RANS-FGM simulation of n-heptane spray flame in OpenFOAM

A new implementation of flamelet generated manifold to account for enthalpy loss with detailed reaction mechanisms

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Abstract

The efficient and clean combustion of liquid fuels is a fundamental requirement in the design of future energy systems. Simulation plays a more and more important role in the design of such burners. In this work the spray combustion simulation approach introduced by Ma (2016) is improved, and validated against the CORIA Jet Spray Flame database (Verdier et al., 2017). The database presents droplet temperatures measured by global rainbow refractometry technique, which gives a unique insight in the flame structure. The two phase flow is treated with an Eulerian-Lagrangian approach. Flamelet Generated Manifold (FGM) is used to model the gas phase combustion. The RANS equations are solved using final volume method, with standard $k - \epsilon$ turbulence modelling. The turbulence-chemistry interaction is addressed with assumed probability density function method. The spray cloud is modelled with the Lagrangian transport of droplets including heat and mass transfer. Ma (2016) developed a solver based on the OpenFOAM 2.3.x libraries. His development is complemented in this work with a novel spray model. The improved spray modelling allows the treatment of droplet evaporation in the context of FGM without limiting the complexity of the chemical mechanism. This enhancement is crucial for the modelling of complex fuels and the correct prediction of emissions. The modelling concept is rather light-weight considering the RANS approach. Despite the low computational expenses, most of the results agree fairly well with the measurement data. However the correct prediction of droplet temperature remains an an unresolved problem.

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Nomenclature

Acronyms

FGM	Flamelet Generated Manifold
GRT	Global Rainbow refractometry Technique
NR	Non-reacting
ODE	Ordinary diferential equation
PDA	Phase Doppler Anemometry
PDE	Partial differential equation
PDF	Probability density function
PLIF	Planar Laser Induced Fluorescence
R	Reacting
RANS	Reynolds-averaged Navier-Stokes
RMS	Root mean square
Greek	s Symbols
χ	Scalar dissipation rate
δ_{ij}	Kronecker delta
$\dot{\omega}_k$	Reaction source term of species k
ϵ	Dissipation rate of turbulent kinetic energy
λ	Thermal conductivity
μ	Dynamic viscosity

- ho Density
- τ_{ij} Viscous stress tensor
- ζ_h Normalised enthalpy loss
- ζ_C Normalised variance of scaled progress variable
- ζ_Z Normalised variance of mixture fraction

Roman Symbols

$\Delta h^0_{f,k}$	Mass enthalpy of formation of species k
a	Strain rate
C	Scaled progress variable
c_p	Isobaric specific heat
D	Diameter
D_k	Diffusivity of species k
Da	Damköhler number
h	Enthalpy
K	Stretch rate
k	Turbulent kinetic energy
Le_k	Lewis number of species k
m	Mass flux
Nu	Nusselt number
p	Pressure
Pr	Prandtl number
R_u	Universal gas constant (8314 J/(kmol K))
S	Source term
S_{ij}	Strain rate tensor
Sc	Schmidt number
T	Temperature
u	Velocity
$V_{k,j}$	Diffusion velocity of species k (in j direction)
W	Molar mass
X	Molar fraction
Y_c	Progress variable
Y_k	Mass fraction of species k
Ζ	Mixture fraction
Р	Probability density function
Super	rscripts
b	Burnt
D	Deviatoric part of tensor

u Unburnt

Subscripts

- ann Annulus
- f Fuel
- m Mean value in bounday layer of droplet
- o Oxidizer
- p Droplet (parcel)
- st Stoichiometric
- t Turbulent

Chapter 1

Introduction

The worldwide consumption of liquid fuels is predicted to increase in the coming decades. (EIA, 2016) The combustion systems, that process this increasing demand are subjected to stricter and stricter requirements regarding efficiency, emissions, noise, etc. The development of these systems substantially depends on numerical tools. (Poinsot and Veynante, 2005) This graduation project focuses on a promising simulation method for combustion of liquid fuels.

Ma (2016) developed a numerical solver for the simulation of spray flames, his work is continued in this project. The simulation of spray combustion is a demanding task for multiple reasons. On top of the difficulties of gas phase combustion, a liquid phase model has to be included, which interacts with the already complex gas phase models in multiple ways.

The solver uses Flamelet Generated Manifold (FGM) to model the chemistry. In the FGM method, the equations that describe the reactions are solved in a preprocessing step in a simplified one dimensional domain. (van Oijen et al., 2016) This way the simulation of the 3D case is decoupled from the chemistry, which spares significant computational expenses. RANS simulation is applied to resolve the governing equations of the 3D case. The combined RANS-FGM approach provides an exceptionally low computational cost, yet it is capable of considering detailed chemistry.

The software is based on the C++ libraries of OpenFOAM 2.3.x. OpenFOAM is an open source platform, thus it enables the drastic modifications of the source code that are performed in this research.

1.1 Validation database

The simulation method is validated using the CORIA Jet Spray Flame database. The atmospheric, open burner geometry is illustrated in Fig.1.1, while Fig.1.2 shows a photograph of the flame. The burner structure is based on the KIAI burner introduced by Cordier et al. (2013), which is originally applied for premixed swirled flames. It has two inlets: one central and one annular, latter can be swirled. To modify this design for the CORIA Jet Spray Flame, the swirling is omitted and the central inlet is replaced by a liquid fuel injector.

The fuel is atomised using a Danfoss 80° hollow cone simplex injector (OD 030H8103.) Pure n-heptane is injected at a flow rate of 0.28 g/s and a temperature of 298 ± 2 K. The diameter of the injector orifice is 200 μ m.



Figure 1.1: Structure of the injection system (Verdier et al., 2017)

The annular inlet delivers 6 g/s air, also at 298 ± 2 K. The inner and outer diameter of the air inlet annulus is 10 mm and 20 mm respectively. Considering an air density of 1.180 kg/m³ (corresponding to p = 101325 Pa and T = 298 K) the average axial velocity at the inlet is 21.58 m/s. The tangential velocity at the inlet is negligible, as swirling is not applied. However the radial component is significant, since the annulus contracts suddenly (the flow is not fully developed at the outlet.) Moreover the annulus' inner wall is inclined. (See Fig.3.4.)



Figure 1.2: Photo of CORIA Jet spray flame

Considering the global reaction of n-heptane in air:

$$C_{7}H_{16} + aO_{2} + a\frac{X_{N_{2},air}}{X_{O_{2},air}}N_{2} \rightarrow bCO_{2} + cH_{2}O + a\frac{X_{N_{2},air}}{X_{O_{2},air}}N_{2}$$
(1.1)
$$a = b + c/2 = 11, \ b = 7, \ c = 16/2, \ X_{N_{2},air} = 0.789, \ X_{O_{2},air} = 0.211$$

for the full combustion of each mole of n-heptane 11 mol of oxygen and 41.13 mol of nitrogen has to be supplied as air. The mass stoichiometric ratio is:

$$\left(\frac{Y_o}{Y_f}\right)_{st} = \frac{aW_{O_2} + aW_{N_2}\frac{X_{N_2,air}}{X_{O_2,air}}}{W_{C_7H_{16}}} = 14.98\tag{1.2}$$

Based on the air and fuel inlet mass flows the global equivalence ratio is:

$$\frac{\dot{m}_o}{\dot{m}_f} \bigg/ \left(\frac{Y_o}{Y_f}\right)_{st} = \frac{6/0.28}{14.98} = 1.431 \tag{1.3}$$

which illustrates the amount of supplied air, however otherwise meaningless in non-premixed combustion. The global equivalence ration is further increased by the entrainment of ambient air. The flame is better characterised by local parameters, like the mixture fraction (see in subsection 2.1.4). At stoichiometric mixture of air and n-heptane the mixture fraction is:

$$Z_{st} = \frac{1}{1 + \left(\frac{Y_o}{Y_f}\right)_{st}} = 0.06258 \tag{1.4}$$

The reactions are significantly faster in the vicinity of stoichiometric mixture fraction, than for leaner or richer mixtures (see, Fig.2.7.) Thus the reaction zone is confined to a thin layer: the flame front, where the mixture is near to stoichiometric conditions. Fig.1.3 gives insight in the flame structure: it shows regions rich in OH radicals, which is a distinctive attribute of the reaction zone. A double flame structure cn be observed, which is typical to spray flames with room temperature oxidizer inlets and hollow cone spray structures. (Verdier et al., 2017) (Ma, 2016) The inner flame is corrugated by the turbulent jet of the annular air inlet, while the outer flame is rather undisturbed.

1.1.1 Measurements

The CORIA Jet Spray Flame database contains measurement results of the set-up described above in reacting and non-reacting case. The measurement data used in this study are listed in Tab.1.1.

Phase Doppler anemometry is used to determine droplet velocities and diameter. The smallest droplets ($D < 10 \ \mu m$) relax to the gas phase velocity considerably fast, thus the gas phase velocity is assumed to be equal to the velocity of these droplets. The air co-flow is seeded with 2.5 μm olive oil droplets to facilitate this measurement technique at all locations.

