the flame cover the entire low-speed recirculation zones for higher gas temperatures and eventually reaches to the spray droplets at the liquid penetration point. Figure 3.13 compares the computed and measured liftoff lengths as a function of initial oxygen concentration for $T=1000$ K and as a function of initial temperature for 21% O_2 concentration. The reported liftoff length is averaged for a short period of time between 0.5 to 1 ms since it fluctuates in time. In contrast to ignition delay, which is sensitive to the chemical kinetics and its level of comprehensiveness, the liftoff length is primarily dependent to the flow and TCI. Therefore it is expected that regardless of the ignition delay, the liftoff length predictions to be accurate, provided that TCI is well predicted. This is supported by the overall good agreement of the LES/FMDF results with the experiment. The flame liftoff length increases with the decrease in oxygen concentration but decreases by increasing the ambient gas temperature. The very small liftoff length on the other hand suggests that the flame may significantly interact with small droplets and their evaporation at the tip of liquid spray, creating a hotter environment for faster evaporation. This in turn makes the non-linear liquid droplet interface equations stiff and the numerical simulation of spray more challenging. Nevertheless, we have been able to

simulate the spray combustion under all tested conditions.

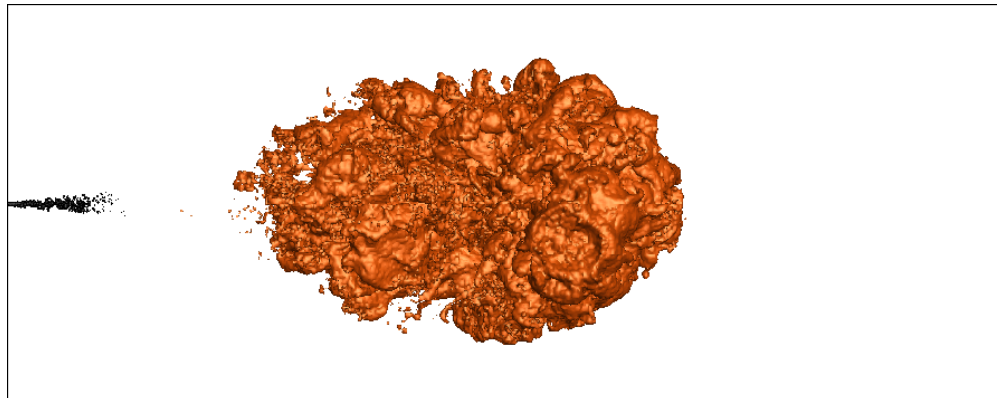


Figure 3.12: Flame visualization via iso-surfaces of OH mass fraction at $t=2.00\text{ms}$.

Figure 3.14 compares the liftoff length as a function of temperature predicted by the LES/FMDF /spray model with global and complex kinetics mechanisms with the experimental data. Although the simulations with the global model perform rather poorly in terms of ignition delay and the computed liftoff lengths are generally shorter than the experiment, the trend in the liftoff length is similar and become closer to the experiment at higher ambient gas temperatures. This is expected as the reaction is faster at higher chamber temperatures. This comparison indicates that while the global reaction model is not quantitatively accurate, it is still useful for the overall study of the spray and testing of LES/FMDF/Spray submodels [154].

High-speed chemiluminescence imaging [149] showed that high temperature self-ignition occasionally occurs in kernels that are upstream of, and detached from, the high temperature reaction zone, suggesting that the liftoff and stabilization of the flame is not controlled by the flame propagation into upstream of the vapour saturated jet. As mentioned before, the “liftoff region” overlaps with the low-speed recirculation zones around the core of vapour jet at intermediate to high chamber temperatures. At these locations, mixing rate is relatively

low and therefore a high temperature flame cannot be established. Figure 3.15 shows the temperature field obtained from the LES-FD and FMDF-MC data with skeletal reaction mechanism at $t=2.00$ ms. It is clear that the temperature at the liftoff region is much higher than that in ambient gas and much lower compared to that in the main flame zone. At the liftoff region, due to low speed recirculation and large-scale eddies, mixing time scales are relatively large, therefore the reaction is less effective in establishing a high temperature flame. It is also clear from the contour plots in Figure 3.15 that the LES-FD and FMDF-MC parts of the two-phase LES/FMDF solver are consistent and generate similar results at all locations and times. To further investigate the consistency of the LES-FD and FMDF-MC methods, scatter plots of the filtered gas temperature and filtered fuel vapour mass fraction as obtained from these two parts of the LES/FMDF are also computed and compared in Figure 3.16. These scatter plots again show a good overall consistency between the LES-FD and FMDF-MC predictions, confirming the overall numerical accuracy of the LES/FMDF/Spray model.

Figure 3.17 compares the O_2 mass fractions in the chamber, normalized with respect to the initial O_2 mass fraction, for the two initial O_2 concentrations of %21 and %8. It is clear that for the higher initial oxygen concentration, O_2 is fairly diminished as it entrains to the turbulent flame; however for the lower O_2 level, the rate of consumption of O_2 is comparatively lower. This suggests that more mixing occur in the upstream of the flame before reaction for the lower O_2 concentration case. Figure 3.17 also shows that the total amount of oxygen entrained upstream of the liftoff flame location does not change with the ambient gas oxygen concentration. Similar observation has been reported in experiments [131]. Comparison of the LES/FMDF and experimental flame liftoff length for the gas with

%15 oxygen level in Figure 3.18 indicates a good agreement between them at later times. At the onset of ignition, the predicted liftoff length is high but gradually decreases as the flame spreads upstream.

3.3.2.3 Flame Structure

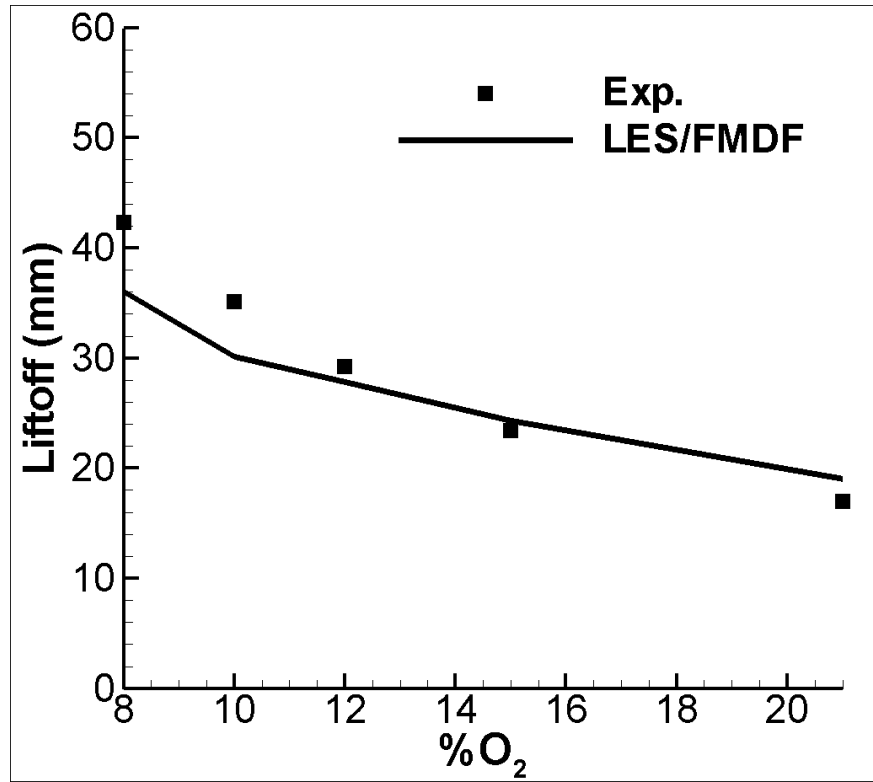
Flame structure can be studied by examining the contour plots of flame variables and maps of equivalence ratio and temperature for the simulated flames. Figure 3.19 shows the instantaneous flame temperature for the base case at different times well after the ignition. It is clear that the low temperature, fuel rich gas jet breaks into smaller structures with much more effective mixing by the spray generated turbulence before disappearing into the complicated flame plume. Figure 3.19 shows that the temperature field, although oscillatory and highly turbulent, does not significantly change in time after the ignition, suggesting that the flame stays nearly steady at these times. Similar trend is also observed in the OH radical contours (not shown).

Figure 3.20 shows the effect of oxygen concentration on the flame structure by comparing flames with %8 and %21 of O_2 molar concentration on the $\varepsilon - T$ map. Clearly, the effect of oxygen concentration on the flame is very significant, which is expected. It is observed that with lower oxygen concentration, the thickness of the outer diffusion flame on the $\varepsilon - T$ map increases. This is attributed to the fact that with lower ambient oxygen, more mixing is required before reactions can occur. Comparison of OH radical contours for different initial oxygen concentration in Figure 3.21 indicates that with lower oxygen concentration in the initial chamber gas, not only the peak temperature will be lower but the OH concentration values will also be much lower. The scatter plots in Figure 3.20 shows that at

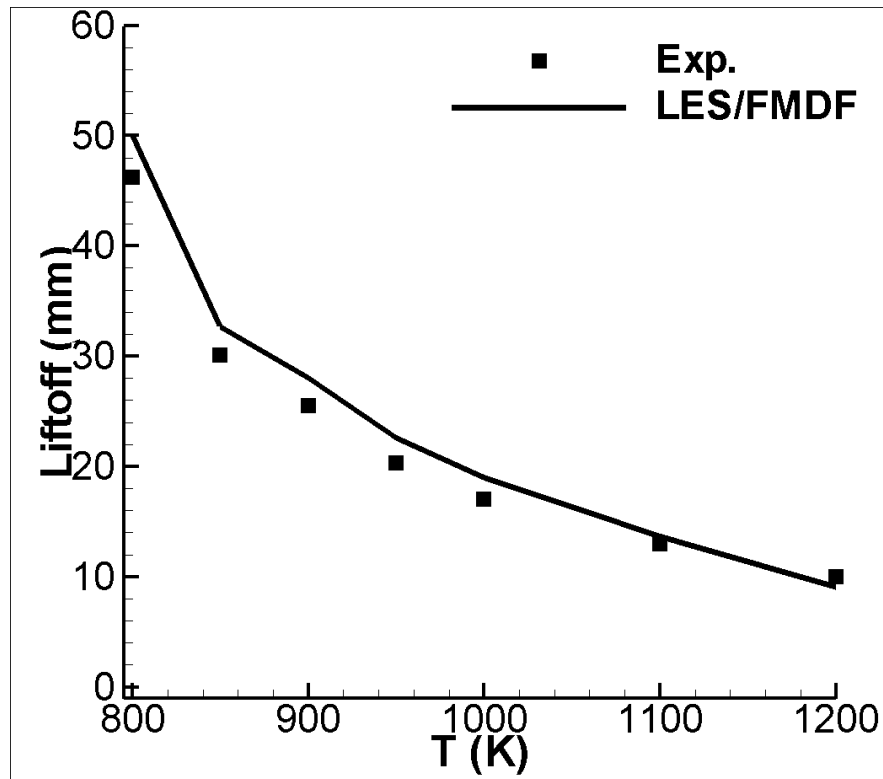
high oxygen levels the flame is not very different than an equilibrium flame, even though the finite-chemistry and non-equilibrium effects are still important in some regions of the flow. However, for the lower initial O_2 level, the non-equilibrium effects are very significant. At various regions in the flow, there is significant mixing and localized flame extinction due to turbulence generated by the spray and lack of oxygen. On average the flame tends to move toward a premixed condition as substantial mixing occur before combustion. The main difference between the flame structures for different oxygen concentrations is that many more thermochemical states are accessed by the flame that has lower oxygen concentration, indicating a higher level of TCI. This is also an indication of higher computational cost for the chemistry calculations with ISAT that needs to cover more points in the $N_s + 1$ dimensional space of scalars. Figure 3.22 compares the iso-surfaces of stoichiometric unity equivalence ratio for the two oxygen concentrations of %21 and %8. It is inferred from the figure that for the lower oxygen concentration, the flame front, identified by the iso-surface of unity equivalence ratio mainly establishes on the periphery of the turbulent flame and due to lack of oxygen does not penetrate significantly to the core of the turbulent plume.

Figure 3.23 compares the flame structures for the two initial ambient gas temperatures of 800 and 1200 K for the same oxygen level of %21. Compared to the base case flame with ambient gas temperature of 1000 K or the flame with high ambient gas temperature of 1200 K, the low temperature ($T=800$ K) flame establishes at equivalence ratios below and up to unity on the ambient side of the $\varepsilon - T$ map, with the highest temperature corresponding to unity equivalence ratio. This is expected as the initial energy content of the gas is low and the fuel rich areas are too cold to react. On the other hand, at higher ambient gas temperature of 1200 K, the energy content of the gas is high enough for a rich premixed

flame to be developed at very high equivalence ratios in addition to the outer diffusion flame and the intermediate premixed flame regions. At this temperature chemical time scales are small and the mixing and reaction compete with each other.



(a)



(b)

Figure 3.13: Comparison of computed flame liftoff length with the experimental data for different chamber gas conditions. (a) liftoff length versus O₂ concentration for T=1000 K, and (b) liftoff length versus chamber temperature for %21O₂ concentration..

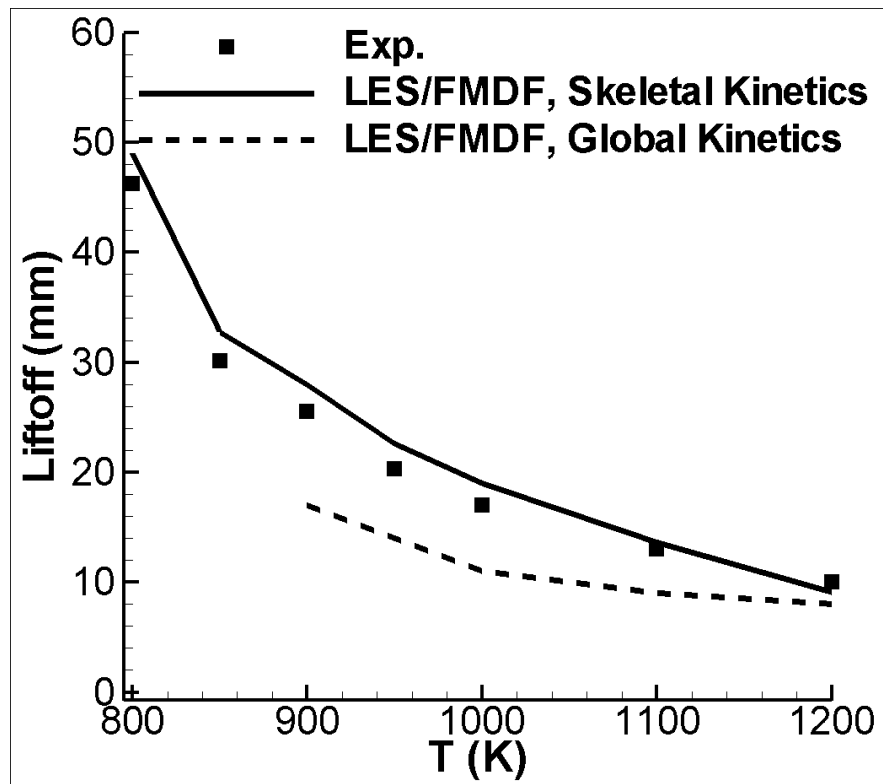
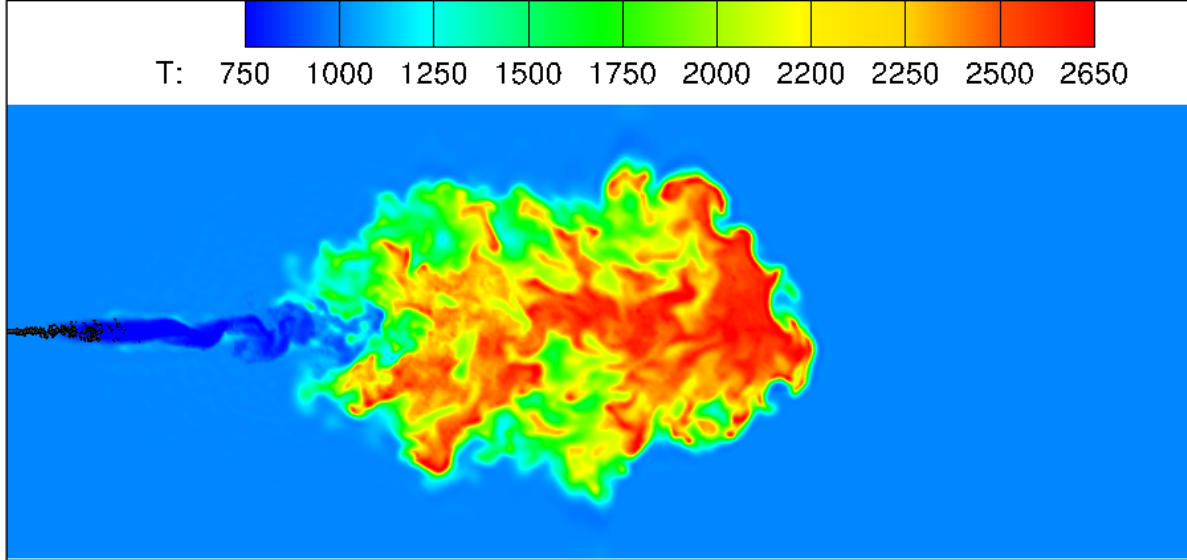
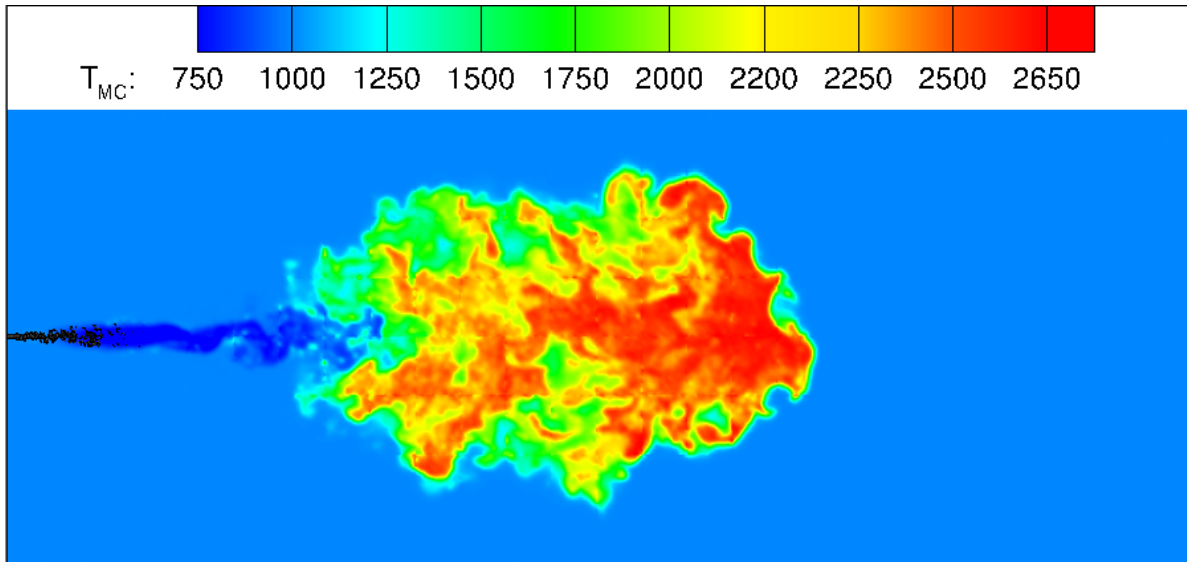


Figure 3.14: Liftoff length versus temperature computed by LES/FMDF/Spray model with global and skeletal chemical kinetics mechanisms.

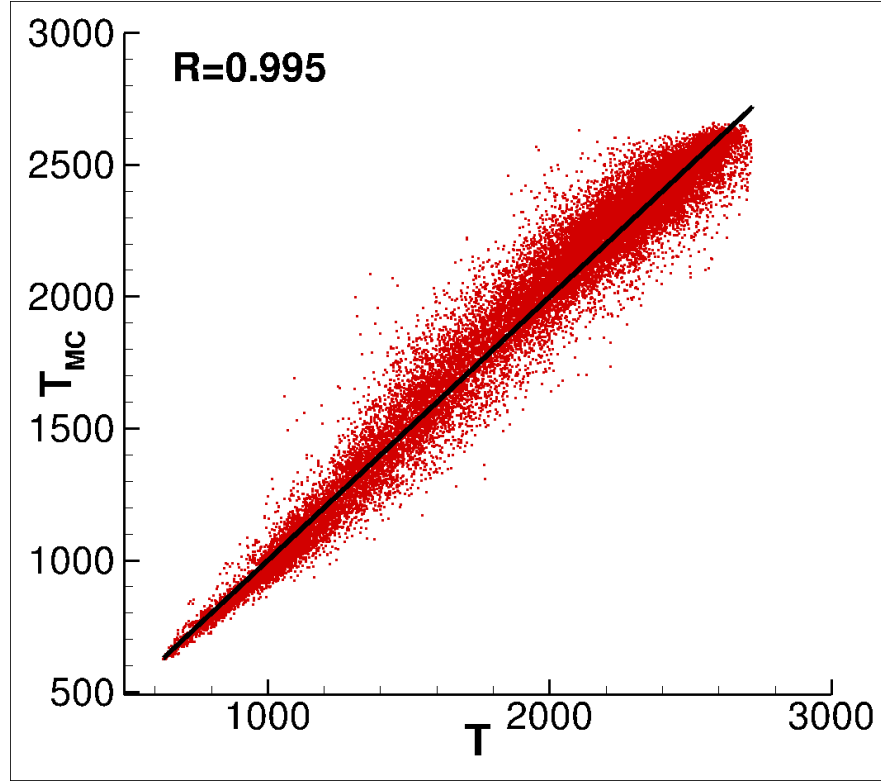


(a) LES-FD

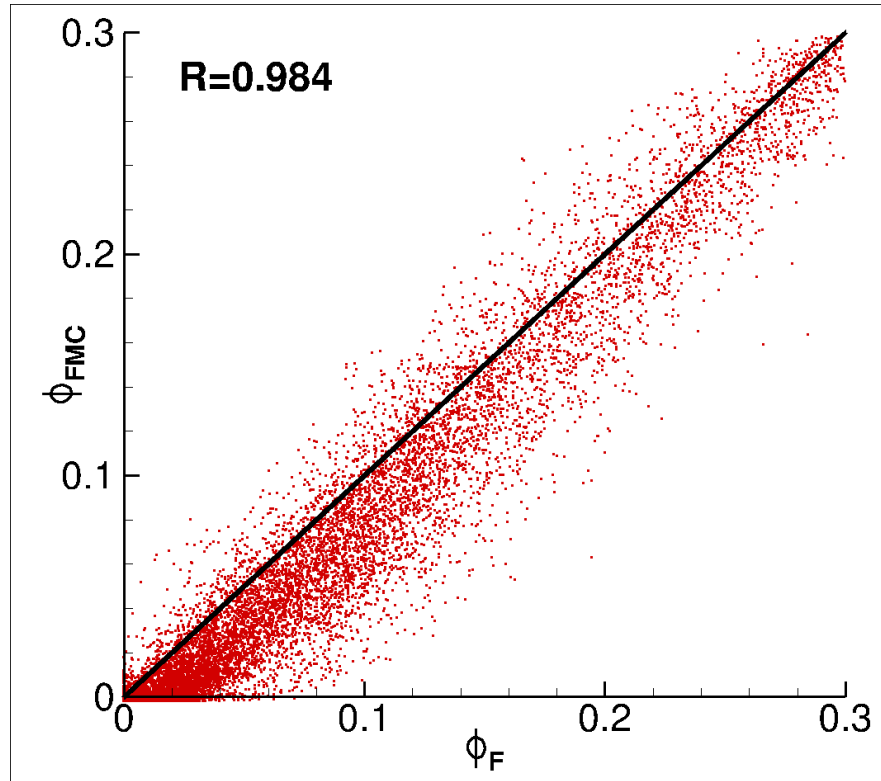


(b) FMDF-MC

Figure 3.15: Gas temperature contours obtained from (a) LES-FD, and (b) FMDF-MC data at $t=2.00$ ms for $T=1000$ K, $\rho = 14.8 \text{ kg/m}^3$, $\%21\text{O}_2$ concentration.



(a) temperature



(b) fuel mass fraction

Figure 3.16: Scatter plots of temperature and gas fuel mass fraction for $T=1000$ K, $\rho = 14.8 \text{ kg/m}^3$, %21 O_2 concentration.

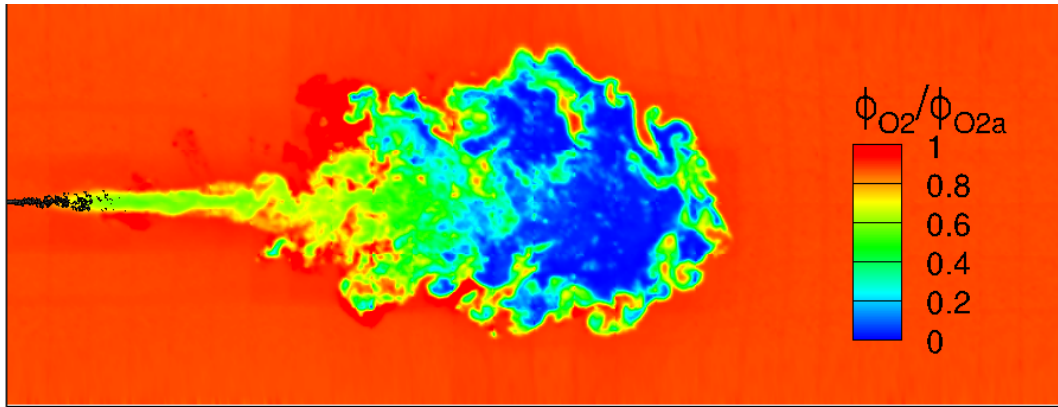
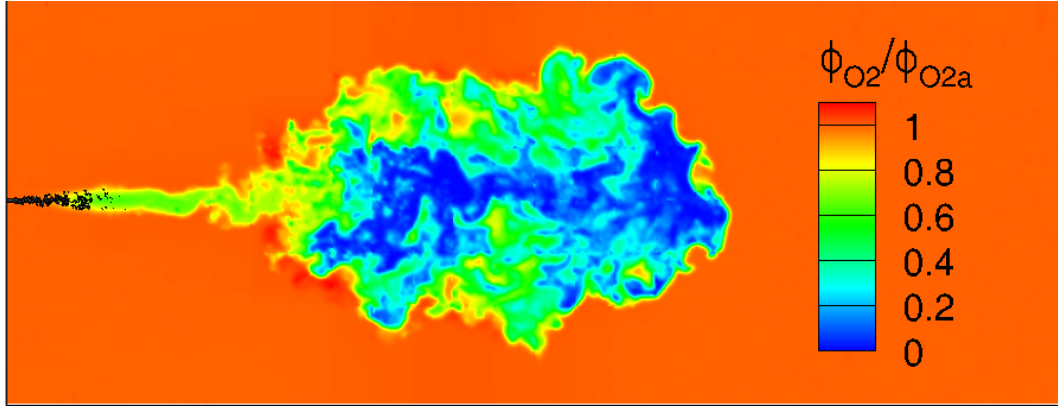


Figure 3.17: Comparison of relative O_2 mass fractions for different initial O_2 molar percentages

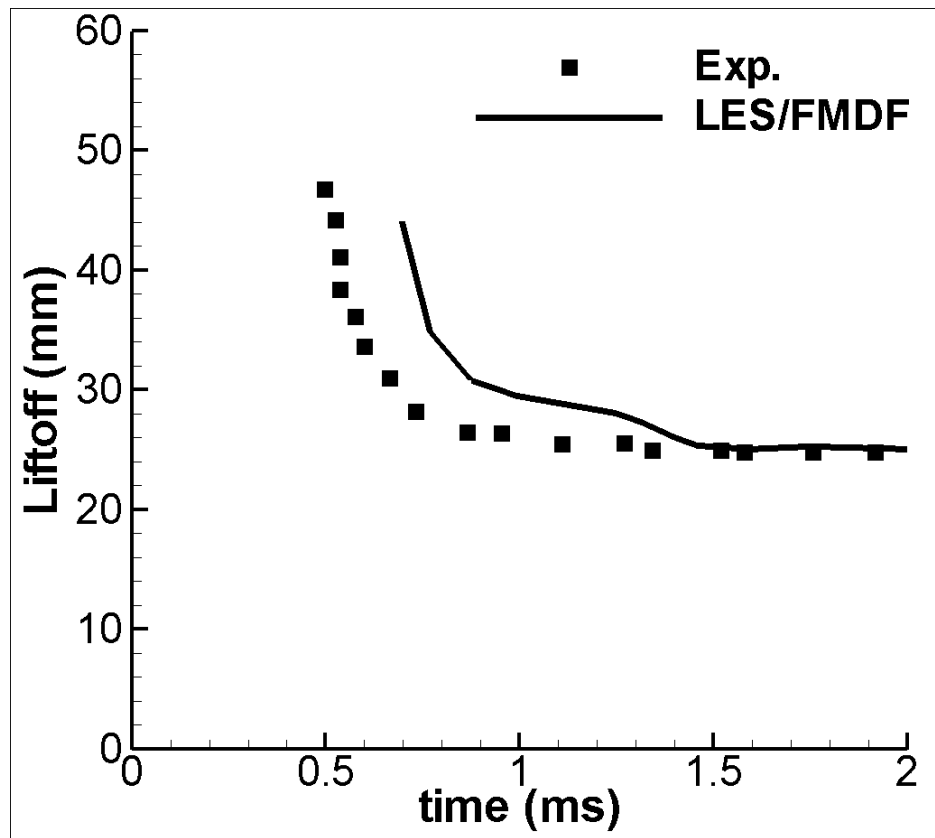


Figure 3.18: Time evolution of liftoff length for $T=1000$ K and $\%15O_2$ level.

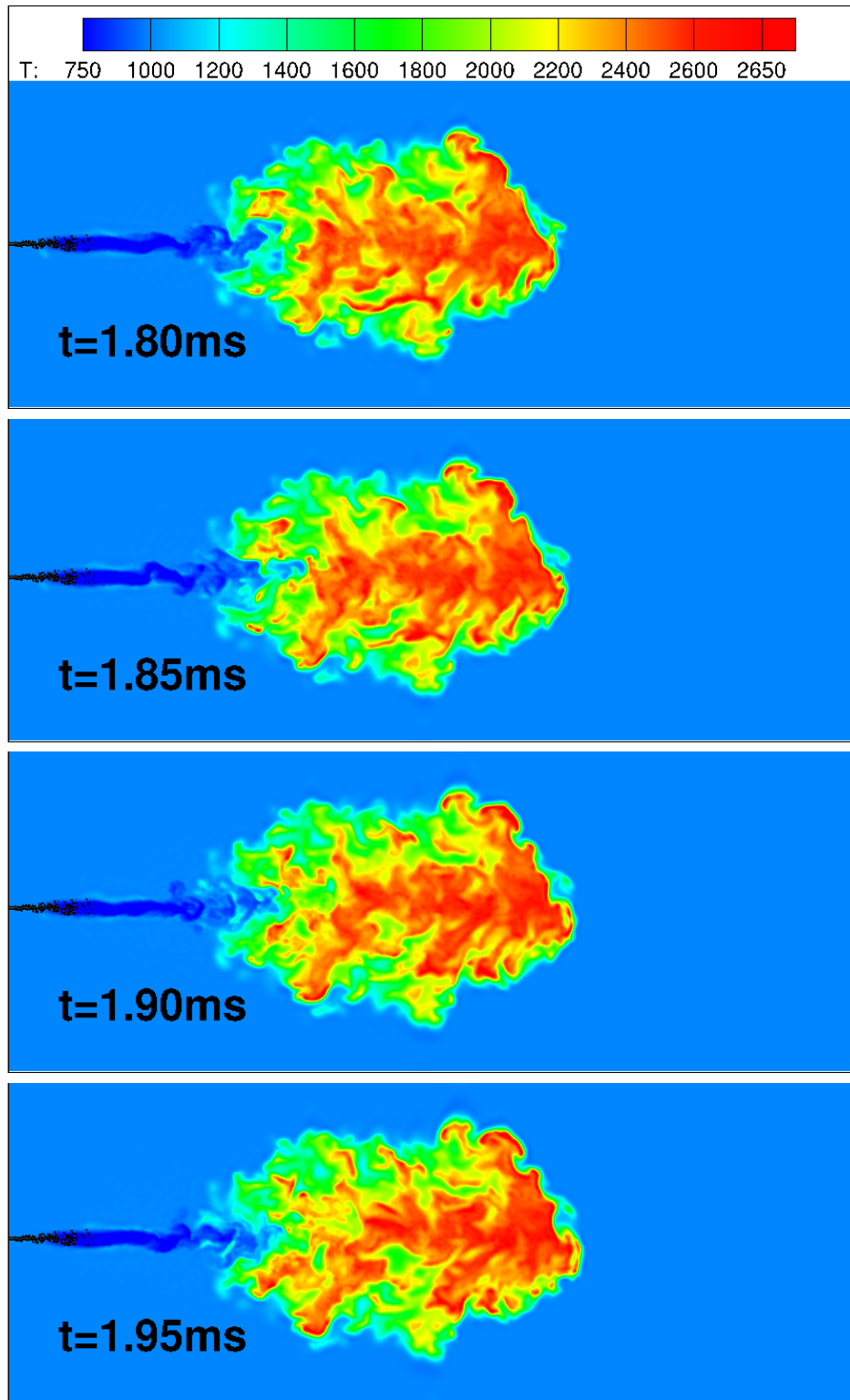
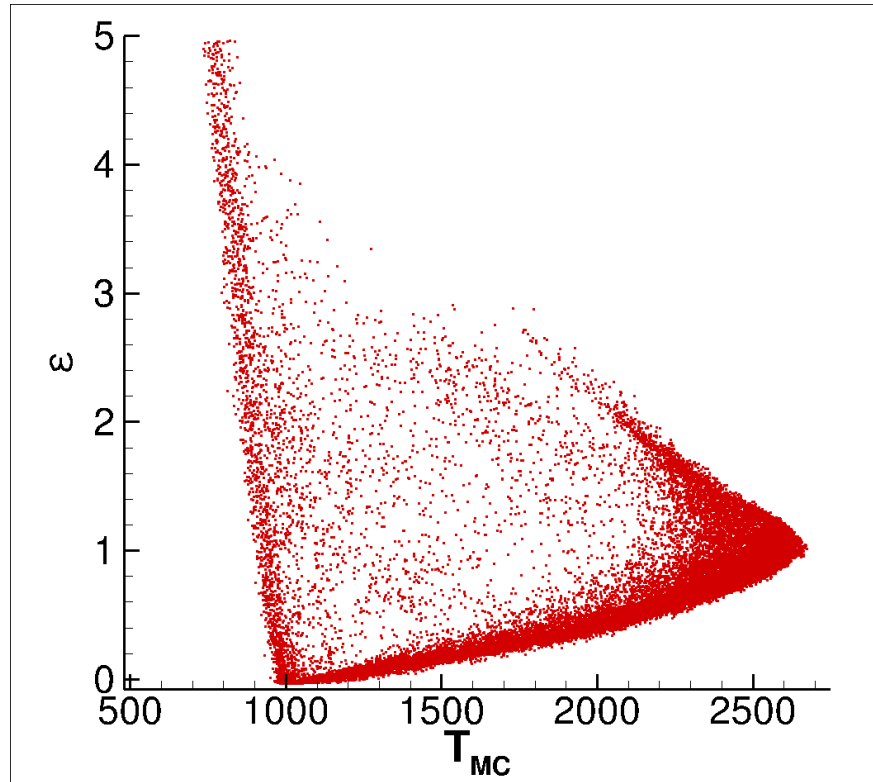
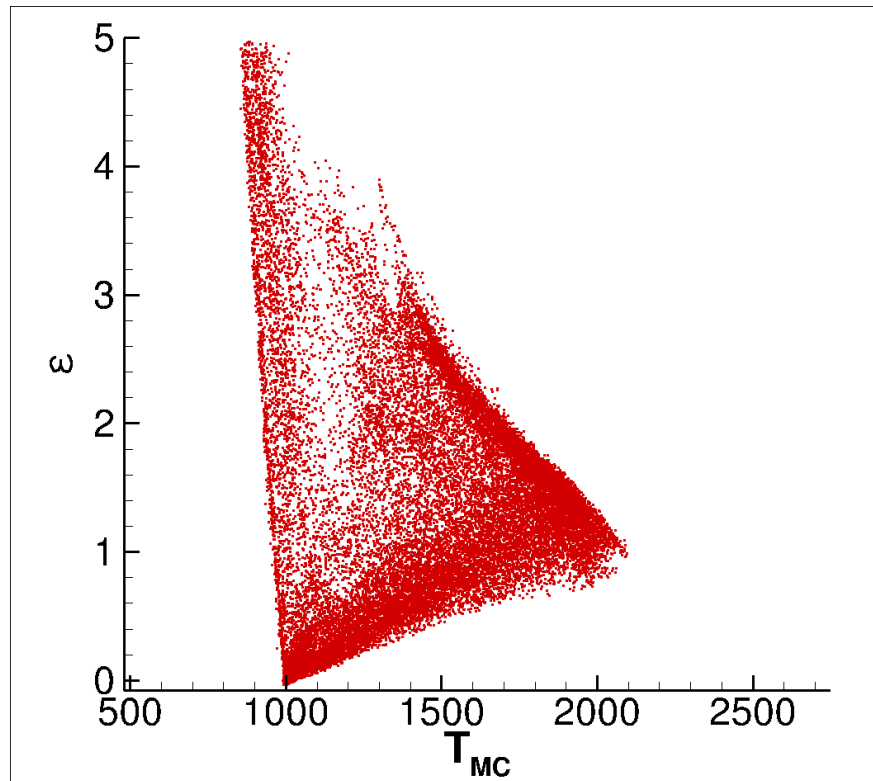


Figure 3.19: Contours of reacting spray temperature at different times for the base case.