Droplet temperatures are measured using global rainbow refractometry technique. As the measuring laser beam reaches a droplet, it goes through refraction, total reflection and refraction again. The total scattering angle is between 140° and 160° depending on the refractive index of n-heptane, which is a temperature dependent property. The average droplet temperature in the measurement volume is related to the distribution of measured scattering angles. Larger



Figure 1.3: Single shot OH-PLIF image of the CORIA Jet spray flame (unfiltered) (Verdier et al., 2017)

Table 1.1: Measurement methods

Data	Technique	Location
Gas phase velocity -axial and radial components -mean and RMS values	Phase Doppler Anemometry	$z \in [5 \text{ mm}, 50 \text{ mm}]$ $x \in [-18 \text{ mm}, 14 \text{ mm}]$
Droplet velocity -axial and radial components -mean and RMS values -average and size classified values	Phase Doppler Anemometry	$z \in [5 \text{ mm}, 50 \text{ mm}]$ $x \in [-25 \text{ mm}, 14 \text{ mm}]$
Droplet size (D_{10}) -mean and RMS values	Phase Doppler Anemometry	$z \in [5 \text{ mm}, 50 \text{ mm}]$ $x \in [-25 \text{ mm}, 14 \text{ mm}]$
Individual droplet data (only non-reacting case) -axial velocity -radial velocity -diameter	Phase Doppler Anemometry	z = 7 mm $x \in [0 \text{ mm}, 10 \text{ mm}]$ $\Delta x = 2 \text{ mm}$
Droplet temperature	Global Rainbow refractometry Technique	$z \in [20 \text{ mm}, 70 \text{ mm}]$ $x \in [0 \text{ mm}, 25 \text{ mm}]$
OH concentration field	Planar Laser Induced Fluorescence	$z \in [0 \text{ mm}, 80 \text{ mm}]$ $x \in [-40 \text{ mm}, 40 \text{ mm}]$

droplets are able to scatter more light, thus the measured temperature is a weighted average of all droplets crossing the measurement volume:

$$T_{measured} = \frac{\sum D^{7/3} T}{\sum D^{7/3}}$$
(1.5)

The OH-PLIF measurements provide qualitative information about the flame shape. OH radicals are excited by a 300 μ m thick laser sheet with a wavelength of 282.75 nm. The radicals emit light on a different wavelength (fluorescence), this light is collected in the [308 nm, 330 nm] band, thus the location of the reaction zones is captured. The average OH field, and the locations of PDA and GRT measurements are illustrated in Fig.1.4.

Note the difference between the OH field in Fig.1.3 and Fig.1.4. The instantaneous image (Fig.1.3) shows that the inner flame is highly corrugated, however the average field (Fig.1.4) suggests that its mean location does not change. On the other hand, the outer flame demonstrates opposite behaviour: it is subject to lower frequency fluctuations: on the instantaneous image it appears to be smooth, but the mean field shows a widened outer flame region.



Figure 1.4: Measurement locations (yellow: PDA, red: GRT, background: average OH-PLIF image)

1.2 Outline

The thesis focuses on the further improvement of the software introduced by Ma (2016). The solver is applied to simulate the CORIA Jet Spray Flame, and its performance is assessed using the measurement database.

Chapter 2 introduces the theory of simulating the gas phase (section 2.1) and the droplet cloud (section 2.2.) Section 2.1 concentrates on the concept of flamelet generated manifold. A 4 and a 5 dimensional manifold is introduced, which simplify the solution of species fields by reducing the number of necessary governing equations. Section 2.2 introduces a novel Lagrangian droplet model, that allows the coupling of droplet equations to the gas phase governing equations, without the need to resolve all the species mass fractions. This new development allows the usage of arbitrarily detailed chemical mechanisms, which used to be a bottleneck of the solver.

Chapter 3 describes the simulation domain and the specific settings applied to model the CORIA Jet Spray Flame. Section 3.1 introduces the computational domain and the strategy to create a structured mesh. Section 3.2 describes a base case for the gas phase and liquid phase boundary conditions. The results of this base case are presented in section 3.3 for 4 and 5 dimensional FGM, and a detailed sensitivity study of the 4D base case is discussed in 3.4.

Chapter 2

Theory

The goal of this work is to solve the conservation equations describing spray combustion. The broad spectrum of length and time scales (E.g. smallest droplets are below the Kolmogorov scale) and the high number of interacting phenomena make the problem computationally demanding. The direct numerical simulation of all details is infeasible in practical cases, thus approximations are necessary. The applied models are introduced in this chapter.

2.1 Gas phase theory

The notations presented in this chapter are in in accordance with Poinsot and Veynante (2005) and Ma (2016). The Einstein summation convention is used, except for the index k, which is reserved to denote different species.

The conservation of following properties are considered:

- mass Eq.(2.1),
- momentum Eq.(2.2),
- species Eq.(2.3),
- total enthalpy Eq.(2.4).

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = S_{\rho}^e \tag{2.1}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \left(\rho u_j u_i\right)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + S_{M,i} + S_{u_i}^e$$
(2.2)

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \left(\rho u_j Y_k\right)}{\partial x_i} = -\frac{\partial \left(\rho V_{k,j} Y_k\right)}{\partial x_i} + \dot{\omega}_k + S^e_{Y_k} \quad k = 1..S$$
(2.3)

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \left(\rho u_j h\right)}{\partial x_j} = \frac{Dp}{Dt} - \frac{\partial q_j}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + S_H + S_H^e \tag{2.4}$$

The source terms mentioned in the above equations are the following:

- S^e_{\dots} : source terms due to evaporation,
- $S_{M,i}$: momentum source term except evaporative part (E.g.: body force),
- $\dot{\omega}_k$: species source term due to reactions,
- S_H : total enthalpy source term (E.g.: radiation).

In conventional combustion systems (such as the CORIA Jet Spray Flame) the gas phase can be modelled well as a Newtonian fluid. The viscous stress tensor is related to the strain rate as follows:

$$\tau_{ij} = 2\mu S_{ij} - \frac{2}{3}\mu \delta_{ij} S_{ll} = 2\mu \left(S_{ij} - \frac{1}{3}\delta_{ij} S_{ll} \right) = 2\mu S_{ij}^D$$
(2.5)

where the strain rate tensor is composed as:

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$
(2.6)

The deviatoric part of the strain rate is: $S_{ij}^D = \left(S_{ij} - \frac{1}{3}\delta_{ij}S_{ll}\right)$

The molecular diffusion of species is usually described by "Fick's law"-like relations. The diffusivity (D) can be different for each species and can depend on the local state. The general expression for the diffusive species volume flux is:

$$V_{k,j}Y_k = -D_k \frac{\partial Y_k}{\partial x_j} \tag{2.7}$$

Fourier's law treats the heat conduction in a similar manner. It gives the sensible enthalpy diffusion (first term in Eq.(2.8).) Furthermore total enthalpy is also transported solely by diffusion of species (second term in Eq.(2.8).)

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{S} h_k Y_k V_{k,j}$$
(2.8)

The thermodynamic properties are calculated using an equation of state assuming local thermodynamic equilibrium. In this work multicomponent ideal gas is assumed. The equation of state is:

$$\frac{p}{\rho} = \frac{R_u}{W}T\tag{2.9}$$

where the mean molar mass (W) is given by Eq.(2.10). The specific enthalpy of species k is calculated as the sum of chemical and sensible enthalpies (Eq.(2.11)), the mean enthalpy is a weighted average, where the weight factors are the mass fractions (Eq.(2.12).) The specific heat of the mixture is calculated similarly (Eq.(2.13).)

$$W = \frac{1}{\sum_{k=1}^{S} \frac{Y_k}{W_k}}$$
(2.10)

$$h_k = \Delta h_{f,k}^0 + \int_{T_0}^T c_{pk} \mathrm{d}T$$
 (2.11)

$$h = \sum_{k=1}^{S} h_k Y_k \tag{2.12}$$

$$c_p = \sum_{k=1}^{S} c_{pk} Y_k \tag{2.13}$$

As mentioned before the direct numerical simulation of all equations is infeasible in practical cases. The following simplifications are introduced to simplify the problem in the gas phase:

- Reynolds-averaged Navier-Stokes equations,
- standard $k \epsilon$ turbulence modelling,
- Flamelet Generated Manifold

2.1.1 Reynolds-averaged Navier-Stokes Equations

To simplify the numerical treatment of the governing equations (Eq.(2.1), Eq.(2.2), Eq.(2.3), Eq.(2.4).) the conserved quantities are decomposed to average and fluctuating parts. An arbitrary quantity ϕ , is decomposed to the Reynolds-average ($\overline{\phi}$) and the corresponding fluctuation (ϕ'):

$$\phi = \overline{\phi} + \phi' \tag{2.14}$$

where the Reynolds-average stands for the ensemble average, however in statistically steady cases it is equal to the temporal average:

$$\overline{\phi} = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \phi(\tau) \mathrm{d}\tau$$
(2.15)

In reacting flows, Favre-averaging is a useful tool to simplify the averaged equations. The Favre-average of a quantity and the corresponding fluctuation is denoted as:

$$\phi = \widetilde{\phi} + \phi'' \tag{2.16}$$

where the Favre-average is the density-weighted ensemble average. Similarly as above it can be treated as a temporal average:

$$\widetilde{\phi} = \frac{\int_{t}^{t+\Delta t} \rho(\tau)\phi(\tau)\mathrm{d}\tau}{\int_{t}^{t+\Delta t} \rho(\tau)\mathrm{d}\tau} = \frac{\overline{\rho\phi}}{\overline{\rho}}$$
(2.17)

The RANS equations are derived by applying Reynolds- and Favre-averaging on the governing equations (Eq.(2.1), Eq.(2.2), Eq.(2.3), Eq.(2.4).)