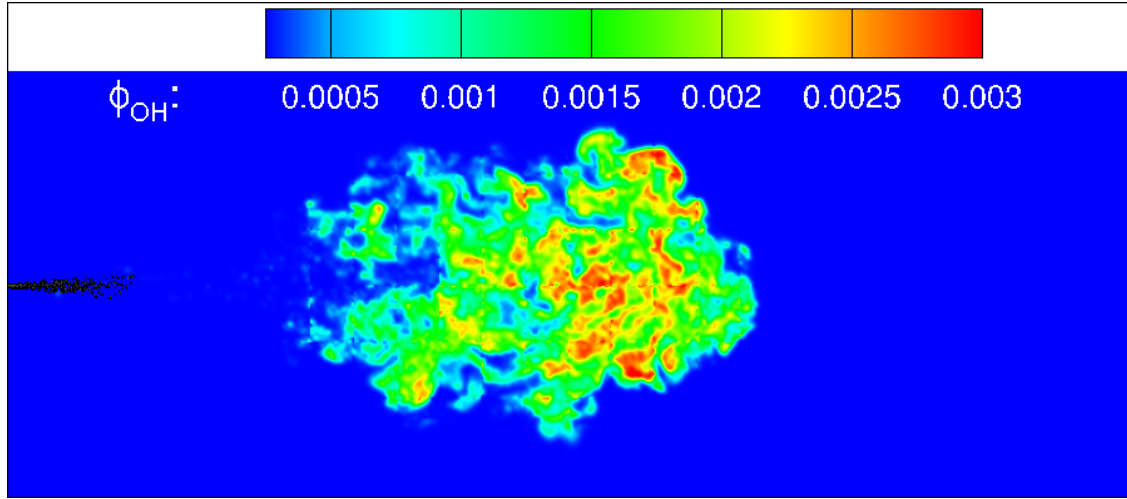


(a) %21 O_2

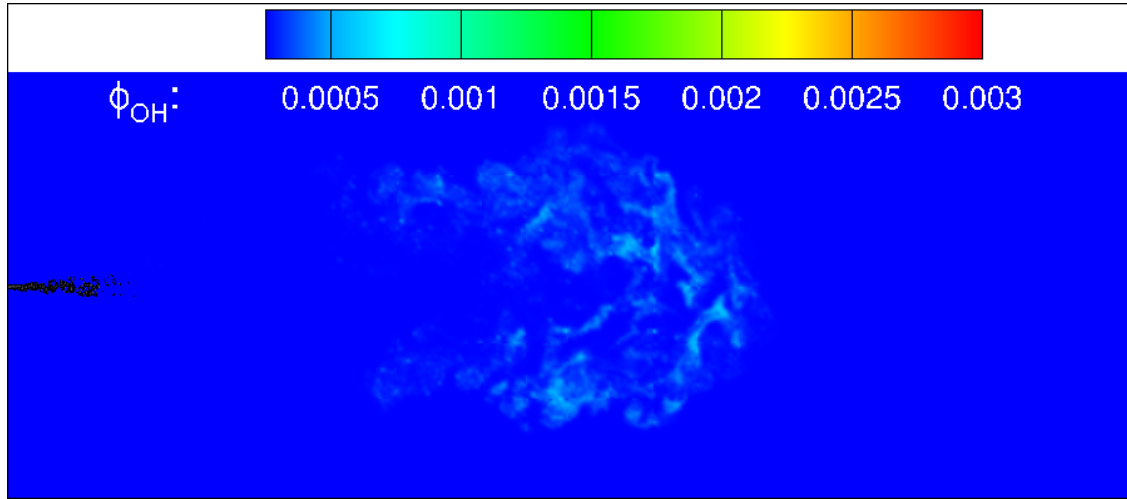


(b) %8 O_2

Figure 3.20: Maps of equivalence ratio versus temperature for different oxygen concentrations.

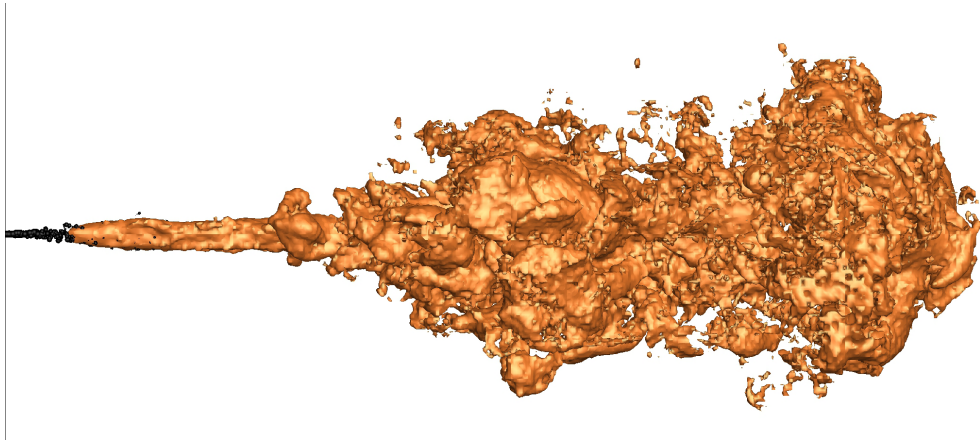


(a) %21 O_2

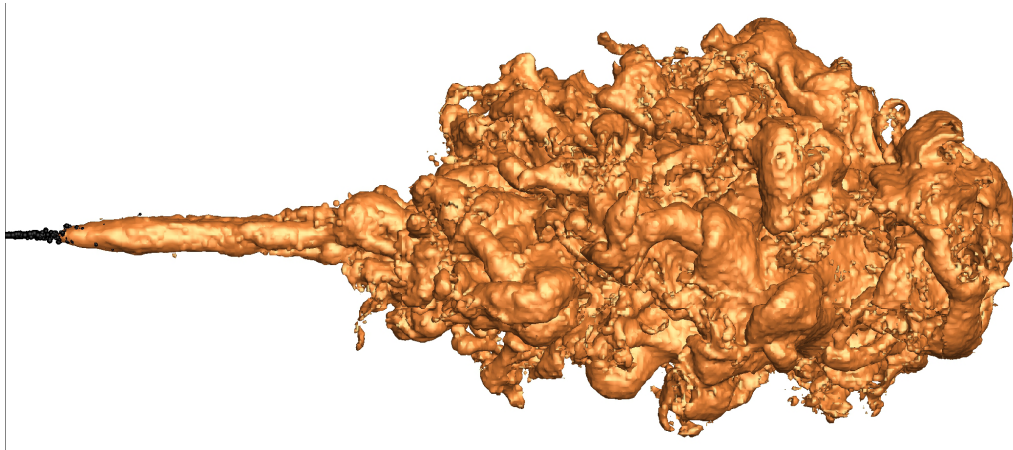


(b) %8 O_2

Figure 3.21: OH mass fraction contours for different initial oxygen concentrations at $T=1000$ K, $\rho = 14.8 kg/m^3$.

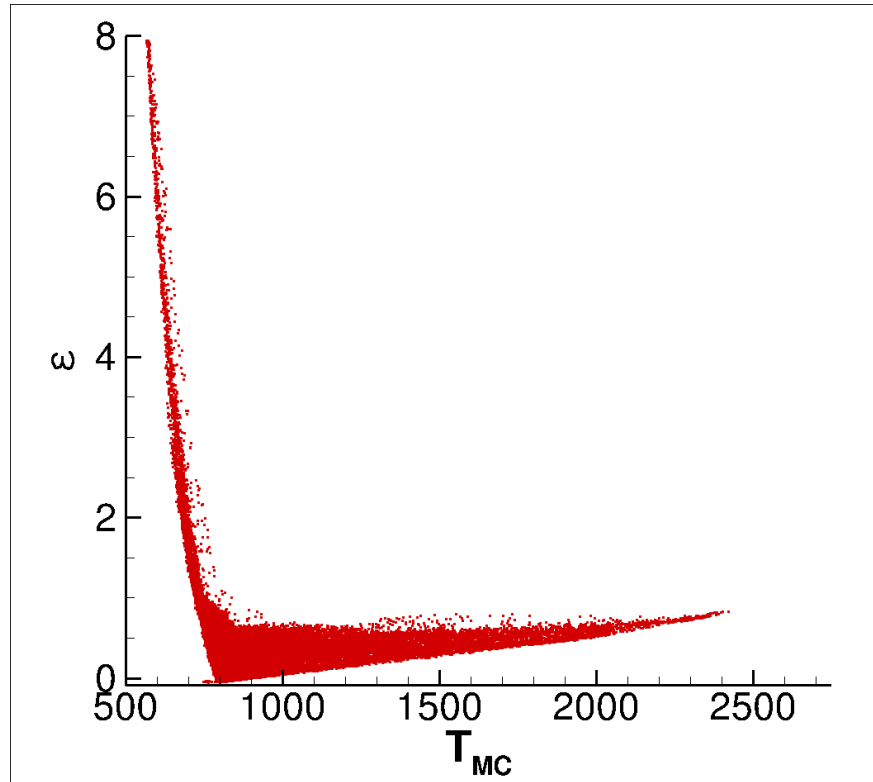


(a) %21 O_2

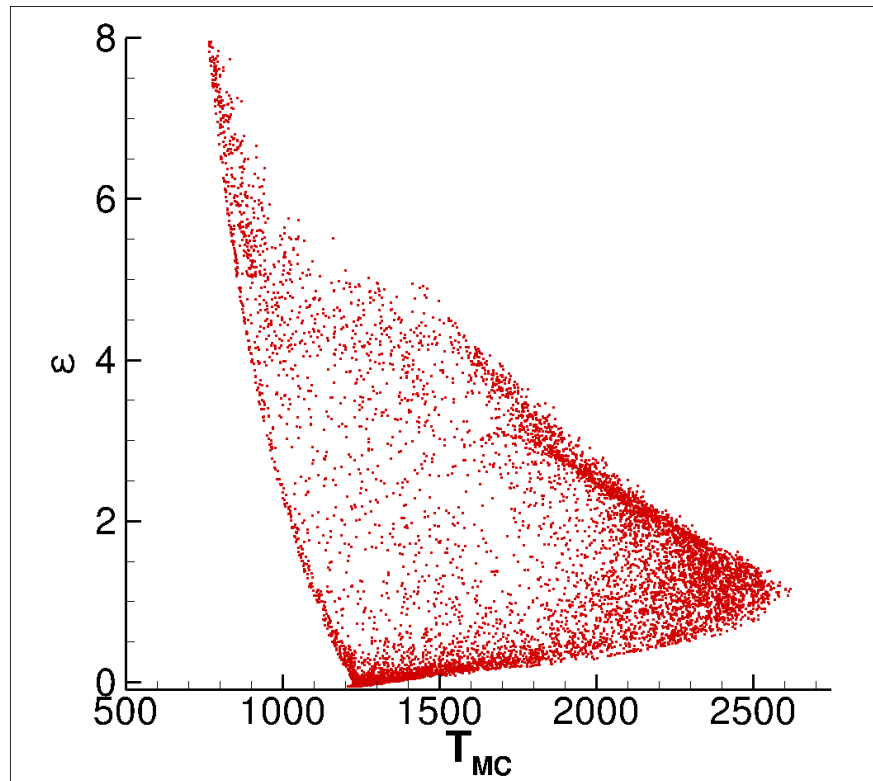


(b) %8 O_2

Figure 3.22: Iso-surfaces of stoichiometric (unity) equivalence ratio for different oxygen concentrations at $t=2.00$ ms.



(a) $T=800$ K



(b) $T=1200$ K

Figure 3.23: Maps of equivalence ratio versus temperature for two different ambient gas temperatures.

3.4 Summary and Conclusions

Hybrid two-phase spray LES/FMDF/ISAT model is used for simulation of evaporating and combusting n-heptane sprays with a 44 species skeletal reaction mechanism. The developed mathematical/computational methodology for the solution of the two-phase LES/FMDF has one Eulerian and two Lagrangian solvers. The fluid velocity and pressure field is obtained by solving the filtered form of the compressible Navier-Stokes equations by high-order finite difference methods via a grid-based Eulerian multiblock flow solver. A Lagrangian droplet model with a stochastic breakup model is employed in which the subgrid turbulence effects on the spray/droplet and the modification of droplet and gas aerodynamics by the wake of nearby droplets are included. Finite rate heat and mass transfer between phases and the local evaporation are considered by solving the spherically symmetric inner droplet conservation equations together with the droplet surface interface equations. The scalar field (species mass fractions and temperature) in the gas and all the complex nonlinear reactions are implemented through the two-phase version of the filtered mass density function (FMDF) methodology. All reaction terms in the FMDF equation appear in closed form. The FMDF is obtained by solution of its transport equation with an efficient stochastic Lagrangian Monte Carlo method with spray effects included. There are two-way interactions between the phases and all the Eulerian and Lagrangian fields. Combustion chemistry calculation is accelerated by using in situ adaptive tabulation (ISAT) and the P-URAN distribution strategy is used to balance the work of ISAT tables on the participating cores. Simulations are conducted for high pressure n-heptane non-reacting evaporating and reacting sprays. For the non-reacting spray, liquid and vapour penetration as well as fuel mass fraction profiles are compared with the experiment. For reacting sprays, ignition delay times and flame liftoff lengths for different

ambient temperatures and oxygen concentrations are compared. Simulations of evaporating sprays, with and without combustion, indicate that the two-phase LES/FMDF results are consistent and compare well with the available experimental data. Our LES/FMDF/Spray results indicate that for low to moderately high ambient gas temperatures, auto-ignition occurs in turbulent eddies at the tip of spray-induced, vapour-saturated jet and the flame lift-off region has a low temperature flame behaviour, meaning that it does not reach the high temperature of the main flame. The ignition delay is overpredicted for lower ambient gas temperature by the model. It was shown that the skeletal mechanism perform less accurate compared to detailed kinetics for the low temperature combustion. The liftoff length is less sensitive to the kinetics and is tied to turbulence chemistry interaction for the quasi-steady flame. Detailed analysis of the flame structure shows that the flame tends to move from a diffusion structure toward to a more premixed structure as the oxygen concentration in the ambient gas decreases and the effect of mixing on the flame is increased. On the other hand, with increase in the ambient gas temperature, the mixing effect on the flame is reduced.

Chapter 4

Volumetric Effects of Dispersed Liquid in Simulation of Moderately Dense Turbulent Droplet Laden Flows

4.1 Introduction

The analytical methods that have been developed for two-phase turbulent flows are generally based on three different approaches: (i) Eulerian-Eulerian, (ii) Eulerian-Lagrangian and (iii) Lagrangian-Lagrangian. In turbulent spray flow computations, the choice of the analytical approach is motivated by three parameters, namely, the Stokes number of the dispersed phase, the grid resolution available in the simulation and the volume loading. These parameters classify the flow regime as dilute, moderately dense and very dense [35],[85]. The grid resolution (Δ) used for the solution of the gas phase could be such that the particles are much smaller than the grid size and subgrid ($d_p \ll \Delta$), partially resolved ($d_p \sim \Delta$), or fully resolved ($d_p \gg \Delta$). For very dense two-phase flows such as that in primary atomization region

of sprays, Eulerian-Eulerian method can be used [21]. These types of models are expected to better capture the interface evolution and breakup of liquid jet ([22],[23] and [24]), but they are not currently practical and cannot be employed for evaporating and reacting sprays in realistic combustion systems. Typical spray combustion systems involve millions of dispersed droplets in a turbulent flow with the droplet diameters often being smaller than, or comparable to the Kolmogorov length scale. The liquid phase in the form of small droplets then is far from being a continuum and it is more appropriate to treat it as a collection of dispersed particles. In this approach, the particle/droplet size is assumed to be smaller than the grid size and the effects exerted by the particles onto the fluid are represented as point-sources at the centroid of spherical particles. Normally, a significant portion of the physical activities associated with the carrier fluid-particle and particle-particle interactions takes place at the subgrid level and has to be modelled. In the majority of studies using Eulerian-Lagrangian methods for dilute sprays particle-particle interactions and volume loading of the droplets are assumed to be negligible ([35], [85] and [78]). These assumptions are not generally valid for moderately dense particle- or droplet-laden flows. However, the Lagrangian particle tracking may still be used for these flows, provided that the particle-particle interactions and volume displacement effects of particles are accounted for [78].

Point particle direct numerical simulations (DNS) and large eddy Simulations (LES) of particle-laden turbulent flows have been used to solve various types of fundamental two-phase turbulent flows such as particle-laden homogeneous turbulence, temporal mixing layers and spatially developing mixing layers ([65],[86],[87], [88], [111], [155] and [156]). These simulations have often been done for the dilute cases with negligible particle-particle interactions, even though particle collisions have been included in some of DNS and LES studies

([157], [158],[159] and [160]). To obtain the particle terms in DNS and LES equations, some form of averaging has to be done for the particles or droplets which is different than the space averaging (or filtering) in LES. Sirignano [161] attempted to unify droplet averaging and LES filtering into one operation and developed filtered equations for both phases which include fluid volume fraction. Few other recent studies also considered the volumetric effect of the dispersed phase on the carrier fluid for moderately dense two-phase flows ([162],[163] and [164]). Most of these studies are, however, on dispersed flows laden with solid particles. On the other hand, when dealing with evaporating droplets, additional interactions between phases due to heat and mass transfer arise. Also following collisions, droplets may coalesce or break. Efficient and comprehensive droplet-droplet collision models have been developed that can be incorporated into Lagrangian droplet simulations [53],[165].

In the present chapter, the emphasis is placed on improving the point-particle assumption for evaporating droplets in LES by accounting for their finite volume effects. The effect of droplets on the carrier gas is implemented through a series of mass, momentum and energy source/sink terms in the gas equations for droplets that undergo collision/coalescence, transport, heat and mass transfer. Here, the particles are still assumed to be small in comparison to LES grid or filter size and the forces acting on them are modelled using modified Stokes, Nusselt and Sherwood number correlations. However, the finite volume effect of droplets is included in the formulation by including the volume fraction variable in the carrier gas equations.

The rate of evaporation is increasing with relative velocity between droplet and the surrounding gas phase. Therefore, the statistics of turbulent slip velocity fluctuations is relevant for the mean heat and mass transfer rates between phases. To account for the influence of

unresolved subgrid turbulence on droplet motion in the LES calculations, Langevin type stochastic models can be used ([31],[32], [33] and [166]). The effects of SGS fluctuations of gas variables like temperature and species mass fractions on the droplet heat and mass transfer rates can also be included by reconstructing the instantaneous values of these gas variables as seen by the individual droplets in a stochastic manner ([102], [167] and [168]). Alternatively, we can directly capture these effects in the two-phase filtered mass density function (FMDF) model described below.

FMDF represents the subgrid-scale (SGS) probability density function (PDF) of the gas energy and species mass fractions [105] and is obtained by solving its transport equation with a stochastic Lagrangian Monte Carlo method. One of the important features of the FMDF is that the single-point process like chemical reaction appears in a closed form in its formulation, making the FMDF very attractive for simulations of various types of reactions (slow, fast, premixed, non-premixed, etc.) with different chemical kinetics ([57],[99], [106], [107], [108],[109] and [110]). As long as the reaction mechanism is known and is computationally affordable it can be used in the LES/FMDF calculations. Recently, the FMDF model is extended and used for simulations of dilute two-phase reacting flows ([58],[111]). Here, the two-phase FMDF is further extended to account for the finite volume of the dispersed phase. The model is capable of computing turbulence-combustion-spray interactions in complex flow configurations in conjunction with non-equilibrium, multi-step reaction models. Several other desirable attributes of the proposed model are noteworthy: (1) LES/FMDF directly computes large-scale unsteady flow structures, while also accounting for mixing and reaction processes at subgrid level, (2) FMDF provides all higher moments of the scalar variables within the subgrid scales, whereas current LES strategies can at best predict the first mo-

ment or filtered values, (3) with a Lagrangian treatment of the FMDF, the LES procedure is free of artificial numerical diffusion errors, (4) in the two-phase LES/FMDF model proposed here the SGS fluctuations of the scalar field in the carrier gas affects the heat and mass transfers between gas and liquid locally through Lagrangian particles, independent of relatively coarse Eulerian grids. This can provide the subgrid scale effects of the gas scalar field on the liquid droplet field. In the following sections, the mathematical formulation and submodels of the two-phase LES/FMDF model for moderately dense droplet laden flows are described. The results obtained by the model for a planar turbulent jet, laden with significant number of evaporating droplets are presented next to show the volumetric effect of droplets on the gas turbulence and evaporation.

4.2 Mathematical Formulations and Modelling

The compressible LES/FMDF/Spray model has three main mathematical components: (1) the (two-phase filtered) gas dynamics equations, (2) the two-phase FMDF and its equivalent stochastic equations and (3) the Lagrangian spray equations with its submodels. These three components are presented in the following sections

4.2.1 Continuum Conservation Equations

Before presenting the LES equations, it is useful to consider the unfiltered (DNS) gas equations. For a compressible two-phase reacting flow, the unfiltered conservation equations for mass, momentum, energy and chemical species mass fractions and the equation of state

are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = \dot{S}_{Mass}^{sp}, \quad (4.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\Theta \frac{\partial \hat{p}}{\partial x_i} + \Theta \frac{\partial \hat{\tau}_{ij}}{\partial x_j} + \dot{S}_{m_i}^{sp}, \quad (4.2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u_i}{\partial x_i} + \Theta \frac{\partial \hat{p} u_i}{\partial x_i} = -\frac{\partial q_i}{\partial x_i} + \Theta \frac{\partial \hat{\tau}_{ij} u_j}{\partial x_i} + \dot{Q} + \dot{S}_E^{sp}, \quad (4.3)$$

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho \phi_\alpha u_i}{\partial x_i} = -\frac{\partial J_i^\alpha}{\partial x_i} + \rho \dot{S}_\alpha + \dot{S}_\alpha^{sp}, \quad (4.4)$$

$$\Theta \hat{p} = \rho R^0 T \sum_{\alpha=1}^{N_s} \frac{\phi_\alpha}{MW_\alpha}. \quad (4.5)$$

Here, $\rho = \Theta \rho_g + (1 - \Theta) \rho_l$ is the fluid density and Θ is the local volume fraction of the carrier gas to the liquid. Also, u_i is the gas velocity component and $E = e + u_i u_i / 2$ is the gas total energy. The original gas pressure and viscous stresses, represented by hat symbols, are directly affected by the volume fraction as $p = \Theta \hat{p}$ and $\tau_{ij} = \Theta \hat{\tau}_{ij}$. The explicit appearance of Θ in these variables facilitates the computations of gas equations affected by liquid volume fraction [161]. The viscous stress tensor τ_{ij} , and the heat and mass fluxes J_i^α , $q_i = J_i^{\alpha=N_s+1}$ are calculated based on Newtonian Fluid and Fourier and Fick's Models:

$$\hat{\tau}_{ij} = 2\mu(S_{ij} - \frac{1}{3}S_{kk}\delta_{ij}) = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}), \quad (4.6)$$

$$J_i^\alpha = -\frac{mu}{Sc} \frac{\partial \phi_\alpha}{\partial x_i}. \quad (4.7)$$

The Favre-filtered forms of gas continuity, momentum, energy and scalar equations are:

$$\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_i} = \langle \dot{S}_{Mass}^{sp} \rangle_l, \quad (4.8)$$

$$\frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_j} = -\langle \Theta \rangle_l \frac{\partial \langle p \rangle_l}{\partial x_i} + \langle \Theta \rangle_l \frac{\partial \langle \tau_{ij} \rangle_l}{\partial x_j} - \frac{\partial \langle \tau_{ij}^{sgs} \rangle_l}{\partial x_j} + \langle \dot{S}_{mi}^{sp} \rangle_l, \quad (4.9)$$

$$\begin{aligned} \frac{\partial \langle \rho \rangle_l \langle E \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle E \rangle_L \langle u_i \rangle_L}{\partial x_i} + \langle \Theta \rangle_l \frac{\partial \langle p \rangle_l}{\partial x_i} = & -\frac{\partial \langle q_i \rangle_l + H_i^{sgs}}{\partial x_i} + \langle \dot{Q} \rangle_l + \langle \dot{S}_E^{sp} \rangle_l \\ & + \langle \Theta \rangle_l \frac{\partial [\langle \tau_{ij} \rangle_l \langle u_j \rangle_L]}{\partial x_i} - \frac{\partial \tau_{ij}^{sgs} \langle u_j \rangle_L}{\partial x_i}, \end{aligned} \quad (4.10)$$

$$\frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = -\frac{\partial \langle J_i^\alpha \rangle_l + J_i^{\alpha sgs}}{\partial x_i} + \langle \rho \dot{S}_\alpha \rangle_l + \langle \dot{S}_\phi^{sp} \rangle_l, \quad (4.11)$$

where the two-phase filtered density is defined as

$$\langle \rho(\mathbf{x}, t) \rangle_l = \int_{-\infty}^{+\infty} G(\mathbf{x} - \mathbf{x}') \Theta(\mathbf{x}', t) \rho(\mathbf{x}', t) d\mathbf{x}'. \quad (4.12)$$

Note that the gas filtered density is related to the two-phase filtered density as $\langle \rho \rangle_l \equiv \langle \Theta \rangle_l \langle \rho_g \rangle_l$. The Favre-filtered variable Υ is defined as

$$\langle \rho(\mathbf{x}, t) \Upsilon(\mathbf{x}, t) \rangle_l = \langle \rho(\mathbf{x}, t) \rangle_l \langle \Upsilon(\mathbf{x}, t) \rangle_L = \int_{-\infty}^{+\infty} G(\mathbf{x} - \mathbf{x}') \Theta(\mathbf{x}', t) \rho(\mathbf{x}', t) \Upsilon(\mathbf{x}', t) d\mathbf{x}' \quad (4.13)$$

The definitions for the filtered pressure and viscous stress tensor (identified by a “hat” symbol) are:

$$\langle \Theta(\mathbf{x}, t) \rangle_l \langle \hat{p}(\mathbf{x}, t) \rangle_l \equiv \langle p(\mathbf{x}, t) \rangle_l \equiv \int_{-\infty}^{+\infty} G(\mathbf{x} - \mathbf{x}') \Theta(\mathbf{x}', t) p(\mathbf{x}', t) d\mathbf{x}', \quad (4.14)$$

$$\langle \Theta(\mathbf{x}, t) \rangle_l \langle \hat{\tau}_{ij}(\mathbf{x}, t) \rangle_l \equiv \langle \tau_{ij}(\mathbf{x}, t) \rangle_l \equiv \int_{-\infty}^{+\infty} G(\mathbf{x} - \mathbf{x}') \Theta(\mathbf{x}', t) \tau_{ij}(\mathbf{x}', t) d\mathbf{x}'. \quad (4.15)$$

The filtered equation of state will be $\langle \Theta \rangle_l \langle \hat{p} \rangle_l = \langle \rho \rangle_l \langle R \rangle_L \langle T \rangle_L$, in which the mixture gas constant is obtained from the filtered species mass fractions and the universal gas constant. The filtered viscous stress tensor $\langle \hat{\tau}_{ij} \rangle_l$ is computed based on the filtered strain rate, and the filtered heat and mass flux vectors are assumed to be proportional to the filtered temperature and species mass fractions. The filtered heat of reaction and rate of species production are obtained from the two-phase FMDF.

To include the liquid volumetric effect on the thermodynamic field, the filtered enthalpy equation is presented as

$$\frac{\partial \langle \rho \rangle_l \langle h \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle h \rangle_L}{\partial x_i} = - \frac{\partial (\langle q_i \rangle_l + q_i^{sgs})}{\partial x_i} + \langle \dot{Q} \rangle_l + \langle \Theta \rangle_l \left[\frac{\partial \hat{p}}{\partial t} + \langle u_i \rangle_L \frac{\partial \hat{p}}{\partial x_i} \right] + \langle \dot{S}_h^{sp} \rangle_l \quad (4.16)$$

4.2.1.1 Two-Phase Filtered Mass Density Function

According to the PDF theory [138], the fine-grained density for the scalar vector (which includes the enthalpy and species mass fractions) represents one measured value or realization of the scalar in a turbulent flow and is defined as [133]:

$$\xi(\Psi, \Phi(\mathbf{x}, t)) = \delta(\Psi, \Phi(\mathbf{x}, t)) = \prod_{\alpha=1}^{N_s+1} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}, t)). \quad (4.17)$$

The transport equation for the fine-grained density in a variable density flow is

$$\frac{\partial \rho \xi}{\partial t} + \frac{\partial (\rho u_i \xi)}{\partial x_i} = \frac{\partial \xi}{\partial \psi_\alpha} \frac{\partial J_i^\alpha}{\partial x_i} - \frac{\partial (\rho \dot{S}_\alpha \xi)}{\partial \psi_\alpha}. \quad (4.18)$$

The two-phase mass density function is a joint probability density function of the scalars at the subgrid-level for the gas-phase and is defined as

$$F_L(\Psi; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \xi(\Psi, \Phi(\mathbf{x}', t)) (\mathbf{x}' - \mathbf{x}) \Theta(\mathbf{x}', t) d\mathbf{x}'. \quad (4.19)$$

The integral property of FMDF is such that

$$\int_{-\infty}^{+\infty} F_L(\Psi; \mathbf{x}, t) d\Psi = \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) G(\mathbf{x}' - \mathbf{x}) \Theta(\mathbf{x}', t) d\mathbf{x}' = \langle \rho(\mathbf{x}, t) \rangle_l. \quad (4.20)$$

The mass-weighted conditional filtered mean of the variable $\Upsilon(\mathbf{x}, t)$ is defined as

$$\langle \Upsilon(\mathbf{x}, t) | \Psi \rangle_l = \frac{\int_{-\infty}^{+\infty} \Upsilon(\mathbf{x}', t) \rho(\mathbf{x}', t) \xi(\Psi, \Phi(\mathbf{x}', t)) G(\mathbf{x}' - \mathbf{x}) \Theta(\mathbf{x}', t) d\mathbf{x}'}{F_L(\Psi; \mathbf{x}, t)}. \quad (4.21)$$

Multiplying both sides of the fine-grained density equation by $G\Theta$ and integrating it term by term in the physical domain over the filter domain yields

$$\begin{aligned} \frac{\partial F_L}{\partial t} + \frac{\partial}{\partial x_i} [\langle u_i(\mathbf{x}, t) | \Psi \rangle_l F_L] &= \frac{\partial}{\partial \psi_\alpha} \left[\left\langle \frac{1}{\rho(\Phi)} \frac{\partial J_i^\alpha}{\partial x_i} | \Psi \right\rangle_l F_L \right] - \frac{\partial}{\partial \psi_\alpha} (\dot{S}_\alpha(\Psi) F_L) \\ &+ \int_{\mathbf{A}} G(\mathbf{x}' - \mathbf{x}) [\rho(\mathbf{x}', t) \xi(\Psi, \Phi(\mathbf{x}', t)) (\mathbf{u}(\mathbf{x}', t) - \mathbf{u}_\Theta(\mathbf{x}', t))] d\mathbf{A}. \end{aligned} \quad (4.22)$$

Note that the molecular diffusion has contributions to the gas-liquid interface due to molecular diffusion at the liquid surface. This contribution explicitly appears when the scalar equation is derived from the two-phase FMDF equation. Having multiplied the FMDF equation by the scalar or composition variable ψ_α and integrating in composition ψ space

we get

$$\begin{aligned} \frac{\partial \langle \rho \rangle_l \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \phi_\alpha \rangle_L}{\partial x_i} = & -\frac{\partial \langle J_i^\alpha \rangle_l}{\partial x_i} + \langle \rho \dot{S}_\alpha \rangle_l \\ & + \int_{\mathbf{A}} G(\mathbf{x}' - \mathbf{x}) [\rho(\mathbf{x}', t) \phi_\alpha(\mathbf{x}', t) (\mathbf{u}(\mathbf{x}', t) - \mathbf{u}_\Theta(\mathbf{x}, t)) + J_i^\alpha] d\mathbf{A}. \end{aligned} \quad (4.23)$$

The scalar equation, as obtained from the two-phase FMDF equation, is equivalent with the filtered scalar equation derived directly from the DNS equations by multiplying the unfiltered scalar equation with $G\Theta$ and integration in space [161]. The surface integral in the FMDF equation, reflects the liquid phase source terms to mass and scalar space arising from droplets. The first term represents the scalar flux at the interface due to Stephan flow and the second term accounts for scalar flux due to scalar diffusion at the interface. To avoid expensive Monte Carlo particle to droplet particle interactions in the moderately dense flow, the liquid contributions to the FMDF equation are computed by volume averaging of droplet terms over the Eulerian grid points ([58],[111]).

In the present hybrid methodology, the filtered scalar values like temperature may be calculated from both the Eulerian finite difference (FD) grid data and the Lagrangian Monte Carlo (MC) particle data. This provides the unique opportunity for the assessment of LES-FD and FMDF-MC parts of the LES/FMDF method. Mathematically, FD and MC results should be the same. Consistency of MC and FD data implies numerical accuracy of both. For establishing the consistency between FD and MC methods in reacting flows, the chemical source terms in the FD equations which are closed in the FMDF formulation are calculated from the MC particles.