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j} = \overline{S_{\rho}^e}$$
(2.18)

$$\frac{\partial \overline{\rho} \widetilde{u}_i}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u}_j \widetilde{u}_i\right)}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\overline{\tau_{ij}} - \overline{\rho} \widetilde{u''_j u''_i}\right) + \overline{S_{M,i}} + \overline{S_{u_i}^e}$$
(2.19)

$$\frac{\partial \overline{\rho} \widetilde{Y_k}}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u_j} \overline{Y_k}\right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(-\overline{\rho} \widetilde{V_{k,j}} \overline{Y_k} - \overline{\rho} \widetilde{u_j'} \overline{Y_k''} \right) + \overline{\dot{\omega}_k} + \overline{S_{Y_k}^e} \quad k = 1..S$$
(2.20)

$$\frac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_{j}h\right)}{\partial x_{j}} = \frac{D\overline{p}}{Dt} - \frac{\partial}{\partial x_{j}}\left(\overline{q_{j}} + \overline{\rho}\widetilde{u_{j}''h''}\right) + \overline{\tau_{ij}}\frac{\partial u_{i}}{\partial x_{j}} + \overline{S_{H}} + \overline{S_{H}}$$
(2.21)

The term in the enthalpy equation that corresponds to work done by viscous forces $\left(\overline{\tau_{ij}\frac{\partial u_i}{\partial x_j}}\right)$ is neglected, as this is an acceptable approximation in subsonic combustion problems. (Poinsot and Veynante, 2005) The following terms need closure:

- Reynolds stress tensor: $R_{ij} = \widetilde{u''_j u''_i}$
- Turbulent flux of species: $\overline{\rho} \widetilde{u_j'' Y_k''}$
- Turbulent flux of enthalpy: $\overline{\rho}\widetilde{u''_ih''}$
- Reynolds-averaged reaction source term: $\overline{\dot{\omega}_k}$

2.1.2 Closure of Reynolds stresses

The Reynolds stress tensor (R_{ij}) is an unclosed term in Eq.(2.19). The turbulent viscosity hypothesis provides a simple way to model it. An analogy is drawn between the viscous stress tensor (Eq.(2.5)) and the Reynolds stresses:

$$\overline{\rho}R_{ij} = \overline{\rho u_j'' u_i''} = \overline{\rho}\widetilde{u_j'' u_i''} \equiv -\mu_t \left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \widetilde{u}_l}{\partial x_l}\delta_{ij}\right) + \frac{2}{3}\overline{\rho}k\delta_{ij} = -2\mu_t \widetilde{S}_{ij}^D + \frac{2}{3}\overline{\rho}k\delta_{ij} \quad (2.22)$$

where μ_t is the turbulent viscosity. The closure of this term is described below. Note the extra term introduced compared to Eq.(2.5): $\frac{2}{3}\overline{\rho}k\delta_{ij}$, where k is the turbulent kinetic energy, defined as:

$$k = \frac{1}{2} \sum_{i=1}^{3} \widetilde{u_{(i)}'' u_{(i)}''}$$
(2.23)

(Parenthesis is used to show that the Einstein summation is not applied here.) The extra term in Eq.(2.22) ensures that the trace of the Reynolds stress tensor takes the correct value, which is by definition 2k.

Closure of μ_t : the $k - \epsilon$ model

As mentioned before the standard $k - \epsilon$ turbulence model is used in this study. The turbulent viscosity is proportional to the density, the turbulent velocity scale, and the turbulent length scale as described in Eq.(2.24).

$$\mu_t = C_\mu \overline{\rho} u_t l_t \tag{2.24}$$

where the turbulent velocity scale (u_t) , and the turbulent length scale (l_t) are defined as:

$$u_t = k^{1/2}$$
 and $l_t = \frac{k^{3/2}}{\epsilon}$ (2.25)

thus the turbulent viscosity is:

$$\mu_t = C_\mu \overline{\rho} \frac{k^2}{\epsilon} \tag{2.26}$$

Two governing equations are added to describe the transport, production, and dissipation of turbulent kinetic energy (Eq.(2.27)) and its dissipation rate (Eq.(2.28).)

$$\frac{\partial \overline{\rho}k}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_{j}k\right)}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left[\left(\mu + \frac{\mu_{t}}{\sigma_{k}}\right) \frac{\partial k}{\partial x_{j}} \right] + P_{k} - \overline{\rho}\epsilon + \overline{S}_{k}^{e}$$
(2.27)

$$\frac{\partial \overline{\rho}\epsilon}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_{j}\epsilon\right)}{\partial x_{j}} = \frac{\partial}{\partial x_{j}} \left[\left(\mu + \frac{\mu_{t}}{\sigma_{\epsilon}} \right) \frac{\partial \epsilon}{\partial x_{j}} \right] + C_{\epsilon 1} \frac{\epsilon}{k} P_{k} - C_{\epsilon 1} \overline{\rho} \frac{\epsilon^{2}}{k} + \overline{S_{\epsilon}^{e}}$$
(2.28)

where the production term P_k is the work done by the Reynolds stresses on the deforming flow (velocity gradients) as presented in Eq.(2.29). Substituting the expression of Reynolds stresses (Eq.(2.22)) the production term only depends on the averaged strain rate tensor and the turbulent viscosity:

$$P_{k} = -\overline{\rho}\widetilde{u_{i}''u_{j}''}\frac{\partial\widetilde{u_{j}}}{\partial x_{j}} = 2\mu_{t}\widetilde{S}_{ij}\widetilde{S}_{ij}$$

$$(2.29)$$

In this work the standard $k - \epsilon$ model (Launder and Sharma, 1974) is used with the constants :

 $C_{\mu} = 0.09, \quad \sigma_k = 1.00, \quad \sigma_{\epsilon} = 1.30, \quad C_{1\epsilon} = 1.44, \quad C_{2\epsilon} = 1.92$ (2.30)

2.1.3 Closure of turbulent scalar fluxes

The turbulent transport of scalars (enthalpy and species) is modelled using the gradient diffusion assumption. The diffusion coefficients are related to the turbulent viscosity by assumed turbulent Schmidt and Prandtl numbers:

$$\overline{\rho}\widetilde{u_j'Y_k''} = -\frac{\mu_t}{Sc_t}\frac{\partial\widetilde{Y_k}}{\partial x_j}$$
(2.31)

$$\overline{\rho}\widetilde{u_j'h''} = -\frac{\mu_t}{Pr_t}\frac{\partial h}{\partial x_j} \tag{2.32}$$

2.1.4 Flamelet Generated Manifold model

In simulation of reacting flows one of the main difficulties come from the high number of species, which significantly increases with the increasing complexity of fuel. The FGM model is one of the tabulated chemistry methods which simplifies this problem by reducing the number of governing equations. The detailed reaction mechanism is solved only in a simplified case: 1D flamelets. In the first applications of FGM freely propagating premixed flamelets were used. Additional complexity can be introduced by modelling heat loss, straining, preferential diffusion of species, etc. A review of FGM is presented by van Oijen et al. (2016) for the modelling of premixed flames, the authors state that premixed and non-premixed flames are best represented by premixed and non-premixed flamelets respectively. In this work 1D non-premixed counterflow flamelets are used for the FGM generation as proposed by Ma (2016). In the 3D domain a significantly smaller set of governing equations is solved.