4.2.1.2 Dispersed Liquid Droplet Equations

For small droplets, the evolution of the droplet displacement vector, velocity vector, temperature and mass is based on a set of non-equilibrium Lagrangian equations [42]:

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p, \quad (4.24)$$

$$\frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{u}_{rel}}{\tau_p}, \quad (4.25)$$

$$\frac{d(me)_p}{dt} = c_l m_p \frac{dT_p}{dt} + c_{pv} T_p \dot{m}_p + \dot{m}_p (h_v^0 - L_v), \quad (4.26)$$

$$\frac{dT_p}{dt} = \frac{1}{3} \frac{Nu}{Pr} \frac{c_p}{c_l} \frac{(T_g - T_p)}{\tau_{evap}} + \frac{\dot{m}_p}{m_p} \frac{L_v}{c_l}, \quad (4.27)$$

$$\dot{m}_p = -\frac{Sh}{3Sc} \frac{m_p}{\tau_{st}} \ln(1 + B_M) \quad (4.28)$$

where the relative velocity is $\mathbf{u}_{rel} = \mathbf{u}_g - \mathbf{u}_p$ and the particle response time is defined as $\tau_p = \tau_{st}/f_1(\Theta, Re_{sl})$. The particle response time is a combination of droplet Stokes time $\tau_{st} = d_p^2 \rho_l / 18 \mu_g$ and the modified drag factor, which is the finite Reynolds number ($Re_{sl} = \rho_g d_p u_{rel} / \mu_g$) correction to the Stokes drag. Here, the drag factor correlation is obtained from the correlation developed by Tenneti et al. [169] from the particle resolved simulations which include the effect of liquid volume fraction. For the heat and mass transfer between droplets and the surrounding gas, the well known Ranz-Marshall correlations for the Sherwood and Nusselt numbers are used. The evaporation time scale is defined as $\tau_{evap} = \tau_{st}/f_2(\beta)$, which is calculated from Stokes time scale and the evaporative heat transfer correction as a function of non-dimensional evaporation parameter β (equation 1.18). The Spalding mass transfer number B_M is obtained using the non-equilibrium surface vapour function.

The particle volume fraction in conjunction with the particle velocity fluctuations suggests the relative importance of the advective transport to collisional effects. For moderately dense particulate flows such as those studied here, droplet collision and its outcome could be important as they affect the size distribution of the droplets and consequently the fuel evaporation, mixing and combustion. The collision and its outcome are modelled here based on the model suggested by Munnannur and Reitz [53] and Kim et al. [52]. Four possible collision outcomes of bouncing, coalescence, reflexive separation and stretching separation are considered. Fragmentations in stretching and reflexive separations are modelled by assuming that the interacting droplets form an elongating ligament that either breaks up by capillary wave instability, or retracts to form a single satellite droplet. To facilitate the collision calculation, droplets are sorted according to their positional cells. The search for possible collision partner for each particle is carried out among particles of the same cell and the immediate neighbouring cells. The neighbouring cells whose particles are searched are picked up according to the droplet's relative position at each time step. During the collision-pair search, interacting pairs are marked to avoid multiple collision calculations using a list of possible collision partners for each droplet. For collision calculation at processors' common boundaries, a one-way communication is carried out to move particles at the common cells for collision calculation with remote particles. After collision calculation is carried out with remote particles, particles are communicated back.

4.3 Results and Discussion

In this section, results for a moderately dense droplet-laden planar jet are used to assess the volumetric effect of the dispersed liquid phase on the carrier gas flow and turbulence. The

general behaviour of single-phase planar and round turbulent jets are well known ([170], [171] and [172]). The near field of the shear layer is mainly controlled by the Kelvin-Helmholtz (K-H) instabilities and are strongly dependent on the inlet flow conditions and external forcing [173]. Colucci [174] used the linear stability theory to show that with a lower density at the shear zone, the jet is more stable and the convective wave speed is biased towards the higher density stream. Therefore, if the higher speed stream has a higher density than the lower speed stream, the K-H instabilities will be augmented. Here, a planar jet with basic characteristics similar to the shear layer flow of Li et al. [111] is simulated. The Reynolds number based on the characteristic shear thickness δ_s is 100. The simulated planar jet is assumed to be composed of cold Nitrogen with a velocity of U_{jet} and temperature of T_{jet} . The co-flow is assumed to be hot air with the velocity and temperature of $U_{co} = U_{jet}/3$ and $T_{co} = 2T_{jet}$. The pressure is uniform and atmospheric; therefore the inflow density is almost inversely proportional to the temperature. The jet width or “diameter” is $D_{jet} = 15\delta_s$. The computational domain extends to $20D_{jet}$ in axial direction, where standard subsonic pressure outflow boundary condition is applied [175]. The lateral direction has a length of $8D_{jet}$ and free stream boundary conditions are used for this direction. Finally in the spanwise direction, the computational length is set to $4D_{jet}$ with periodic boundary conditions. Table 4.1 summarizes the main computational parameters of the problem. The LES grid size is set to $\Delta_{LES} = \delta_s$. The inlet flow velocities are perturbed with an isotropic turbulent flow obtained by DNS. The amplitude of the perturbation is set to be about %10 of the convective velocity ($U_\infty = \frac{U_{jet}+U_{co}}{2}$). Figure 4.1 shows the instantaneous temperature field of the developed single phase planar jet. It is clear that the jet becomes highly unstable and three-dimensional with the isotropic turbulent perturbation. The two shear layers grow due to K-H instabilities and reach each other at about $9D_{jet}$ downstream of the inlet. For

N_{core}	56
N_{PC}	11,000,000
N_G	1,550,000
N_{MC}	9,300,000
Δ	0.25 mm

Table 4.1: Computational parameters for LES of moderately dense droplet laden planar jet

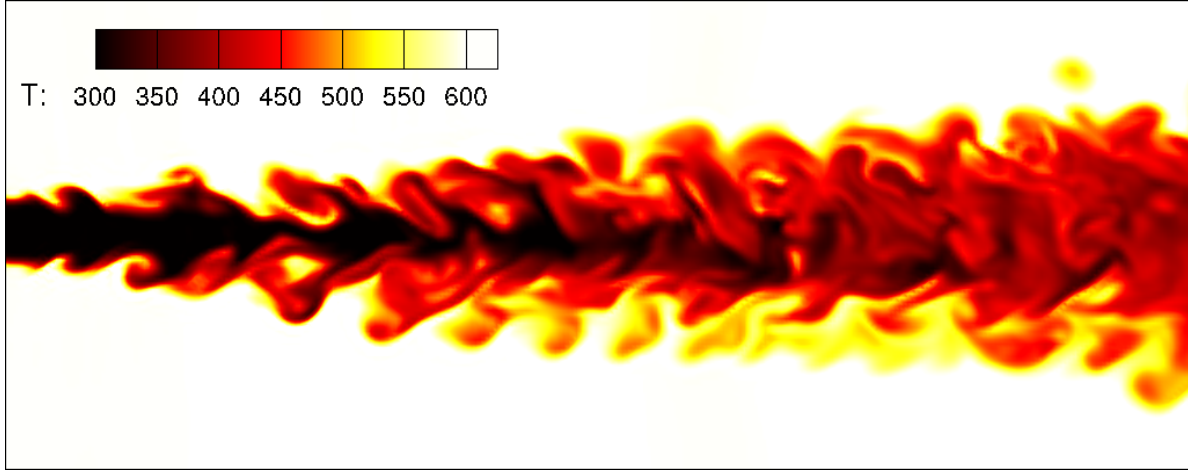


Figure 4.1: Temperature contours for the simulated single-phase planar jet in a x-y plane.

the two-phase planar jet simulations, the inner jet (away from the shear layers) is randomly laden with decane liquid droplets with initially uniform diameter of $10\mu m$. The inlet volume loading of droplets to that of the gaseous nitrogen is set to be about %15. This will lead to a liquid to gas mass loading ratio of about 75, which is very significant. Figure 4.2 shows the liquid volume fraction field in the simulated droplet-laden planar jet. It is clear that those droplets following the shear flow are centrifuging away from the vortex cores and accumulate in the high strain rate zones, causing the liquid volume fraction to reach %20 or more. This phenomenon, known as the preferential concentration [176] leads to local effect of the liquid volume fraction to become significant.

Figure 4.3 compares the temperature field in the two-phase jet flow obtained with and without the liquid volume fraction effect. Figure 4.4 compares the evaporated fuel mass fractions

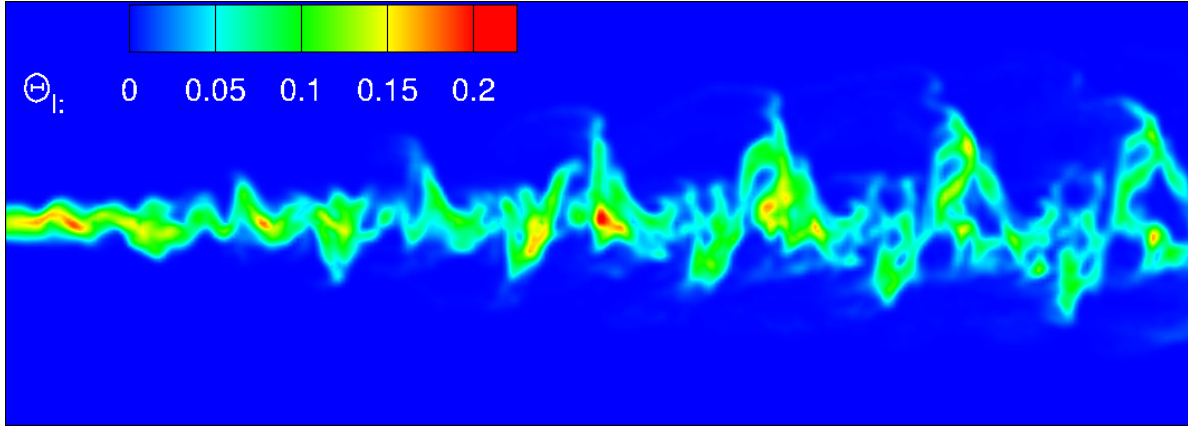
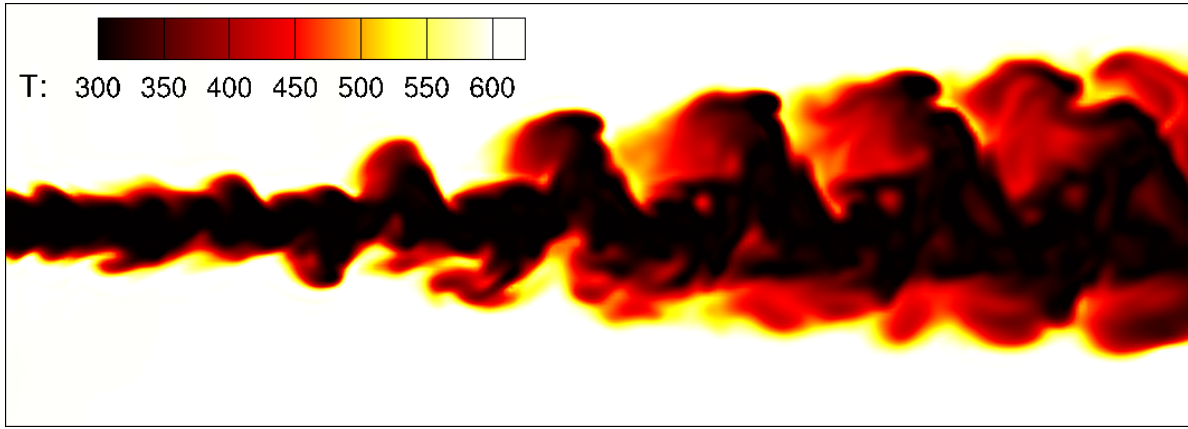
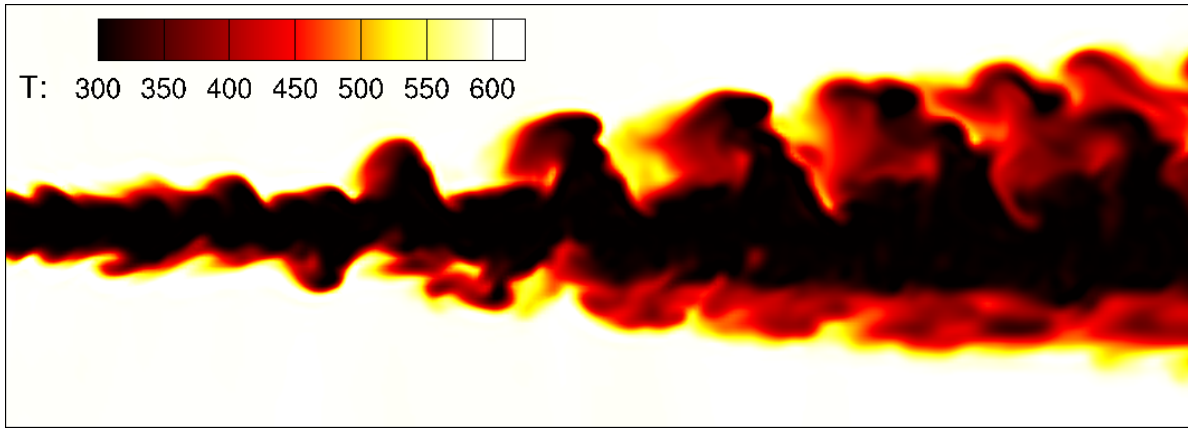


Figure 4.2: Liquid volume fraction field for the droplet laden planar jet.

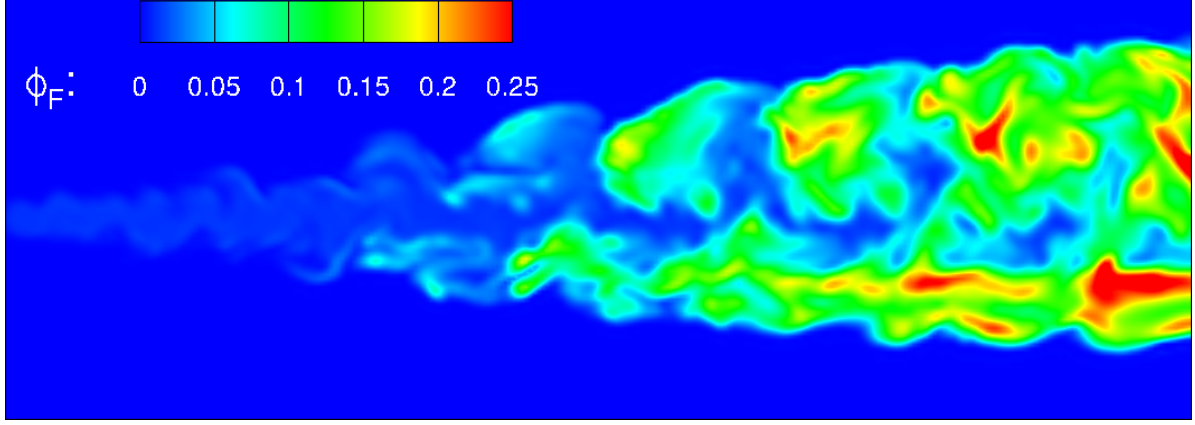


(a)

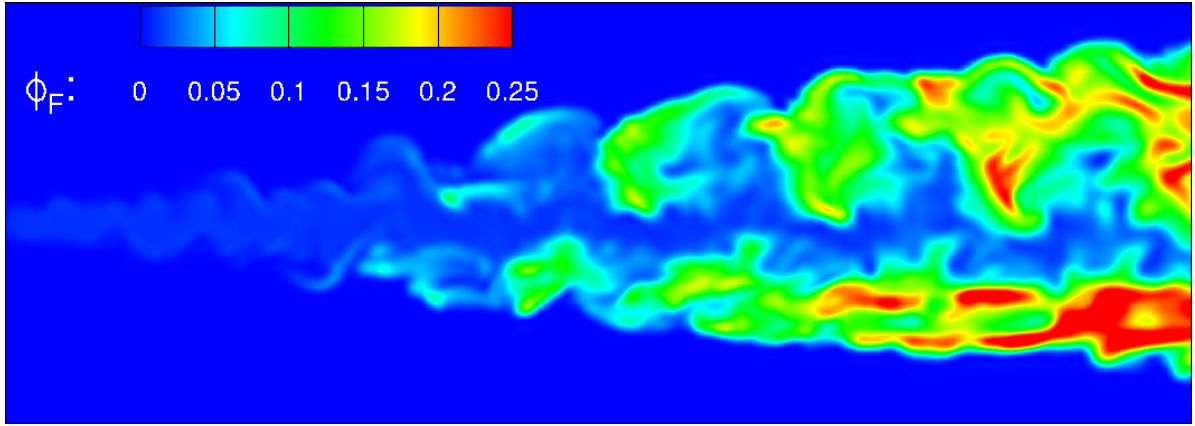


(b)

Figure 4.3: Comparison of the temperature fields of the droplet laden planar jets computed (a) with liquid volume fraction effect, and (b) without liquid volume fraction effect.



(a)



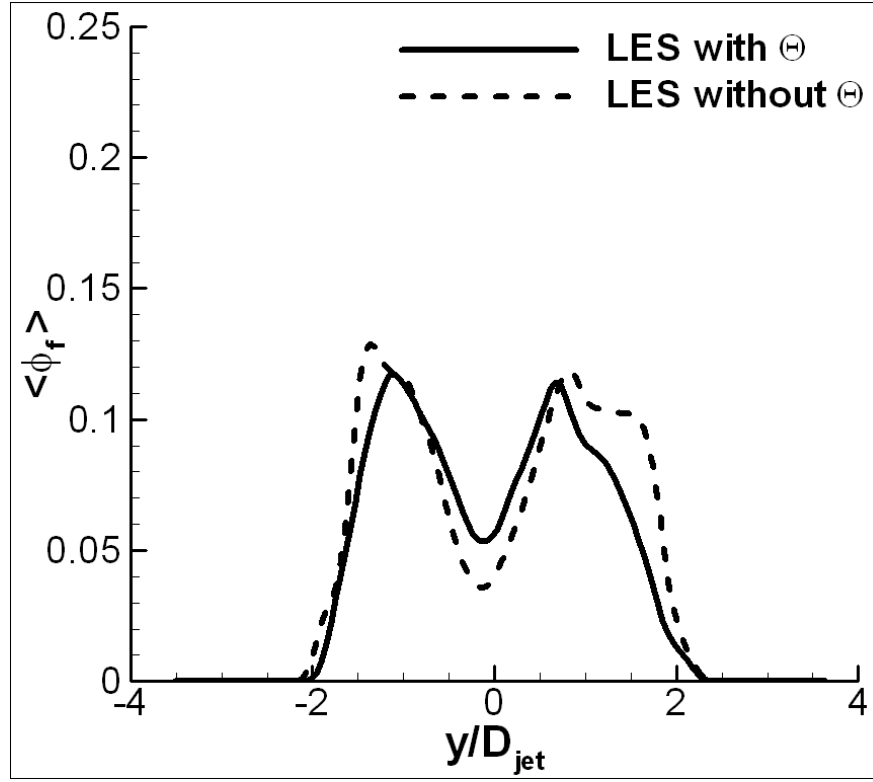
(b)

Figure 4.4: Comparison of the evaporated fuel mass fraction fields of the droplet laden planar jet computed (a) with liquid volume fraction effect, and (b) without liquid volume fraction effect.