Chemistry

A reaction mechanism is described by the species it considers and the elementary reactions between these species. A general form of the elementary reactions r is given in Eq.(2.33) for s = 1..S species. The reaction is described by the rate constant (k_r) , and the stoichiometric coefficients (ν_{rk}) of species on the reactant (e) and product (p) side.

$$\sum_{s=1}^{S} \nu_{rs}^{(e)} A_s \xrightarrow{k_r} \sum_{s=1}^{S} \nu_{rs}^{(p)} A_s$$
(2.33)

The formation rate of a species i in reaction r is:

$$\left(\frac{\partial C_i}{\partial t}\right)_r = k_r \left(\nu_{ri}^{(p)} - \nu_{ri}^{(e)}\right) \prod_{s=1}^S C_s^{\nu_{rs}^{(e)}}$$
(2.34)

where C_s is the molar concentration of species s. The total formation rate of species i from all R reactions is:

$$\frac{\partial C_i}{\partial t} = \sum_{r=1}^{R} \left[k_r \left(\nu_{ri}^{(p)} - \nu_{ri}^{(e)} \right) \prod_{s=1}^{S} C_s^{\nu_{rs}^{(e)}} \right] \quad i = 1..S$$
(2.35)

The rate constant is given by the Arrhenius law:

$$k_r = A_r T^{b_r} e^{-\frac{E_{ar}}{R_u T}}$$
(2.36)

where b_r is a dimensionless constant, E_{ar} is the activation energy associated with the reaction, and A_r is the pre-exponential constant (with a unit such that Eq.(2.35) is dimensionally correct). The reaction source term is the produced mass of a species per unit volume and unit time:

$$\dot{\omega}_i = W_i \frac{\partial C_i}{\partial t} = W_i \sum_{r=1}^R \left[k_r \left(\nu_{ri}^{(p)} - \nu_{ri}^{(e)} \right) \prod_{s=1}^S \left(\frac{\rho Y_s}{W_s} \right)^{\nu_{rs}^{(e)}} \right] \quad i = 1..S$$
(2.37)

where the molar concentration is expressed with the mass fraction. Eq.(2.37) represents an ordinary differential equation system. This ODE system is usually very stiff due to the different time scales, furthermore it is strongly coupled to the temperature field through Eq.(2.36), and causes a strong coupling between each species transport equation too (Eq.(2.20).)

FGM

The computational difficulties mentioned above underline the importance of decoupling the flow field calculation from the chemistry. In this study the decoupling is executed with FGM. The usage of FGM inherently assumes that the flame structures are quasi-1D, thus they are well represented by 1D counterflow flamelets.

The quasi-1D nature of the flame means that gradients along the flame front are negligible compared to gradients normal to the flame front. This condition can be quantified by the ratio of Kolmogorov and chemical time scales (the Damköhler number.) The 1D assumption holds if the reactions are significantly faster than the turbulent mixing, which is equivalent to Da > 1. (Poinsot and Veynante, 2005). Judged by the instantaneous OH-PLIF image of the flame (Fig.1.3) the flame mostly consists of thin flamelets, thus the application of FGM is reasonable. The FGM method used in this study can be summarised in the following steps:

- 1. Calculation of representative 1D flamelets using a chemical mechanism, that is too complex to solve in the 3D domain.
- 2. Transformation of 1D flamelets to the control variable space.
- 3. Tabulation of relevant gas properties as function of the control variables.
- 4. PDF-integration of said properties using assumed PDF method. (The probability density functions are characterised by the average and the variance values of the control variables.)
- 5. Tabulation as function of average and variance values of the control variables.
- 6. Solution of gas phase governing equations including equations describing the FGM control variables and their variances.
- 7. Retrieval (interpolation) of properties from the manifold, that are necessary for the calculation of the governing equations. E.g.: temperature, viscosity, mass fractions of species, source therm of progress variable (definition below), etc.

A detailed explanation of this process is provided below. The greatest benefit of this FGM method, is that steps 1.-5. are executed in the preprocessing phase. Once the gas properties and the progress variable source term are finally tabulated (5.), there is no need to repeat the preprocessing.



Figure 2.1: Laminar counterflow flame

FGM: counterflow flamelets In this study the FGM is constructed from laminar counterflow flamelets computed at different strain rates using Chem1D: a 1D chemistry solver developed at TU Eindhoven (Chem1D, 2002). The counterflow flamelets are illustrated in Fig.2.1, fuel and air are impinging on a stagnation plane, and in the process they mix and react. The 1D counterflow equations used in Chem1D are proposed by Van Oijen and De Goey (2002) for premixed flamelets and by Ramaekers (2011) for non-premixed flamelets. In steady state the non-premixed governing

equations are the following:

$$\frac{\mathrm{d}m}{\mathrm{d}x} = -\rho K \tag{2.38}$$

$$\frac{\mathrm{d}mK}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\mu \frac{\mathrm{d}K}{\mathrm{d}x} \right) = \rho_{air} a_{air}^2 - 2\rho K^2 \tag{2.39}$$

$$\frac{\mathrm{d}mY_k}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\lambda}{Le_k c_p} \frac{\mathrm{d}Y_k}{\mathrm{d}x}\right) - \dot{\omega}_k = -\rho K Y_k \qquad \qquad k = 1..S \qquad (2.40)$$

$$\frac{\mathrm{d}mh}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\lambda}{c_p} \frac{\mathrm{d}h}{\mathrm{d}x}\right) = \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\lambda}{c_p} \sum_{k=1}^{S} h_k \left(\frac{1}{Le_k} - 1\right) \frac{\mathrm{d}Y_k}{\mathrm{d}x}\right) - \rho Kh \tag{2.41}$$

The strain rate a_{air} is applied on the air side. Hereafter the air side strain rate will be simply referred to as "strain rate." The fuel side strain rate is set such that $\rho_{air}a_{air}^2 = \rho_{fuel}a_{fuel}^2$ thus it is indifferent weather the air or fuel side quantities are used in Eq.(2.39).

The diffusion of species is treated a "Fick-like" way. The mass diffusivity of each species is defined with the Lewis number: the ratio of thermal and mass diffusivity. In this work unity Lewis numbers are assumed in the 1D laminar calculations. A qualitative justification of this choice is the following: in the simulated flame the diffusion of enthalpy and species is dominated by turbulent transport, which affects every species equally, thus the effect of preferential diffusion is negligible (Ma, 2016). Consequently the preferential diffusion term in Eq.(2.41) is zero.

FGM: boundary conditions The fuel and air boundaries are at x = -15 mm and x = 45 mm respectively. Dirichlet boundary conditions are applied for composition (Y_k) and temperature (which defines the enthalpy (h).) The stretch rate (K) is treated with Dirichlet boundary condition on the air side, and a zero-gradient Neumann boundary condition on the fuel side. The stagnation point is fixed to the origin, thus $m_{|x=0} = 0$ kg/m²s. (Ramaekers, 2011) Only nitrogen and oxygen are considered in the air composition, their mass fractions are: $Y_{N_2} = 0.767621$ and $Y_{O_2} = 0.232379$. The fuel is pure n-heptane (C_7H_{16}) . The pressure is constant 101325*Pa* through the entire domain. Depending on whether the enthalpy loss is treated or not, two types of FGM are distinguished in this study. The temperature boundary conditions are the following in the two case:

1. Adiabatic FGM:

The temperature of fuel on the boundary is the saturation temperature of n-heptane at atmospheric pressure: $T_{fuel} = T_{C_7H_{16},sat}(101325 \text{ Pa}) = 371.55 \text{ K}.$ The boundary temperature of air is the environment temperature: $T_{air} = 298 \text{ K}$

2. FGM including enthalpy loss:

The flamelets of the adiabatic FGM are taken as a basis, additionally a set of flamelets is generated with lower enthalpy at the inlets: $T_{fuel} = T_{air} = 240$ K. According to Ottino et al. (2016) this temperature is considered admissible.

The strain rate is varied on the boundaries. With increasing strain rate the low temperature fuel and oxidant is mixed more intensely with the flame region, thus the reaction zone becomes thinner and the temperature in the flame decreases. The effect is illustrated in Fig.2.2. The flame extinguishes above a certain strain rate, as the reaction source terms can no longer balance the effect of stretching. (See Eq.(2.40).) The steady state solution in this case is the pure mixing of fuel and oxidant.

To cover the range between the last steady solution and pure mixing, an extinguishing flamelet is computed. This is the unsteady solution of the flamelet equations where the initial



Figure 2.2: Temperature in the physical domain (solid lines: steady flamelets, dashed lines: extinguishing flamelet sampled at different time steps, the colour represents the strain rate: shifts from red to black as the strain rate increases)

condition is the last steady flamelet, but the strain rate is slightly higher $(+5 \text{ s}^{-1})$. This flamelet is also visualised in Fig.2.2 with a few samples at different time steps.

The manifold generated from such flamelets is named extinguishing FGM after the treatment of the unsteady part. For cold inlets of air and n-heptane there is no other way to sweep through all possible states of counterflow flamelets. Note that if autoignition is viable (at least one boundary temperature is high enough) then a single unsteady igniting flamelet can cover most of the states. (Ma, 2016)

FGM: chemical mechanisms In this study two different chemical mechanisms are used. The mechanisms are identified with their authors:

- 1. Lu and Law mechanism:
 - A skeletal reaction mechanism for n-heptane developed by Lu and Law (2006), which contains 188 species and 939 elementary reactions.
- 2. Patel et al. mechanism:

A reduced reaction mechanism for n-heptane combustion developed by Patel et al. (2004), containing 29 species and 52 reactions.