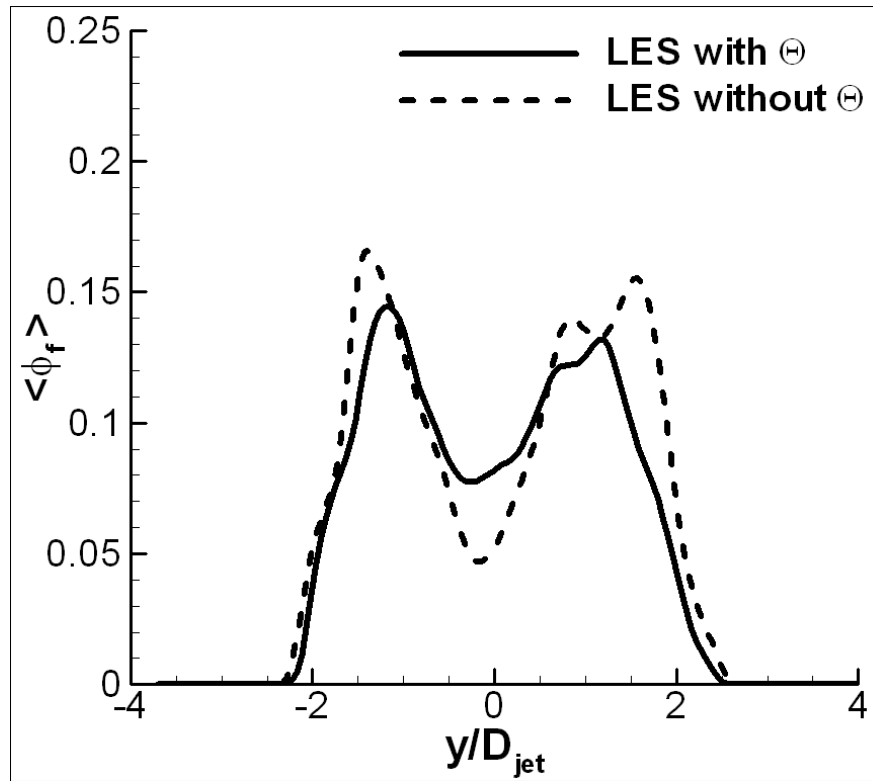
for the two cases. Compared to the single-phase flow, the droplets significantly damp the turbulence in the shear layers, which is very significant due to a very high mass loading ratio. The significance of this damping is due to the drag force of the highly loaded jet and also later on due to droplet evaporation at downstream locations. It is clear from the figure that the volume fraction effect is pronounced at downstream locations, where the turbulence modulation is higher without volume fraction effect. Figure 4.4 shows that in general there is more liquid droplet evaporation when the liquid volume fraction is neglected.

To further investigate the liquid volume fraction effect on the evaporation, profiles of mean evaporated vapour at different axial locations are compared in Figure 4.5 . It is clear that when the liquid volume fraction is neglected in the formulation and computations, the evaporation is higher in the shear zones and is lower in the core of the jet. When the liquid volume fraction is ignored, the available gas mass in the shear zones are higher than it really should be. This higher gas mass enhances the evaporation in this regions. On the other hand, when the volume fraction effects are included in the calculations, the volume displaced by the dispersed droplets causes a relatively higher gas entrainment into the core of the droplet-laden jet, hence paving the way for further evaporation in the dense regions.

In order to investigate the volumetric effect of the liquid phase on the FMDF predictions, simulations are carried out with the liquid volume effect in the LES-FD part of the hybrid LES/FMDF included, but ignored in the FMDF equation. Figures 4.6 and 4.7 compare the temperatures and evaporated fuel mass fractions obtained from FD and MC data with and without liquid volume effect in the FMDF equation. It is clear that although the overall agreement between the FD and MC data is good for both cases, the correlation between FD and MC is slightly better when the liquid volume effect is included in the FMDF equation. It should be noted, however, that more significant difference between FD and MC data is expected for higher liquid volume areas. The FMDF should correctly represent the gas mass temperature and species mass fractions in the moderately dense droplet laden flows. With the liquid volume fraction included, the FMDF correctly captures the gas variables at all locations and times in the simulated droplet-laden jet even with high mass and liquid volume loading.



(a) $x/D_{jet} = 12$

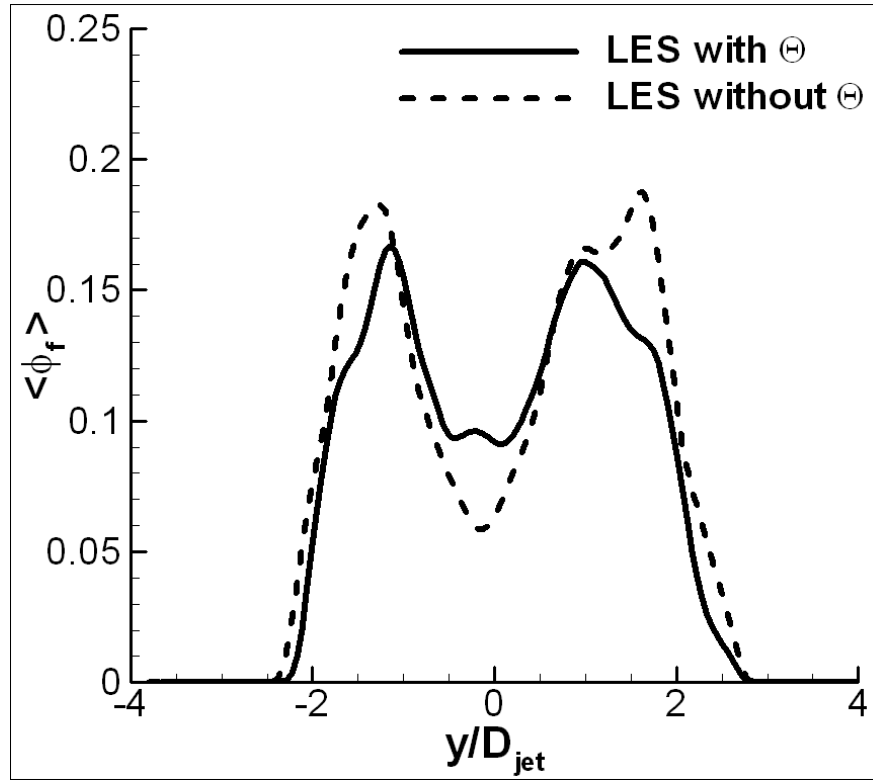


(b) $x/D_{jet} = 14$

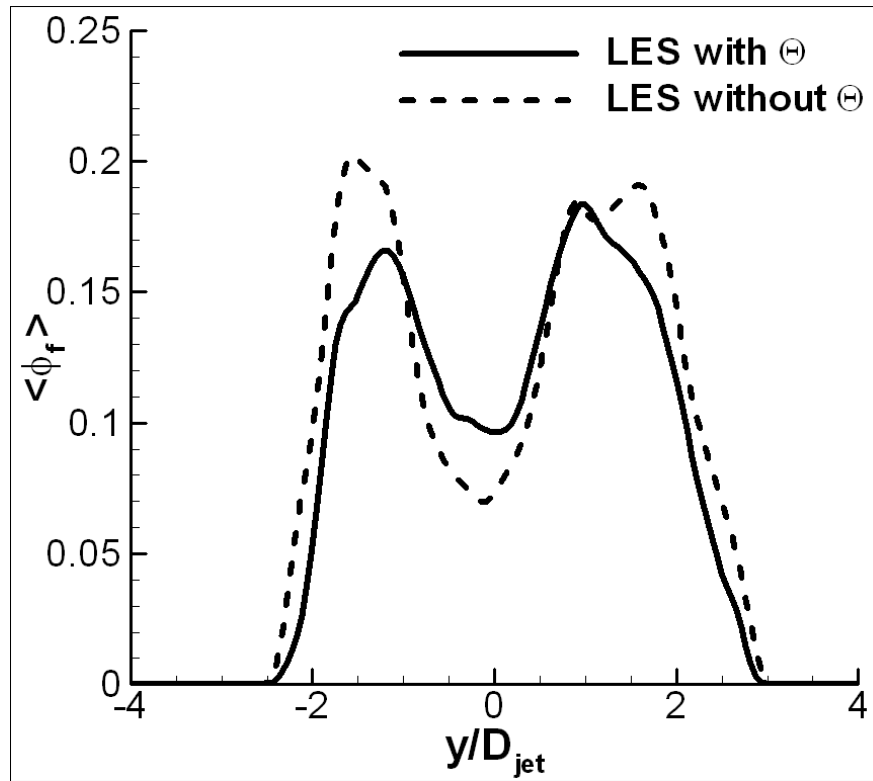
Figure 4.5: Mean evaporated fuel mass fractions predicted by LES with and without liquid volume fraction at different axial locations.

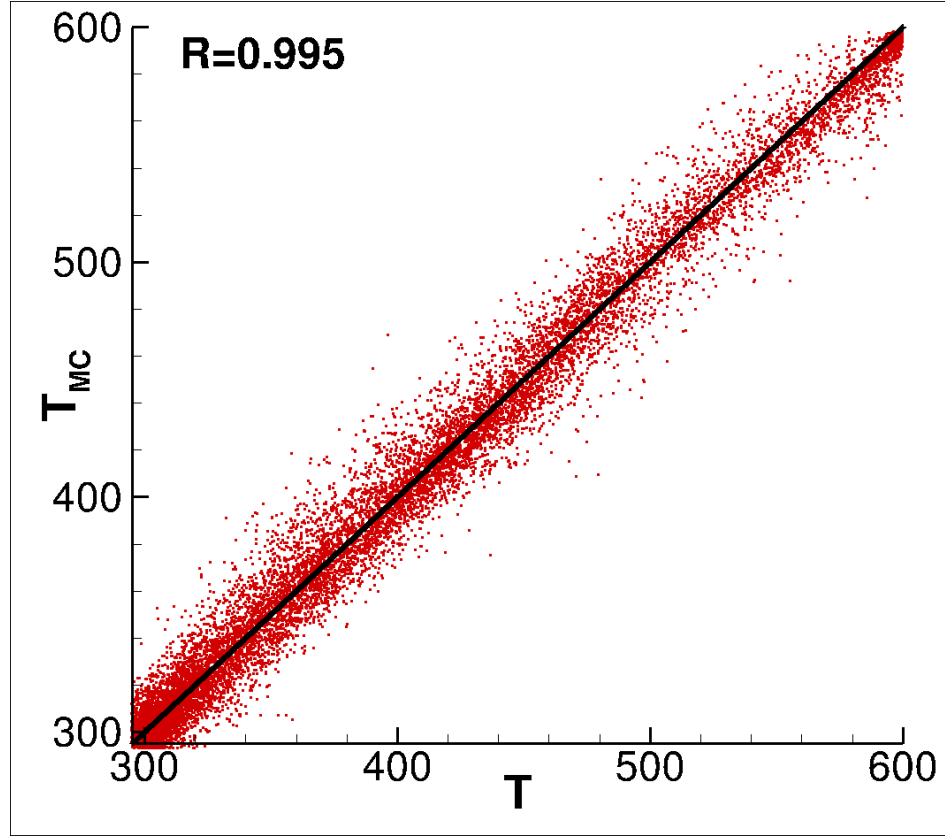
Figure 4.5: (cont'd)

(c) $x/D_{jet} = 16$



(d) $x/D_{jet} = 18$



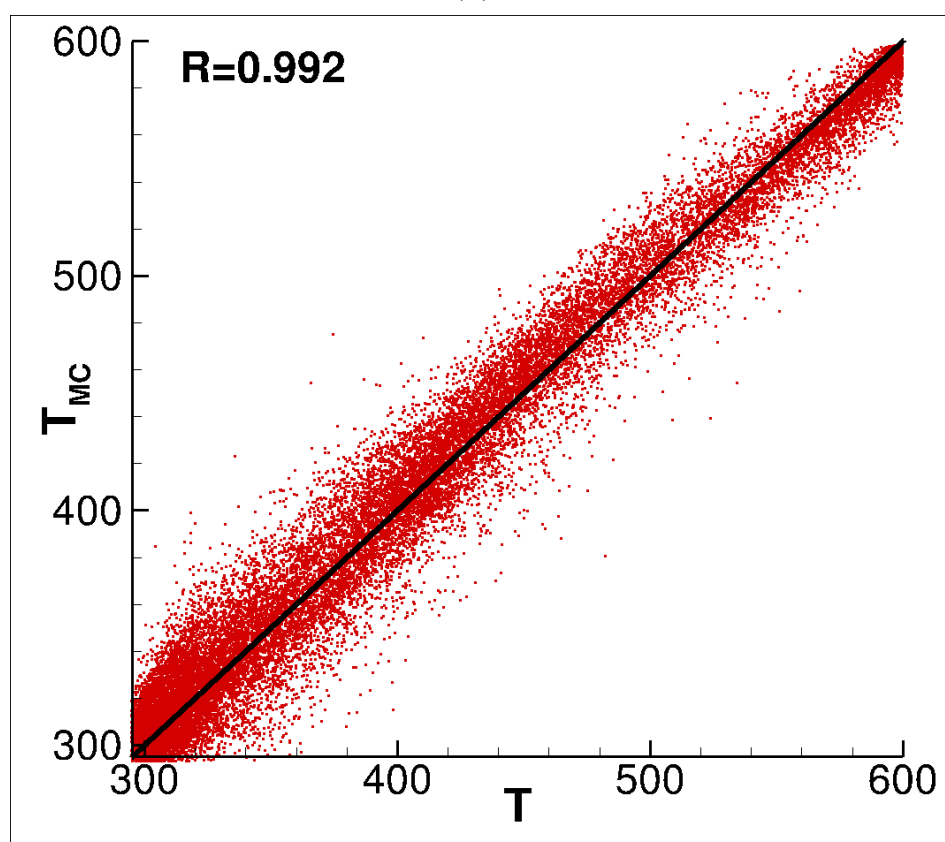


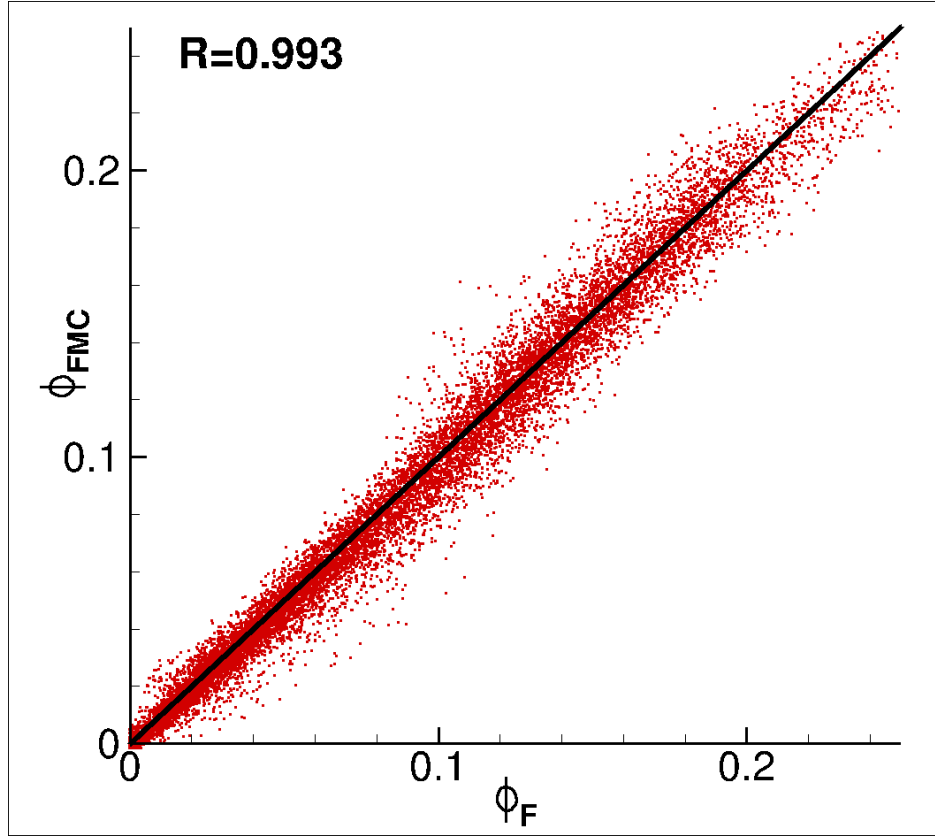
(a)

Figure 4.6: Gas temperatures obtained from the finite difference (FD) and Monte Carlo (MC) parts of the hybrid LES/FMDF model in the planar jet, (a) with liquid volume fraction effect in the FMDF and (b) without volume fraction effect in the FMDF.