Based on the inclusion of enthalpy loss, and on the mechanism, 3 different sets of flamelets are generated:

- 1. Lu and Law mechanism with adiabatic temperature boundary conditions.
- 2. Lu and Law mechanism with lowered temperature boundary conditions.
- 3. Patel et al. mechanism with adiabatic temperature boundary conditions.

The process of increasing the strain rate till extinction is represented in Fig.2.3 (b), (d), and (f) for the three sets of flamelets. For the steady flamelets the temperature at stoichiometric mixture fraction decreases with increasing strain rates. At the extinguishing strain rate this temperature decreases until it reaches the pure mixing temperature.

The most distinct difference between the three sets is in the extinguishing strain rates, 1485 s^{-1} , 1110 s^{-1} , and 1335 s^{-1} respectively. The highest temperatures always occur at the lowest strain rates (1 s⁻¹ in this work), the maximum temperatures are respectively: 2231 K, 2189 K, and 2204 K. The difference in extinguishing strain rates outlines the importance of using a more comprehensive mechanism, as the difference between the two adiabatic sets is significant.

It is interesting to notice that the reduction of the temperature peak in the Lu and Law flamelets between the adiabatic and reduced enthalpy sets (42 K) is smaller than the temperature reduction on the boundaries (131.55 K and 58 K.) This suggests that the temperature peak is influenced more by the dissociation of species in the reaction zone than by the value of inlet enthalpies.

FGM: coordinate transformation As seen in Fig.2.2 the flame thickness varies substantially with strain rate. Because of the varying length scales and high local gradients, handling the flamelets in physical space is unreasonable. Furthermore by introducing a normalised variable instead of the spatial coordinate, the flamelet states can be mapped to any 3D domain where the normalised variable is evaluated. The flamelets are transformed to mixture fractions space, which provides a normalised coordinate.

Mixture fraction is a dimensionless quantity expressing the mass fraction originating from the fuel. Since the mass of elements is conserved during chemical reactions, the mixture fraction behaves as a passive scalar (no chemical source term). In this work Bilger's formula is used to calculate the mixture fraction. (Bilger, 1976) A quantity b is formed as a linear combination of element mass fractions such that it is zero for stoichiometric mixtures. For hydrocarbon fuels it is:

$$b = 2\frac{Y_C}{W_C} + \frac{1}{2}\frac{Y_H}{W_H} - \frac{Y_O}{W_O}$$
(2.42)

where Y_C , Y_H and Y_O are the mass fractions of carbon, hydrogen, and oxygen respectively and W_C , W_H and W_O are the molar masses of these elements. This quantity is normalised to a range between 0 and 1 using the values associated with the oxidizer (b_o) and fuel (b_f) boundaries:

$$Z = \frac{b - b_o}{b_f - b_o} \tag{2.43}$$

The 1D species and energy transport equations (Eq.(2.40) and Eq.(2.41)) can be transformed to mixture fraction space. Considering mass and mixture fraction conservation, assuming $Le_k = 1$, and quasi-constant diffusivity, the steady state flamelet equations become:

$$0 = \rho D \left(\frac{\partial Z}{\partial x}\frac{\partial Z}{\partial x}\right) \frac{\partial^2 \phi_k}{\partial Z^2} + \dot{\omega}_k = \rho \frac{\chi}{2} \frac{\partial^2 \phi_k}{\partial Z^2} + \dot{\omega}_k \qquad k = 1..S + 1$$
(2.44)

where ϕ_k can represent species or enthalpy. (Poinsot and Veynante, 2005) Eq.(2.44) shows that the species and enthalpy profiles of flamelets only depend on mixture fraction and the scalar dissipation rate:

$$\chi = 2D\left(\frac{\partial Z}{\partial x}\frac{\partial Z}{\partial x}\right) \tag{2.45}$$

As shown in Fig.2.3 the scalar dissipation rate (at stoichiometric mixture) scales well with the strain rate for steady flamelets. However Eq.(2.44) suggests, that in unsteady cases (introducing time dependence) the flamelets degree of freedom increases (i.e. $\phi_k = \phi_k(Z, \chi, t)$). Indeed, as seen in Fig.2.3 the same stoichiometric scalar dissipation rate can correspond to many samples of the unsteady flamelet.



Figure 2.3: Temperature at stoichiometric mixture fraction (T_{st}) as a function of scalar dissipation rate at the same location (a, c, e) and strain rate at the air inlet (b, d, f)

The introduction of progress variable eliminates the need for a third control variable. It is defined as a linear combination of the species mass fractions such, that it monotonically increases from the pure mixing to the fully burnt (equilibrium) condition. The mixture fraction and the progress variable together uniquely define the flamelet and the location within the flamelet, hence this is a 2D FGM. Ma (2016) showed the benefit of including intermediate species in the progress variable. In this study the definition is the following:

$$Y_c = 4\frac{Y_{CO_2}}{W_{CO_2}} + 2\frac{Y_{H_2O}}{W_{H_2O}} + 0.5\frac{Y_{H_2}}{W_{H_2}} + 1\frac{Y_{CO}}{W_{CO}}$$
(2.46)

Fig.2.4 illustrates that on the rich part of the manifold (Z > 0.06258) there are regions where Y_{CO_2} and Y_{H_2O} do not provide one-to-one correspondence, since higher mass fractions do not correspond to lower strain rates. Opposite behaviour is seen in the H_2 mass fractions, as it shows a similar inversion on the lean part of the manifold. The CO mass fraction is non-unique for all mixture fractions. Note that the flamelets slightly overlap at the high progress variables of rich mixtures. Nevertheless the progress variable is unique on most part of the manifold. There is a trade-off between accuracy on rich and lean sides, here the lean accuracy is prioritized.

The tabulation and retrieval of flamelet properties is simpler if the progress variable is normalised:

$$C(Y_c, Z) = \frac{Y_c - Y_c^u(Z)}{Y_c^b(Z) - Y_c^u(Z)}$$
(2.47)

where the unburnt progress variable $(Y_c^u(Z))$ is zero for all mixture fractions in this study. The burnt progress variable ranges from zero (on the boundaries) to approximately 25 near the stoichiometric mixture fraction. (Normalization is not applied on the boundaries.) Based on the scaled progress variable and mixture fraction, the location in the manifold is identified and the gas properties are interpolated:

$$\phi = \phi(Z, C) \tag{2.48}$$

where ϕ can be any scalar property. This is a two dimensional manifold as there are two control variables: mixture fraction and progress variable. Note that the scaled progress variable (C) is beneficial for the interpolation, however the formulation of conservation laws is simpler for the progress variable $(Y_C.)$ E.g.: the chemical source term of progress variable is calculated simply by substituting the corresponding reaction source terms in Eq.(2.46). Consequently a governing equation (Eq.(2.77)) is formed for the progress variable, and scaling is executed when properties are retrieved from the manifold.

FGM: enthalpy loss Enthalpy loss is introduced as a third control variable. This is motivated by the importance of evaporative enthalpy source term (S_H^e) in Eq.(2.4). The evaporation of droplets is significant in the base of the flame (e.q.: Fig.1.3 x = 20 mm z = 40 mm), as they enter a high temperature region.

The non-adiabatic FGM is formulated by combining two different sets of flamelets. In this work the two sets are "Lu and Law adiabatic" and "Lu and Law lowest enthalpy". Note that additional sets of flamelets could be incorporated in the manifold between these two extremes, but the difference between the "adiabatic" and "lowest enthalpy" sets is relatively low. Ma (2016) uses only 3 layers, while the oxidizer temperature changes up to 600 K between the sets of lowest and highest enthalpy. However in this study the temperature changes are much smaller (131.55 K and 58 K.)

Analogously to the 2D FGM a three dimensional manifold is created using mixture fraction, progress variable, and enthalpy loss as control variables. The tabulated properties are interpolated between the two sets of flamelets based on the enthalpy loss. As mentioned previously



Figure 2.4: Progress variable and its components (solid lines: steady flamelets, dashed lines: extinguishing flamelet sampled at different time steps, the colour represents the strain rate: shifts from red to black as the strain rate increases)

the numerical treatment of the control variables is simpler after normalization. The normalised enthalpy loss is expressed as:

$$\zeta_h(h,Z) = \frac{h - h_{ad}(Z)}{\Delta h_{max}(Z)} \tag{2.49}$$

where $\Delta h_{max}(Z)$ is the maximal enthalpy loss, and $h_{ad}(Z)$ is the adiabatic enthalpy. Note that without the preferential diffusion of species (unity Lewis number assumption) the maximal enthalpy loss and the adiabatic enthalpy only depend on mixture fraction. The enthalpy is linear in the mixture fraction space, since combustion does not change the enthalpy of a mixture, it only transforms chemical enthalpy to sensible enthalpy (Eq.(2.11).)



Figure 2.5: Enthalpy of different mixtures

Fig.2.5 shows the enthalpies of the two sets of flamelets. The enthalpy difference between the two sets of flamelets is not the same on the fuel and air boundary, thus the maximal enthalpy loss at a given mixture fraction is:

$$\Delta h_{max}(Z) = \Delta h_{max,Z=0} + Z \left(\Delta h_{max,Z=1} - \Delta h_{max,Z=0} \right)$$
(2.50)

and the adiabatic enthalpy is defined similarly:

$$h_{ad}(Z) = h_{ad,Z=0} + Z \left(h_{ad,Z=1} - h_{ad,Z=0} \right)$$
(2.51)

The adiabatic enthalpy of oxidizer and fuel, and the maximal enthalpy loss are presented in Tab.2.1.

The interpolation in the 3D FGM is executed using the mixture fraction, the scaled progress variable and the normalised enthalpy loss:

$$\phi = \phi(Z, C, \zeta_h) \tag{2.52}$$

note that $\zeta_h = 0$ corresponds to the adiabatic flamelets.

Table 2.1: Enthalpies of fuel and oxidizer for Lu and Law flamelets [J/kg]

	Oxidizer $(Z = 0)$	Fuel $(Z = 1)$
adiabatic (h_{ad})	-118.42	-1744032.71
lowest enthalpy	-58446.25	-1968602.54
difference (Δh_{max})	-58327.83	-224569.83

FGM: assumed PDF method The properties retrieved from the 2D or 3D FGM table show strong non-linearity as function of mixture fraction and progress variable (see the scaled mass fractions in Fig.2.4 or the progress variable source term in Fig.2.7.) In turbulent combustion the control variables $(Z, Y_c \text{ and } h)$ are fluctuating in the intervals: $Z \in [0,1], Y_c \in [Y_c^u, Y_c^b]$, and $h \in [h_{ad} - |\Delta h_{max}|, h_{ad}]$. To retrieve the mean value of the strongly non-linear properties in a statistically steady case, information about the joint probability density function of the control variables is necessary.

A joint PDF can be applied for the mixture fraction and the scaled progress variable $(\tilde{P}(Z, C))$. The scaled progress variable is used for simpler numerical treatment. The effect of the enthalpy fluctuations is neglected, as they are insignificant. (Ma, 2016) Using the joint PDF the Favre-average of a property is:

$$\widetilde{\phi} = \int_0^1 \int_0^1 \phi(Z, C, \zeta_h) \widetilde{P}(Z, C) \mathrm{d}Z \mathrm{d}C$$
(2.53)

where ζ_h is optional depending on the dimensions of the FGM. The Reynolds-averaged quantities are calculated as:

$$\overline{\phi} = \overline{\rho} \int_0^1 \int_0^1 \frac{\phi(Z, C, \zeta_h)}{\rho(Z, C, \zeta_h)} \widetilde{P}(Z, C) dZ dC$$
(2.54)

where the average density is:

$$\overline{\rho} = \left[\int_0^1 \int_0^1 \frac{1}{\rho(Z, C, \zeta_h)} \widetilde{P}(Z, C) \mathrm{d}Z \mathrm{d}C \right]^{-1}$$
(2.55)

In this work the joint PDF is simplified using the assumption that the mixture fraction and the scaled progress variable are statistically independent, thus the joint PDF is the product of the PDFs:

$$\widetilde{P}(Z,C) = \widetilde{P}(Z)\widetilde{P}(C) \tag{2.56}$$

Further simplification is reached by assuming the PDF is β -function which is parametrized with the average and variance of mixture fraction and progress variable:

$$\widetilde{P}(\xi) = \frac{(\xi)^{\alpha-1} \left(1-\xi\right)^{\beta-1} \Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}$$
(2.57)

where:

$$\alpha = \widetilde{\xi} \left[\frac{\widetilde{\xi}(1 - \widetilde{\xi})}{\widetilde{\xi''^2}} - 1 \right], \qquad \beta = (1 - \widetilde{\xi}) \left[\frac{\widetilde{\xi}(1 - \widetilde{\xi})}{\widetilde{\xi''^2}} - 1 \right]$$
(2.58)

and

$$\Gamma(\eta) = \int_0^\infty x^{\eta - 1} e^{-x} \mathrm{d}x \tag{2.59}$$

The Favre-averaged mixture fraction and scaled progress variable (\widetilde{Z} and \widetilde{C}) and their variances $(\widetilde{Z''^2})$ and $\widetilde{C''^2}$) are substituted in the place of $\widetilde{\xi}$ and $\widetilde{\xi''^2}$ respectively to obtain the parameters α and β . The variable ξ and its mean value are restricted to the]0,1[interval, furthermore α

and β are restricted to \mathbb{R}^+ , thus $\widetilde{\xi''^2} \in]0, \widetilde{\xi}(1-\widetilde{\xi})[$. The mixture fraction and progress variable variances are normalised to simplify interpolation. The normalised variances are:

$$\zeta_{\xi} = \frac{\xi''^2}{\tilde{\xi}(1-\tilde{\xi})} \tag{2.60}$$



A few examples of the β -function are presented in Fig.2.6. As the normalised variance approaches zero, the PDF becomes a Dirac δ around the mean value. For low normalised variances the PDF has its mode in the vicinity of the mean value, for high normalised variances the PDF becomes bimodal the two modes are at the limiting values: 0 and 1. This corresponds to the expectations about mixture fraction and progress variable:

- In fluctuating flame fronts bimodal behaviour is expected, with the two modes located at the burnt and unburnt conditions.
- In regions characterised by low turbulence the variances are low, thus the "Dirac δ "-like treatment is adequate.

The Favre-averaged scaled progress variable is defined as:

$$\widetilde{C}\left(\widetilde{Y}_{c}, \widetilde{Z}, \widetilde{Z''^{2}}\right) = \frac{\widetilde{Y}_{c} - \widetilde{Y}_{c}^{u}(\widetilde{Z}, Z''^{2})}{\widetilde{Y}_{c}^{b}(\widetilde{Z}, \widetilde{Z''^{2}}) - \widetilde{Y}_{c}^{u}(\widetilde{Z}, \widetilde{Z''^{2}})}$$
(2.61)

where the burnt and unburnt average values are already PDF integrated in the mixture fraction space and tabulated. The conversion between the variance of progress variable and scaled progress variable is derived below:

$$C = \widetilde{C} + C'' \tag{2.62}$$

$$C^2 = \tilde{C}^2 + 2\tilde{C}C'' + C''^2 \tag{2.63}$$

$$\widetilde{C}^2 = \widetilde{\widetilde{C}}^2 + 2\widetilde{\widetilde{C}}\widetilde{C}'' + \widetilde{C}''^2$$
(2.64)

$$\widetilde{C}^2 = \widetilde{C}^2 + \widetilde{C''^2} \tag{2.65}$$

$$\left(\frac{Y_c - \overline{Y_c^u}}{Y_c^b - \overline{Y_c^u}}\right)^2 = \widetilde{C}^2 + \widetilde{C''^2}$$
(2.66)

$$\widetilde{C''^2} = \left(\frac{Y_c - \overline{Y_c^u}}{Y_c^b - \overline{Y_c^u}}\right)^2 - \widetilde{C}^2$$
(2.67)

$$\widetilde{C}^{\prime\prime\prime 2} = \frac{\widetilde{Y_c^2 - 2\widetilde{Y_cY_c^u} + (Y_c^u)^2}}{(\widetilde{Y_c^b - Y_c^u})^2} - \widetilde{C}^2$$
(2.68)

$$\widetilde{C''^2} = \frac{\widetilde{(Y_c + Y_c'')^2} + \widetilde{(Y_c^u)^2 - 2[C(Y_c^b - Y_c^u) + Y_c^u]Y_c^u}}{\widetilde{(Y_c^b)^2 - 2Y_c^bY_c^u + (Y_c^u)^2}} - \widetilde{C}^2$$
(2.69)

$$\widetilde{C''^2} = \frac{\widetilde{Y_c''^2} + \widetilde{Y_c}^2 - (Y_c^u)^2 + 2C(Y_c^b Y_c^u - (Y_c^u)^2)}{(\widetilde{Y_c^b})^2 - 2\widetilde{Y_c^b} \widetilde{Y_c^u} + (\widetilde{Y_c^u})^2} - \widetilde{C}^2$$
(2.70)

$$\widetilde{C''^2} = \frac{\widetilde{Y_c''^2} + \widetilde{Y_c}^2 - \widetilde{(Y_c^u)^2} - 2}{\widetilde{(Y_c^b)^2} - 2\widetilde{(V_c^b)^2} + \widetilde{(Y_c^u)^2}} - \widetilde{C}^2$$
(2.71)

$$\widetilde{C''^2} = \frac{\widetilde{Y_c''^2} + \widetilde{Y_c}^2 - \widetilde{(Y_c^u)^2} - 2\widetilde{C}\left(\widetilde{Y_c^bY_c^u} - \widetilde{(Y_c^u)^2}\right)}{\widetilde{(Y_c^b)^2} - 2\widetilde{Y_c^bY_c^u} + \widetilde{(Y_c^u)^2}} - \widetilde{C}^2$$
(2.72)

where $(Y_c^u)^2 = (Y_c^u)^2 (\widetilde{Z}, \widetilde{Z''^2}), (\widetilde{Y_c^b})^2 = (Y_c^b)^2 (\widetilde{Z}, \widetilde{Z''^2})$ and $\widetilde{Y_c^b Y_c^u} = \widetilde{Y_c^b Y_c^u} (\widetilde{Z}, \widetilde{Z''^2})$ are PDF integrated in the mixture fraction space and tabulated.