Figure 4.6: (cont'd)

(b)



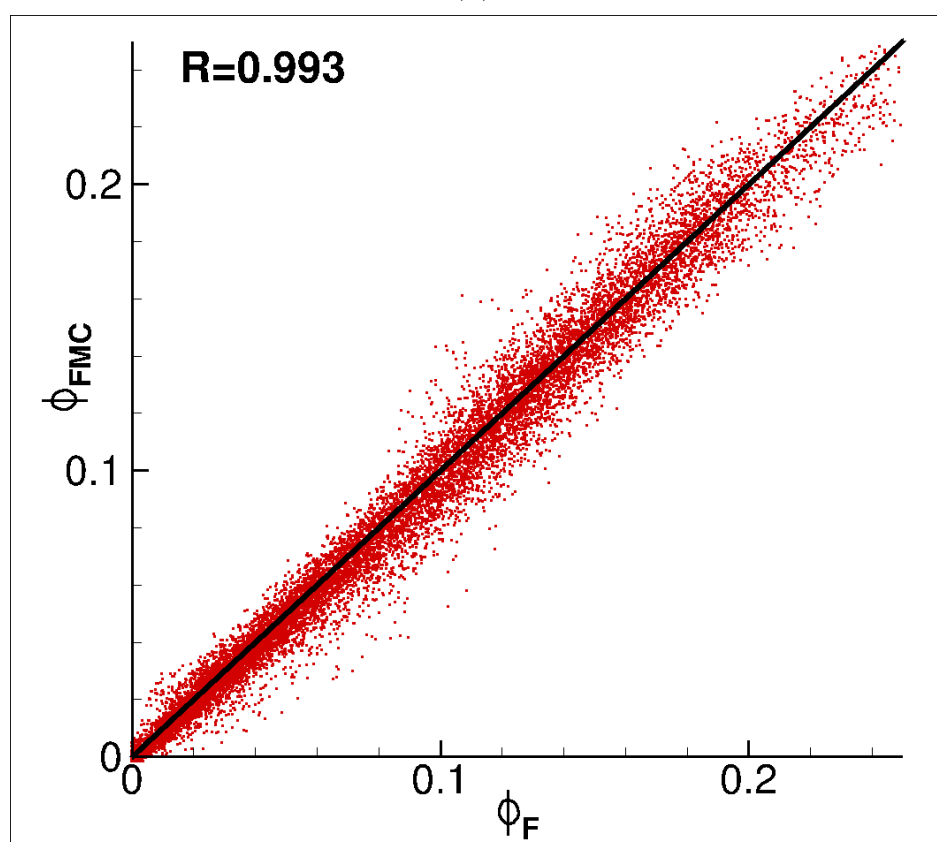


(a)

Figure 4.7: Evaporated fuel mass fractions obtained from the finite difference (FD) and Monte Carlo (MC) parts of the hybrid LES/FMDF model in the planar jet, (a) with liquid volume fraction effect in the FMDF and (b) without volume fraction effect in the FMDF.

Figure 4.7: (cont'd)

(b)



4.4 Summary and Conclusions

The Eulerian-Lagrangian LES model is used together with the two-phase FMDF model for moderately dense droplet laden turbulent flows. This is accomplished by introducing the fluid volume fraction into the Eulerian carrier gas LES equations and also into the stochastic Lagrangian FMDF model. The two-way interactions between gas and liquid phases and the Eulerian and Lagrangian fields are included in the new two-phase LES/FMDF formulation. A moderately dense, droplet-laden, planar jet is simulated to study the liquid volume fraction effects. In these simulations, the carrier gas jet is perturbed with an isotropic turbulence at the jet inflow. Both single-phase and two-phase flow simulations are considered. The two-phase simulations are conducted with and without liquid volume fractions. The LES results for the moderately dense droplet-laden planar jet indicate that the neglect of the volume fraction of the liquid phase will lead to excessive evaporation and turbulence modulation. This is because the available gas mass in the shear zones will be higher than it really should be, causing higher evaporation in these regions. On the other hand, when volume fraction effects are included, the volume displaced by the dispersed droplets leads to relatively higher gas entrainment into the core of the droplet-laden jet. It is also shown that for the LES/FMDF results to be consistent, it is necessary to include the volume fraction effect into the FMDF formulation as the FMDF represent the gas mass in the domain and not in the liquid phase.

BIBLIOGRAPHY

BIBLIOGRAPHY

- [1] Plich, M., Erdman, C.A., 1987. Use of breakup time data and velocity history data to predict the maximum size of stable fragments for accelartion induced breakup of a liquid drop, *Int. J. of Multiphase Flow* 13, 741-757.
- [2] Gel'fand, B. E., 1996. Droplet breakup phenomena in flows with velocity lag, *Prog. Energy Combust. Sci.* 22, 201-265.
- [3] Liu, Z., Reitz, R. D., 1997. An analysis of the distortion and breakup mechanisms of high speed liquid drops, *Int. J. Multiphase Flow* 23,6-31.
- [4] Lee, C. H., Reitz, R. D., 2000. An experimental study of the effect of gas density on the distortion and breakup mechanism of drops in high speed gas stream, *Int. J. Multiphase Flow* 26, 229.
- [5] Guildenbecher, D. R., López-Rivera, C., Sojka, P. E., 2009. Secondary atomization. *Exp. Fluids* 46, 371-402.
- [6] Jiang, X., Siamas, G. A., Jagus, K., Karayiannis, T. G., 2010. Physical modeling and advanced simulations of gas-liquid two-phase jet flows in atomization and sprays. *Prog. Energy Combust. Sci.* 36, 131-167.
- [7] Chryssakis, C.A., Assanis, D. N., Tanner, F. X., 2011. Atomization Models, in Ashgriz, N. (Ed.). *Handbook of atomization and sprays: theory and applications*. Springer.
- [8] Reitz, R. D., 1987. Modeling atomization processes in high pressure vaporizing sprays. *Atom. Spray Tech.* 3, 309-337.
- [9] O'Rourke, P. J., Amsden, A. A., 1987. The TAB method for numerical calculations of spray droplet breakup, No. LA-UR-87-2105-Rev.; CONF-871142-1-Rev. Los Alamos National Lab., NM.
- [10] Lasheras, J. C., Eastwood, C., Martinez-Bazan, C., Montanes, J. L., 2002. A review of statiscal models for the breakup of an immiscible fluid immeresd into a fully developed turbulent flow, *Int. J. Multiphase Flow* 28, 247-278.
- [11] Gorokhovski, M. A., Saveliev, V. L., 2003. Analyses of Kolmogorov's model of breakup and its application into Lagrangian computation of liquid sprays under air-blast atomization. *Phys. Fluids* 15, 184-192.
- [12] Apte, S. V., Gorokhovski, M., Moin, P., 2003. LES of atomizing spray with stochastic modeling of secondary breakup, *Int. J. of Multiphase Flow* 29, 1503-1522.

- [13] Liu, H. F., Gong, X., Li, W. F., Wang, F. C., Yu, Z. H., 2006. Prediction of droplet size distribution in sprays of prefilming air-blast atomizers. *Chem. Eng. Sci.* 61, 1741-1747.
- [14] Jones, W. P., Lettieri, C., 2010. Large eddy Simulation of spray atomization with stochastic modeling of breakup, *Phys. Fluids* 15, 115106.
- [15] Kolmogorov, A. N., 1941. On the log-normal distribution of particle sizes during breakup process, *Dokl. Akad. Nauk. SSSR*, 31, 99.
- [16] Shavit, U., Chigier, N. J., 1995. Fractal dimensions of liquid jet interface under breakup, *Atom. Sprays* 5, 525-543.
- [17] Zhou, W. X., Yu. Z. H., 2000. Multifractality of drop breakup in the air-blast nozzle atomization process. *Phys. Rev. E* 63, 016302.
- [18] Andersson, R., Andersson, B., 2006. On the breakup of fluid particles in turbulent flows. *AIChE J.* 2, 2020–2030.
- [19] Zacccone, A., Gäbler, A., Maaß, S., Marchisio, D., Kraume, M., 2007. Drop breakage in liquid–liquid stirred dispersions: modelling of single drop breakage. *Chem. Eng. Sci.* 62, 6297-6307.
- [20] Dukowicz, J. K., 1980. A particle-fluid numerical model for liquid sprays, *J. Comput. Phys.* 35, 229-253.
- [21] Gorokhovski, M., Herrmann, M., 2008. Modeling primary atomization. *Annu. Rev. Fluid Mech.* 40, 343-366.
- [22] Shen, L., Yue, D., 2001. Large-Eddy Simulation of Free-Surface Turbulence, *J. Fluid Mech.* 440, 75-116.
- [23] Li, Z., Jaber, F. A., 2009. Turbulence-interface interactions in a two-fluid homogeneous flow, *Phys. Fluids* 21, 095102.
- [24] Herrmann, M., 2010. A parallel Eulerian interface tracking/Lagrangian point particle multi-scale coupling procedure. *J. Comput. Phys.* 229, 745-759.
- [25] Moin, P., Apte, S. V., 2006. Large-eddy simulation of realistic gas turbine combustors. *AIAA J* 44, 698-708.
- [26] Kastengren, A., Tilocco, F. Z., Powell, C. F., Manin, J., Pickett, L. M., Payri, R., Bazyn, T., 2012. Engine Combustion Network (ECN): Measurements of Nozzle Geometry and Hydraulic behaviour. *Atom. Sprays* 22, 1011-1052.
- [27] Beale, J. C., Reitz, R. D., 1999. Modeling spray atomization with the Kelvin-Helmholtz/Rayleigh-Taylor hybrid model. *Atom. Sprays* 9, 623-650.
- [28] Yi, Y., Reitz, R. D., 2004. Modeling the primary breakup of high-speed jets. *Atom. Sprays* 14, 53-79.
- [29] Arcoumanis, C., Gavaises, M., 1998. Linking nozzle flow with spray characteristics in a diesel fuel injection system. *Atom. Sprays* 8, 307-347.

- [30] Schmidt, D. P., Chiappetta, L. M., Goldin, G. M., Madabhushi, R. K., 2003. Transient multidimensional modeling of air-blast atomizers. *Atom. Sprays* 13, 373-394.
- [31] Shotorban, B., Mashayek, F., 2005. Modeling sub-grid-scale effects on particles by approximate deconvolution, *Phys. Fluids* 17, 081701.
- [32] Almeida, T. G., Jaber, F. A., 2008. Large eddy simulation of a dispersed particle-laden turbulent round jet, *Int. J. Heat Mass Transfer* 51, 683-695.
- [33] Pozorski, J., Apte, S. V., 2009. Filtered particle tracking in isotropic turbulence and stochastic modeling of subgrid-scale dispersion, *Int. J. of Multiphase Flow* 35, 118-28.
- [34] Eaton, J. K., 2009. Two-way coupled turbulence simulations of gas-particle flows using point-particle tracking, *Int. J. of Multiphase Flow* 35, 792-800.
- [35] Balachandar, S., Eaton, J. K., 2010. Turbulent dispersed multiphase flow, *Ann. Rev. Fluid Mech.* 42, 111-133.
- [36] Patel, N., Menon, S., 2008. Simulation of spray-turbulence-flame interactions in a lean direct injection combustor. *Combust. Flame* 153, 228-257.
- [37] Bharadwaj, N., Rutland, C. J., Chang, S. M., 2009. Large eddy simulation modeling of spray-induced turbulence effects. *Int. J. Engine Research* 10, 97-119.
- [38] Tsuji, Y., Morikawa, Y., Terashima, K., 1982. Fluid dynamic interaction between two spheres, *Int. J. of Multiphase Flow* 8, 71-82.
- [39] Poo, J. Y., Ashgriz, N. "Variation of Drag Coefficients in an Interacting Drop Stream", *Experiments In Fluids*, 11, 1-8, 1991.
- [40] Prahl, L., Jadoon, A., Revstedt, J., 2009. Interaction between two spheres placed in tandem arrangement in steady and pulsating flow, *Int. J. Multiphase Flow* 35, 963-969.
- [41] Silverman, I., Sirignano, W. A. , 1994. Multi-droplet interaction effects in dense sprays, *Int. J. of Multiphase Flow* 20, 99-116.
- [42] Miller, R. S., Harstad, K., Bellan, J., 1998. Evaluation of equilibrium and non-equilibrium evaporation models for many-droplet gas-liquid flow simulations. *Int. J. Multiphase Flow* 24, 1025-1055.
- [43] Sazhin, S. S., 2006. Advanced models of fuel droplet heating and evaporation, *Prog. Energy Combust. Sci.* 32, 162-214.
- [44] Sirignano, W. A., 2010. Fluid dynamics and transport of droplets and sprays. Cambridge University Press.
- [45] Torres, D. J., O'Rourke, P. J., Amsden, A. A., 2003. Efficient multicomponent fuel algorithm, *Combust. Theory Modeling* 7, 67-86.

- [46] Crowe, C., Sommerfeld, M., Tsuji, Y., 1998. Multiphase flows with droplets and particles, CRC Press, Boca Raton, FL.
- [47] Loth, E., 2000. Numerical approaches for motion of dispersed particles, droplets and bubbles, *Prog. Energy Combust. Sci.* 26, 161-223.
- [48] Bellan, J., Harstad, K., 1987. The details of the convective evaporation of dense and dilute clusters of drops, *Int. J. Heat Mass Transfer* 30, 1083-1093.
- [49] Clift, R., Gauvin, W.H., 1970. The motion of particles in turbulent gas streams, *Proc. Chemeca'70*, 1,14.
- [50] Liu, A. B., Mather, D., Reitz, R. D., 1993. Modeling the effects of drop drag and breakup on fuel sprays, SAE Tech. Paper, 930072.
- [51] Gardiner, C.W., 1990. Handbook of stochastic methods for physics chemistry and the natural sciences, corrected 2nd edition, Springer-Verlag, Berlin.
- [52] Kim, S., Lee, D. J., Lee, C. S., 2009. Modeling of binary droplet collisions for application to inter-impingement sprays, *Int. J. Multiphase Flow* 35, 533-549.
- [53] Munnannur, A., Reitz, R. D., 2007. A new predictive model for fragmenting and non-fragmenting binary droplet collisions. *Int. J. Multiphase Flow* 33, 873-896.
- [54] Abramzon, B., Sirignano, W. A., 1989. Droplet vaporization model for spray combustion calculations, *Int. J. Heat Mass Transfer* 32, 1605-1618.
- [55] Wu, J. S., Faeth, G. M., 1993. Sphere wakes in still surroundings at intermediate Reynolds numbers. *AIAA J.* 31, 1448.
- [56] Gorokhovski, M. A., Saveliev, V. L., 2008. Statistical universalities in fragmentation under scaling symmetry with a constant frequency of fragmentation, *J. Phys. D: Appl. Phys.* 41, 085405.
- [57] Afshari, A., Jaber, F. A., Shih, T. I. P., 2008. Large-eddy simulations of turbulent flows in an axisymmetric dump combustor, *AIAA J.* 46, 1576-1592.
- [58] Banaeizadeh, A., Afshari, A., Schock, H., Jaber, F., 2013. Large eddy simulations of turbulent flows in internal combustion engines, *Int. J. Heat Mass Transfer* 60, 781-796.
- [59] Visbal, M. R., Gaitonde, D. V., 2000. Pade-type high-order boundary filters for the Navier-Stokes equations, *AIAA J.* 38, 2103-2112.
- [60] Moin, P., Squires, K., Cabot, W., Lee, S., 1991. A dynamic subgrid scale model for compressible turbulence and scalar transport, *Phys. Fluids A* 3, 2746-2757.
- [61] Ghosal, S., Lund, T. S., Moin, P., Akselvoll, K., 1995. A dynamic localization model for large-eddy simulation of turbulent flows, *J. Fluid Mech.* 286, 229-255.

- [62] Yoshizawa, A., Horiuti, K. , 1985. A statistically-derived subgrid-scale kinetic energy model for the large eddy simulation of Tturbulent flows, J. Phys. Soc. Japan 54, 2834-283.
- [63] Germano, M., Piomelli, U., Moin, P., Cabot, W. H., 1991. A dyanamic subgrid-scale eddy viscosity model, Phys. Fluids A, 3, 1760-1765.
- [64] Lilly, D.K., 1992. A proposed modification of the Germano subgrid scale closure method, Phys. Fluids A 4, 633-635.
- [65] Mashayek, F., 1998. Droplet-turbulence interactions in low Mach number homogenous shear two phase flows, J. Fluid Mech. 367, 163-203.
- [66] Hiroyasu, M., Kadota, T. “Fuel Droplet Size Distrubution in Diesel Combustion Chamber.” SAE Paper 74071, 1974.
- [67] Tanner, F.X., 1998. Liquid jet atomization and droplet breakup modeling of non-evaporating diesel fuel sprays. SAE Trans.: J. Engines 106, 127–140.
- [68] Faeth, G. M., Hsiang, L. P., Wu, P. K., 1995. Structure and breakup properties of sprays. Int. J. of Multiphase Flow 21, 99-127.
- [69] Siebers, D.L., 1998. Liquid phase fuel penetration in diesel sprays, SAE Tec. Paper, 980809.
- [70] Siebers, D.L., 1999. Scaling liquid-phase fuel penetration in diesel sprays based on mixing-limited vaporization, SAE Tec. Paper 1999-01-0528.
- [71] Poling, B. E., Prausnitz, J. M., O’Connell, J. P., 2001. The properties of gases and liquids, 5th Edition, NY: McGraw-Hill.
- [72] Kim, H., Sung, N., 2003. The effect of ambient pressure on the evaporation of a single droplet and a spray, Combust. Flame 135, 261-270.
- [73] Segal, C., Polikhov, S. A., 2008. Subcritical to supercritical mixing, Phys. Fluids 20, 052101.
- [74] Poo, J. Y., Ashgriz, N., 1991. Variation of drag Coefficients in an interacting drop stream, Exp. Fluids, 11, 1-8.
- [75] Qian, J., Law, C.K., 1997. Regimes of coalescence and Separation in droplet collision, J. Fluid Mech. 331, 59-80.
- [76] Srivastava, S., Schock, H., Jaber, F., 2013. Numerical Simulations of Turbulent Sprays with a Multicomponent evaporation Model, SAE Tech. Paper 2013-01-1603.
- [77] Prosperetti, A., Tryggvason, G. (Eds.), 2007. Computational methods for multiphase flow. Cambridge University Press.
- [78] Subramaniam, S., 2013. Lagrangian–Eulerian methods for multiphase flows, Prog. Energy Combust. Sci. 39, 215-245.