The PDF integration (Eq.(2.53), Eq.(2.54)) of the tabulated variables is executed in a preprocessing step, and the resulting average values are stored in 4D or 5D lookup tables depending the enthalpy treatment. The properties are interpolated in the tables using the normalised control variables:

$$\widetilde{\phi} = \widetilde{\phi}(\widetilde{Z}, \zeta_Z, \widetilde{C}, \zeta_C, \zeta_h) \quad \text{and} \quad \overline{\phi} = \overline{\phi}(\widetilde{Z}, \zeta_Z, \widetilde{C}, \zeta_C, \zeta_h)$$

$$(2.73)$$

where ζ_h is optional.

FGM: governing equations The reason of applying a tabulated chemistry method is to reduce the complexity of the original PDE system consisting of: Eq.(2.18), Eq.(2.19), Eq.(2.20), and Eq.(2.21), which consists of 5 + S strongly coupled PDEs. Instead of the stiff and numerous species transport equations (Eq.(2.20)) only 4 PDEs are used: the conservation of mixture fraction, progress variable and their variances $(Z, Y_c, \widetilde{Z''}^2, \text{ and } \widetilde{Y''_c}^2)$ The full set of governing equations (except turbulence modelling) is the following:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_j}{\partial x_j} = \overline{S_{\rho}^e}$$
(2.74)

$$\frac{\partial \overline{\rho} \widetilde{u}_i}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u}_j \widetilde{u}_i\right)}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\overline{\tau_{ij}} - \overline{\rho} \widetilde{u''_j u''_i}\right) + \overline{S_{M,i}} + \overline{S_{u_i}^e}$$
(2.75)

$$\frac{\partial \overline{\rho} \widetilde{Z}}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u_j} \widetilde{Z}\right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{D} \frac{\partial \widetilde{Z}}{\partial x_j} - \overline{\rho} \widetilde{u_j'' Z''}\right) + \overline{S_Z^e}$$
(2.76)

$$\frac{\partial \overline{\rho} \widetilde{Y}_c}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u}_j \widetilde{Y}_c\right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{D} \frac{\partial \widetilde{Y}_c}{\partial x_j} - \overline{\rho} \widetilde{u}_j'' \widetilde{Y}_c''\right) + \overline{\dot{\omega}_{Y_c}} + \overline{S_{Y_c}^e}$$
(2.77)

$$\frac{\partial \overline{\rho} \widetilde{Z''^2}}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u_j} \widetilde{Z''^2}\right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{D} \frac{\partial \widetilde{Z''^2}}{\partial x_j} - \overline{\rho} u_j'' \widetilde{Z''^2}''\right) - C_{d,Zv} \overline{\rho} \widetilde{s_{\chi_Z}} - C_g \Phi_{Z,j} \frac{\partial \widetilde{Z}}{\partial x_j}$$
(2.78)

$$\frac{\partial \overline{\rho} \widetilde{Y_c''^2}}{\partial t} + \frac{\partial \left(\overline{\rho} \widetilde{u_j} \widetilde{Y_c''^2}\right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\overline{\rho} \widetilde{D} \frac{\partial \widetilde{Y_c''^2}}{\partial x_j} - \overline{\rho} \widetilde{u_j''} \widetilde{Y_c''^2}''\right) - C_{d,Y_c v} \overline{\rho} \widetilde{s_{\chi Y_c}} - C_g \Phi_{Y_c,j} \frac{\partial \widetilde{Y_c}}{\partial x_j} \qquad (2.79)$$
$$+ 2 \left(\overline{Y_c \dot{\omega}_{Y_c}} - \widetilde{Y_c \dot{\omega}_{Y_c}}\right)$$

$$\frac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u_j}\widetilde{h}\right)}{\partial x_j} = \frac{D\overline{p}}{Dt} - \frac{\partial}{\partial x_j} \left(\overline{q_j} + \overline{\rho}\widetilde{u_j'h''}\right) + \overline{S_H} + \overline{S_H^e}$$
(2.80)

where $\Phi_{Z,j} = \overline{\rho} \widetilde{u_j''Z''}$, and $\Phi_{Y_c,j} = \overline{\rho} \widetilde{u_j''Y_c''}$ are the turbulent fluxes of mixture fraction and progress variable respectively. Tab.2.2 lists the source terms related to the spray cloud.

The diffusive transport of all 4 control variables is treated similarly, assuming a universal diffusion coefficient for these dimensionless quantities. As Eq(2.76) shows, the mixture fraction is a passive scalar, apart of the evaporative source term. The progress variable (Eq.(2.77)) has a source term due to combustion, similarly to Eq.(2.46) this source term is expressed as:

$$\dot{\omega}_{Y_c} = 4\frac{\dot{\omega}_{CO_2}}{W_{CO_2}} + 2\frac{\dot{\omega}_{H_2O}}{W_{H_2O}} + 0.5\frac{\dot{\omega}_{H_2}}{W_{H_2}} + 1\frac{\dot{\omega}_{CO}}{W_{CO}}$$
(2.81)

The progress variable source terms are plotted in in Fig2.7. The source term is negligible for Z > 0.25. It has its maximum near the stoichiometric mixture fraction. At the lowest strain rate the flame is practically unstretched, thus it is close to the chemical equilibrium solution, consequently the source term is zero. With increasing strain rate, the source term increases as it has to balance the effect of stretching (see Eq.(2.40)), and reaches its maximum at the last steady strain rate. The unsteady extinguishing flamelet is characterised by decreasing source terms.



Figure 2.7: Progress variable source term (solid lines: steady flamelets, dashed lines: extinguishing flamelet sampled at different time steps, the colour represents the strain rate: shifts from red to black as the strain rate increases)
The production term of variances is proportional to the turbulent flux of the scalar quantity and its gradient. Note the similarity with the k- ϵ model (Eq.(2.29).) The progress variable variance has an additional production term, since the chemical source term is non-linear in the (Z, Y_c) space. The decay of variances is proportional to their respective turbulent scalar dissipation rates ($\widetilde{s_{\chi_Z}}$ and $\widetilde{s_{\chi_{Y_c}}}$) which need closure. $C_{d,Zv}$, C_{d,Y_cv} , and C_g are modelling constants. $C_g = 2$ is used as it is theoretically coherent. $C_{d,Zv} = C_{d,Y_cv} = 2$ is selected as proposed by Ma (2016).

The enthalpy transport is resolved using Eq.(2.80) only if a 5D FGM is used. For 4D (adiabatic) FGM the enthalpy is in one-to-one correspondence with the mixture fraction:

$$h = h_{ad}(Z) \tag{2.82}$$

thus Eq.(2.80) is unnecessary.

FGM: turbulence modelling The turbulent scalar dissipation rate of mixture fraction and progress variable are modelled similarly to the dissipation in the k- ϵ model:

$$\overline{\rho}\widetilde{s_{\chi_Z}} = \overline{\rho}\frac{\epsilon}{k}\widetilde{Z''^2} \tag{2.83}$$

$$\overline{\rho}\widetilde{s_{\chi_{Y_c}}} = \overline{\rho}\frac{\epsilon}{k}\widetilde{Y_c''^2} \tag{2.84}$$

The turbulent scalar fluxes are modelled with the gradient diffusion assumption. Thus the expressions are simplified to:

$$\Phi_{Z,j} = \overline{\rho} \widetilde{u_j'' Z''} = -\frac{\mu_t}{Sc_t} \frac{\partial \widetilde{Z}}{\partial x_j}$$
(2.85)

$$\Phi_{Y_c,j} = \overline{\rho} \widetilde{u_j'' Y_c''} = -\frac{\mu_t}{Sc_t} \frac{\partial Y_c}{\partial x_j}$$
(2.86)

$$\overline{\rho} u_j'' \widetilde{Z''^2}'' = -\frac{\mu_t}{Sc_t} \frac{\partial \widetilde{Z''^2}}{\partial x_j}$$
(2.87)

$$\overline{\rho}u_j''\overline{Y_c''}'' = -\frac{\mu_t}{Sc_t}\frac{\partial Y_c''^2}{\partial x_j}$$
(2.88)

2.2 Spray theory

In the modelled set-up all the fuel is introduced in liquid state. At the point of injection the whole liquid mass flow is concentrated in the nozzle orifice. Verdier et al. (2017) reported that fuel ligaments are not fund for z > 3 mm, and the droplets are fairly spherical at z > 5 mm.