- [79] Hetsroni, G., 1989. Particles-turbulence interaction. *Int. J. Multiphase Flow* 15, 735-746.
- [80] Elghobashi, S., Truesdell, G. C., 1993. On the two-way interaction between homogeneous turbulence and dispersed solid particles. I: Turbulence modification. *Physics of Fluids A: Fluid Dynamics*, 5, 1790.
- [81] Mashayek, F., Pandya, R.V.R., 2003. Analytical Description Particle/Droplet-laden Turbulent Flows. *Prog. Energy Combust. Sci.* 29, 329-378.
- [82] Crowe, C. T., 2000. On models for turbulence modulation in fluid-particle flows. *Int. J. Multiphase Flow* 26, 719-727.
- [83] Eaton, J. K., 2006. Turbulence modulation by particles. In *Multiphase Flow Handbook*, ed. CT Crowe, Boca Raton, FL: Taylor and Francis, 86-98.
- [84] Chen, J. H., Wu, J. S., Faeth, G. M., 2000. Turbulence generation in homogeneous particle-laden flows. *AIAA J.* 38, 636-642.
- [85] Fox, R. O., 2012. Large-eddy-simulation tools for multiphase flows. *Annu. Rev. Fluid Mech.* 44, 47-76.
- [86] Miller, R. S. Bellan, J., 1999. Direct numerical simulation of a confined three-dimensional gas mixing layer with one evaporating hydrocarbon-droplet-laden stream. *J. Fluid Mech.* 384, 293-338.
- [87] Okong'o, N., Bellan, J., 2004. Consistent large-eddy simulation of a temporal mixing layer laden with evaporating drops. Part 1. Direct numerical simulation, formulation and a priori analysis, *J. Fluid Mech.* 499, 1-47.
- [88] Leboissetier, A., Okong'o, N., Bellan, J., 2005. Consistent large-eddy simulation of a temporal mixing layer laden with evaporating drops. Part 2. A posteriori modelling, *J. Fluid Mech.* 523, 37-78.
- [89] Bini, M., Jones, W. P., 2009. Large eddy simulation of an evaporating acetone spray. *Int. J. Heat and Fluid Flow*, 30, 471-480.
- [90] Pickett, L. M., Genzale, C. L., Bruneaux, G., Malbec, L. M., Hermant, L., Christiansen, C., Schramm, J., 2010. Comparison of diesel spray combustion in different high-temperature, high-pressure facilities, *SAE Technical Paper*, 01-2106.
- [91] Bardi, M., Payri, R., Malbec, L. M., Bruneaux, G., Pickett, L. M., Manin, J., Bazyn, T., Genzale, C., 2012. ENGINE COMBUSTION NETWORK: Comparison of Spray Development, vaporization, and Combustion in Different Combustion Vessels. *Atom. Sprays*, 22, 807-842.
- [92] Naber, J. Siebers, D., 1996. Effects of Gas Density and vaporization on Penetration and Dispersion of Diesel Sprays, *SAE Technical Paper* 960034.

- [93] Kamimoto, T., Yokota, H., and Kobayashi, H., 1987. Effect of high pressure injection on soot formation processes in a rapid compression machine to simulate diesel flames (No. CONF-8709177-). SAE, Warrendale, PA.
- [94] Aggarwal, S. K., 1998. A review of spray ignition phenomena: present status and future research. *Prog. Energy Combust. Sci.* 24, 565-600.
- [95] Venugopal, R., Abraham, J., 2007. A review of fundamental studies relevant to flame lift-off in diesel jets. SAE Tec. paper, 01-0134.
- [96] Mastorakos, E., 2009. Ignition of turbulent non-premixed flames. *Prog. Energy Combust. Sci.* 35, 57-97.
- [97] Borghesi, G., Mastorakos, E., Cant, R. S., 2013. Complex chemistry DNS of n-heptane spray autoignition at high pressure and intermediate temperature conditions. *Combust. Flame* 160, 1254-1275.
- [98] Pitsch, H., 2006. Large-eddy simulation of turbulent combustion. *Annu. Rev. Fluid Mech.* 38, 453-482.
- [99] Haworth, D. C., 2010. Progress in probability density function methods for turbulent reacting flows. *Prog. Energy Combust. Sci.* 36, 168-259.
- [101] Jenny, P., Roekaerts, D., Beishuizen, N., 2012. Modeling of turbulent dilute spray combustion. *Prog. Energy Combustion Sci.* 38, 846-887.
- [101] Haworth, D.C., Pope, S.B., in Echehki, T., Mastorakos, E. (Eds.), 2011. *Turbulent Combustion Modeling: Advances, New Trends and Perspectives*, Springer, Dordrecht, 119-142.
- [102] Jones, W. P., Lira, S., Navarro-Martinez, S., 2012. Numerical investigation of swirling kerosene spray flames using Large Eddy Simulation, *Combust. Flame* 159, 1539-1561.
- [103] Prasad, V. N., Masri, A. R., Navarro-Martinez, S., Luo, K. H., 2013. Investigation of auto-ignition in turbulent methanol spray flames using Large Eddy Simulation. *Combust. Flame* 160, 2941-2954.
- [104] Pei, Y., Hawkes, E. R., Kook, S., 2013. A Comprehensive Study of Effects of Mixing and Chemical Kinetic Models on Predictions of n-heptane Jet Ignitions with the PDF Method. *Flow, Turbul. Combust.*, 1-32.
- [105] Jaber, F. A., Colucci, P. J., James, S., Givi, P., Pope, S. B., 1999. Filtered Mass Density Function for Large Eddy Simulation of Turbulent Reacting Flows, *J. Fluid Mech.* 401, 85-121.
- [106] James, S., Jaber, F. A., 2000. Large Scale Simulations of Two-Dimensional Nonpremixed Methane Jet Flames, *Combust. Flame* 123, 465-487.
- [107] Sheikhi, M. R. H., Drozda, T. G., Givi, P., Jaber, F. A., Pope, S. B., 2005. Large Eddy Simulation of a Turbulent Nonpremixed Piloted Methane Jet Flame, *Proc. Combust. Inst.* 30, 549-556.

- [108] Givi, P., 2006. Filtered density function for subgrid scale modeling of turbulent combustion. *AIAA J* 44, 16-23.
- [109] Raman, V., Pitsch, H., 2006. A Consistent LES/Filtered-Density Function Formulation for the Simulation of Turbulent Flames with Detailed Chemistry,” *Proc. Combust. Inst.* 31, 1711-1719.
- [110] Yaldizli, M., Mehravaran, K., Jaber, F.A., 2010. Large-Eddy Simulations of Turbulent Methane Jet Flames with Filtered Mass Density Function, *Int. J. Heat Mass Transfer* 53, 2551-2562.
- [111] Li, Z., Banaeizadeh, A. Jaber, F. A., 2013. Two-phase filtered mass density function for LES of turbulent reacting flows, *J. Fluid Mech.*, in review.
- [112] Lu, T., Law, C. K., 2009. Toward accommodating realistic fuel chemistry in large-scale computations. *Prog. Energy Combust. Sci.* 35, 192-215.
- [113] Battin-Leclerc, F., 2008. Detailed chemical kinetic models for the low-temperature combustion of hydrocarbons with application to gasoline and diesel fuel surrogates. *Prog. Energy Combust. Sci.* 34, 440-498.
- [114] Seiser, R., Pitsch, H., Seshadri, K., Pitz, W. J., Gurran, H. J., 2000. Extinction and autoignition of n-heptane in counterflow configuration. *Proc. Combust. Inst.* 28, 2029-2037.
- [115] Liu, S., Hewson, J. C., Chen, J. H., Pitsch, H., 2004. Effects of strain rate on high-pressure nonpremixed n-heptane autoignition in counterflow. *Combust. flame*, 137, 320-339.
- [116] Yoo, C. S., Lu, T., Chen, J. H., Law, C. K., 2011. Direct numerical simulations of ignition of a lean n-heptane/air mixture with temperature inhomogeneities at constant volume: Parametric study. *Combust. Flame* 158, 1727-1741.
- [117] Pope, S. B., Ren, Z., 2009. Efficient implementation of chemistry in computational combustion. *Flow, turbulence and combustion* 82, 437-453.
- [118] Chen, J. Y., Kollmann, W., Dibble, R. W. 1989. Pdf modeling of turbulent nonpremixed methane jet flames. *Combust. Sci. Tech.* 64, 315-346.
- [119] Turanyi, T. 1994. Parameterization of reaction mechanisms using orthonormal polynomials. *J. Comput. Chem.* 18, 45-54.
- [120] Christo, F. C., Masri, A. R., Nebot, E. M. 1996. Artificial neural network implementation of chemistry with pdf simulation of H₂/CO₂ flames. *Combust. Flame* 106, 406-427.
- [121] Blasco, J. A., Fueyo, N., Dopazo, C., Ballester, J. 1998. Modelling the temporal evolution of a reduced combustion chemical system with an artificial neural network. *Combust. Flame* 113, 38-52.

- [122] Pope S. B., 1997. Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation. *Combust. Theory Modelling* 1, 41–63.
- [123] Lu, L., Pope, S. B., 2009. An improved algorithm for in situ adaptive tabulation, *J. Comput. Phys.* 228, 361-386.
- [124] Bell, J. B., Brown, N. J., Day, M. S., Frenklach, M., Grcar, J. F., Propp, R. M., Tonse, S. R. 2000. Scaling and efficiency of PRISM in adaptive simulations of turbulent premixed flames. *Proc. Combust. Inst.* 28, 107-113.
- [125] Rabitz, H., Alis, O. F. 1999. General foundations of high dimensional model representations. *J. Mathematical Chemistry* 25, 197-233.
- [126] Cao, R. R., Pope, S. B., 2005. The influence of chemical mechanisms on PDF calculations of nonpremixed piloted jet flames. *Combust. Flame* 143, 450-470.
- [127] Embouazza, M., Haworth, D.C., Darabiha, N., 2002. Implementation of detailed chemical mechanisms into multidimensional CFD using in situ adaptive tabulation: application to HCCI engines, *SAE Tec. Paper* 2002-01-2773.
- [128] Lu, L., Lantz, S. R., Ren, Z., Pope, S. B., 2009. Computationally efficient implementation of combustion chemistry in parallel PDF calculations, *J. Comput. Phys.* 228, 5490-5525.
- [129] Hiremath, V., Lantz, S. R., Wang, H., Pope, S. B., 2012. Computationally-efficient and scalable parallel implementation of chemistry in simulations of turbulent combustion, *Combust. Flame* 159, 3096-3109.
- [130] Siebers, D.L., Higgins, B.S., 2001. Flame lift-off on direct-injection diesel sprays under quiescent conditions, *SAE Paper* 2001-01-0530.
- [131] Siebers, D.L., Higgins, B.S., Pickett, L.M., 2002. Flame lift-off on direct injection diesel fuel jets: Oxygen concentration effects. *SAE Paper* 2002-01-0890
- [132] Bhattacharjee, S., Haworth, D. C., 2013. Simulations of transient n-heptane and n-dodecane spray flames under engine-relevant conditions using a transported PDF method. *Combust. Flame* 160, 2083-2102.
- [133] Colucci, P. J., Jaber, F. A., Givi, P., Pope, S. B., 1998. Filtered density function for large eddy simulation of turbulent reacting flows. *Phys. Fluids* 10, 499-515.
- [134] Banaeizadeh, A., Li, Z., Jaber, F. A., 2011. Compressible Scalar Filtered Mass Density Function Model for High-Speed Turbulent Flows, *AIAA J.* 49, 2130-2143.
- [135] Dopazo, C., O'Brien, E. E., 1976. Statistical treatment of non-isothermal chemical reactions in turbulence. *Combust. Sci. Tech.* 13, 99-122.

- [136] O'Brien, E. E., 1980. The probability density function (PDF) approach to reacting turbulent flows. In *Turbulent Reacting Flows* (pp. 185-218). Springer Berlin Heidelberg.
- [137] Borghi, R., 1988. Turbulent combustion modelling. *Prog. Energy Combust. Sci.* 14, 245-292.
- [138] Pope, S. B., 1985. PDF Methods for Turbulent Reactive Flows, *Prog. Energy Combust. Sci.* 11, 119-192.
- [139] Kloeden, P. E., Platen, E., 1995. *Numerical Solution of Stochastic Differential Equations, Applications of Mathematics, Stochastic Modeling and Applied Probability*, Vol. 23, Springer-Verlag, New York, NY.
- [140] Caracotsios, M., Stewart, W. E. 1985. Sensitivity analysis of initial value problems with mixed ODEs and algebraic equations. *Comput. Chem. Eng.* 9, 359-365.
- [141] Pickett, L., 2012. Engine Combustion Network. <http://www.sandia.gov/ecn/>.
- [142] Pei, Y., Hawkes, E. R., Kook, S., 2012. Transported probability density function modelling of the vapour phase of an n-heptane jet at diesel engine conditions. *Proc. Combust. Inst.* 34, 3039-3047.
- [143] Curran, H. J., Gaffuri, P., Pitz, W. J., Westbrook, C. K., 1998. A comprehensive modeling study of n-heptane oxidation. *Combust. Flame* 114, 149-177.
- [144] Mehl, M., Pitz, W. J., Westbrook, C. K., Curran, H. J., 2011. Kinetic modeling of gasoline surrogate components and mixtures under engine conditions. *Proc. Combust. Inst.* 33, 193-200.
- [145] Patel, A., Kong, S., Reitz, R., 2004. Development and Validation of a Reduced Reaction Mechanism for HCCI Engine Simulations, SAE Tec. Paper 2004-01-0558.
- [146] Chiu, H. H., Liu, T. M., 1977. Group combustion of liquid droplets, *Combust. Sci. Tech.* 17, 127-142.
- [147] Sato, J. I., Konishi, K., Okada, H., Niioka, T. 1988. Ignition process of fuel spray injected into high pressure high temperature atmosphere. *Symposium (International) on Combustion* 21, 695-702.
- [148] Edwards, C., Siebers, D., Hoskin, D., 1992. A Study of the Autoignition Process of a Diesel Spray via High Speed Visualization, SAE Tec. Paper 920108.
- [149] Pickett, L., Siebers, D., Idicheria, C., 2005. Relationship Between Ignition Processes and the Lift-Off Length of Diesel Fuel Jets, SAE Tech. Paper 2005-01-3843.
- [150] Westbrook, C. K., Dryer, F. L., 1981. Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames. *Combust. Sci. Tech.* 27, 31-43.

- [151] Dec, J. E., 2009. Advanced compression-ignition engines—understanding the in-cylinder processes. *Proc. Combust. Inst.* 32, 2727-2742.
- [152] Dec, J. E., 1997. A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet Imaging, SAE Tec. Paper 970873.
- [153] Flynn, P., Durrett, R., Hunter, G., zur Loye, A. et al., 1999. Diesel Combustion: An Integrated View Combining Laser Diagnostics, Chemical Kinetics, And Empirical Validation, SAE Tech. Paper 1999-01-0509
- [154] Irannejad, A., Jaber, F., Large Eddy Simulation of Spray Mixing and Combustion with Two-Phase Filtered Mass Density Function, 43rd AIAA Fluid Dynamics Conf., AIAA-2013-2599, 24-27 June 2013, San Diego, California.
- [155] Jaber, F. A., 1998. Temperature fluctuations in particle-laden homogeneous turbulent flows. *Int. J. Heat Mass Transfer* 41, 4081-4093.
- [156] Mashayek, F., 2000. Numerical investigation of reacting droplets in homogeneous shear turbulence, *J. Fluid Mech.* 405, 1–36.
- [157] Reade, W. C., Collins, L. R., 2000. Effect of preferential concentration on turbulent collision rates. *Phys. Fluids* 12, 2530.
- [158] Wang, L. P., Wexler, A. S., Zhou, Y., 2000. Statistical mechanical description and modelling of turbulent collision of inertial particles. *J. Fluid Mech.* 415, 117-153.
- [159] Yamamoto, Y., Potthoff, M., Tanaka, T., Kajishima, T., Tsuji, Y., 2001. Large-eddy simulation of turbulent gas-particle flow in a vertical channel: effect of considering inter-particle collisions, *J. Fluid Mech.* 442, 303-334.
- [160] Wang, L-P, Rosa, B., Gao, H., He, G., Jin, G., 2009. Turbulent Collision of Inertial Particles: Point-Particle Based, Hybrid Simulations and Beyond, *Int. J. Multiphase Flow* 35, 854-867.
- [161] Sirignano, W. A., 2005. Volume averaging for the analysis of turbulent spray flows. *Int. J. of Multiphase Flow* 31, 675-705.
- [162] Apte, S. V., Mahesh, K., Lundgren, T., 2008. Accounting for finite-size effects in simulations of disperse particle-laden flows. *Int. J. Multiphase Flow* 34, 260-271.
- [163] Capecelatro, J., Desjardins, O., 2012. An Euler-Lagrange strategy for simulating particle-laden flows. *J. Comput. Phys.* 238, 1-31.
- [164] Cihonski, A. J., Finn, J. R., Apte, S. V., 2013. Volume displacement effects during bubble entrainment in a travelling vortex ring, *J. Fluid Mech.* 721, 225-267.
- [165] Post, S. L., Abraham, J., 2002. Modeling the outcome of drop-drop collisions in Diesel sprays. *Int. J. Multiphase Flow* 28, 997-1019.

- [166] Bini, M., Jones, W. P., 2008. Large-eddy simulation of particle-laden turbulent flows. *J. Fluid Mech.*, 614, 207-252.
- [167] Jones, W. P., Lyra, S., Marquis, A. J., 2010. Large eddy simulation of evaporating kerosene and acetone sprays. *Int. J. Heat Mass Transfer* 53, 2491-2505.
- [168] De, S., Kim, S. H., 2013. Large eddy simulation of dilute reacting sprays: Droplet evaporation and scalar mixing. *Combust. Flame* 160, 2048–2066.
- [169] Tenneti, S., Garg, R., Subramaniam, S., 2011. Drag law for monodisperse gas–solid systems using particle-resolved direct numerical simulation of flow past fixed assemblies of spheres. *Int. J. Multiphase Flow* 37, 1072-1092.
- [170] Hinze, J., 1975. *Turbulence*, McGraw-Hill, New York
- [171] Pope, S. B., 2000. *Turbulent Flows*, Cambridge University Press, New York.
- [172] Bernard, P., Wallace, J., 2002. *Turbulent Flow*, John Wiley and Sons, Inc., Hoboken, NJ.
- [173] Hsiao, F. B., Huang, J. M., 1990. On the evolution of instabilities in the near field of a plane jet. *Phys. Fluids A* 2, 400-412.
- [174] Colucci, P., 1994. Linear stability analysis of density stratified parallel shear flows, in: *Proc. 32nd Aerospace Sci. Meeting and Exhibit*, AIAA-94-0011.
- [175] Rudy, D. H., Strikwerda, J. C., 1980. A nonreflecting outflow boundary condition for subsonic Navier-Stokes calculations. *J. Comput. Phys.* 36, 55-70.
- [176] Eaton, J. K., Fessler, J. R., 1994. Preferential concentration of particles by turbulence. *Int. J. Multiphase Flow* 20, 169-209.