In this study a Lagrangian approach is adapted for the spray modelling. The spray is assumed to be dilute, i.e.: the volume fraction of the dispersed phase is under 10^{-3} .(Jenny et al., 2012) This is clearly an invalid assumption near the fuel nozzle. Verdier et al. (2017) stated that for z < 10 mm the validation level of PDA measurements is poor because of too high droplet concentration.

The assumption of dilute spray allows the omission of droplet-droplet interactions (like collision), since the probability of close encounters of droplets is negligible. The droplet cloud is modelled using parcels. One parcel represents multiple droplets with the same parameters

(diameter, temperature, velocity, etc.), thus the computational cost of tracking the Lagrangian cloud is reduced.

The density of the liquid fuel is significantly larger than the surrounding gas density, thus the parcels are assumed to be point like. This means that the mass, momentum, and energy source terms which couple the Lagrangian cloud to the gas phase governing equations ($\overline{S^e}_{...}$ Eq.(2.74), Eq.(2.75), Eq.(2.76), Eq.(2.77), and Eq.(2.80)) are considered as point sources. The gas phase domain is spatially discretized thus the source corresponding to a parcel is considered in the computational cell where the parcel is located. This illustrates one disadvantage of the parcels: the relative dispersion between droplets is neglected, which would occur if each parcel represents only one droplet.

2.2.1 Atomization

During the atomization of fuel the liquid sheet that leaves the nozzle separates into larger ligaments, then these break to droplets. For some extent the unfiltered instantaneous OH-PLIF image (Fig.1.3) shows this process. The liquid sheet emerging form the nozzle is broken to droplets well below z = 10 mm. Kannaiyan et al. (2017) studied the pressure swirl atomization of Jet A-1 fuel, the atomization process is illustrated with a shadowgraphy image from their study: Fig.2.8, which shows the breakup of the liquid sheet to ligaments and the further breakup of ligaments to droplets as well. Two qualitatively different sub-processes are distinguished:

- primary breakup: the atomization of the liquid sheet to ligaments and large droplets,
- secondary breakup: further breakup of large droplets.



Figure 2.8: Pressure swirl atomization of Jet A-1 fuel (L = 3.9 mm) (Kannaiyan et al., 2017)

In this study the conditional droplet injection model is used proposed by Ma (2016). This model assumes that spherical parcels enter the computational domain on a disk (approximately the size of the nozzle throat) at the injection plane (z = 0 mm.) The modelling of primary breakup is circumvented using this approach.

The secondary breakup is treated using Taylor analogy breakup (TAB) model which draws an analogy between an oscillating droplet and a spring-mass system. The aerodynamic forces acting on the droplet, the surface tension force, and the viscous forces in the droplet are corresponding to the exciting, restoring, and damping forces in the spring-mass model.

Two ODEs are defined for each parcel: one describing the distortion of the droplet and another describing the change rate of distortion. If the distortion exceeds a threshold, then breakup occurs. Note that although it is modelled, secondary breakup did not occur in the simulation because the parcels already have considerably small diameter at the injection plane.

2.2.2 Dispersion

Dispersion is the kinetic effect of the gas phase on the droplets. The movement of the parcels is described by the equations of motion:

$$\frac{\mathrm{d}\mathbf{X}_p}{\mathrm{d}t} = \mathbf{U}_p \tag{2.89}$$

$$\frac{\mathrm{d}\mathbf{U}_p}{\mathrm{d}t} = \sum \mathbf{a} \tag{2.90}$$

where \mathbf{X}_p is the location and \mathbf{U}_p is the velocity of the parcel. $\sum \mathbf{a}$ is the cumulative acceleration of the parcel. The buoyant forces are neglected, since the fuel is much denser than the surrounding gas. The rotation of the droplets is also assumed to be negligible. Two significant forces are considered:

Drag force:
$$\mathbf{a}_{drag} = \frac{\mathbf{U}_{seen} - \mathbf{U}_p}{\tau_p}$$
 (2.91)

Gravity force:
$$\mathbf{a}_{grav} = \mathbf{g}$$
 (2.92)

where \mathbf{U}_{seen} is the gas phase velocity, \mathbf{g} is the gravitational acceleration, and τ_p is the droplet relaxation time, the latter is defined assuming Stokes flow with Schiller-Neumann correction:

$$\tau_p^{St} = \frac{\rho_{liquid} D_p^2}{18\mu_m} \tag{2.93}$$

$$\tau_p = \frac{\tau_p^{St}}{C_D} \tag{2.94}$$

where ρ_{liquid} is the density of the fuel, and D_p is the diameter of the droplet. μ_m is the mean viscosity considered in the boundary layer around the droplet. The correction coefficient (C_D) is defined as a function of the droplet Reynolds number:

$$C_D = \begin{cases} 1 + 0.15 R e_p^{0.687}, & R e_p \le 1000\\ 0.44 \frac{R e_p}{24}, & R e_p > 1000 \end{cases}$$
(2.95)

where the Reynolds number is:

$$Re_p = \frac{\rho_m |\mathbf{U}_{seen} - \mathbf{U}_p| D_p}{\mu_m}$$
(2.96)

where ρ_m is the density considered in the boundary layer around the droplet.

The seen gas velocity has an average and a turbulent component. The average component is simply interpolated from the solution of Eq.(2.75) ($\tilde{\mathbf{u}}(\mathbf{X}_p, t)$.) Turbulence is considered with velocity perturbation (\mathbf{u}''_{seen}) that has a random direction and magnitude: the direction is uniformly distributed, while the magnitude is considered with the positive part of a normal distribution with expected value: 0 and standard deviation: $\sqrt{2k/3}$. The total seen velocity is:

$$\mathbf{U}_{seen} = \widetilde{\mathbf{u}}(\mathbf{X}_p, t) + \mathbf{u}_{seen}^{\prime\prime}$$
(2.97)

2.2.3 Heat and mass transfer

In this study the infinite conductivity model is applied to treat the heat transfer inside the droplet. This means that the temperature is uniform in the droplet although it evolves in time, thus the energy conservation in in a droplet is described by a single ODE:

$$\frac{\mathrm{d}T_p}{\mathrm{d}t} = \frac{\pi D_p \lambda_m N u_m}{m_p c_{p,liquid}} (T_{seen} - T_p) + \frac{1}{m_p c_{p,liquid}} L_v(T_p) \dot{m}_p \tag{2.98}$$

where Nu_m is the Nusselt number for forced convection around a sphere, $L_v(T_p)$ is the heat of evaporation at the droplet temperature, and λ_m is the thermal conductivity at the mean conditions in the boundary layer.



Figure 2.9: Boundary layer around droplet

The mass of the droplet changes due to evaporation, the mass transfer rate is:

$$\dot{m}_p = \frac{\mathrm{d}m_p}{\mathrm{d}t} = \pi D_p D_m S h_m m_p \rho_{gas} \ln(1 + B_M) \tag{2.99}$$

where D_m is the diffusivity of fuel, and Sh_m is the Sherwood number evaluated at the boundary layer conditions. B_M is the Spalding number defined as:

$$B_M = \frac{Y_{f,surf} - Y_{f,seen}}{1 - Y_{f,surf}} \tag{2.100}$$

where $Y_{f,surf}$ is the mass fraction of fuel on the droplet surface, and $Y_{f,seen}$ is the mass fraction of fuel in the surrounding gas. The latter is a gas phase property, thus it is retrieved from the FGM tables. The former is calculated by assuming the fuel vapour on the droplet surface is in thermodynamic equilibrium with the liquid phase, thus the partial pressure of fuel is the saturation pressure evaluated at the droplet temperature. Hence the molar fraction of fuel on the droplet surface is:

$$X_{f,surf} = \frac{p_{f,sat}(T_p)}{p} \tag{2.101}$$

where $p_{f,sat}(T_p)$ is the saturation pressure of n-heptane. Modelling function no.101 of the National Standard Reference Data Series (Daubert and Danner, 1985) is used to calculate the saturation pressure (default n-heptane in OpenFOAM):

$$p_{f,sat}(T) = \exp\left(87.829 + \frac{-6996.4 \text{ K}}{T} - 9.8802 \ln\left(\frac{T}{1 \text{ K}}\right) + 7.2099 \ 10^{-6} \text{K}^{-2} \ T^2\right) \text{ Pa} \quad (2.102)$$



Figure 2.10: Saturation pressure of n-heptane according to Eq.(2.102)

The droplets' temperatures are generally below boiling point (371.55 K), thus the molar fraction of fuel is lower than one on the droplet surface. As Fig2.10 shows, the partial pressure of fuel rapidly drops as the droplet temperature decreases.

The rest of the gas mixture on the droplet surface originates from the surrounding gas, however the equilibrium condition determines the fuel content on the surface, so the rest of the surface mixture can only consist of species that are not fuel. It is assumed that the surrounding gas mixes with the evaporated fuel fast, thus the chemical reactions in the boundary layer are neglected. With these conditions the fuel mass fraction on the droplet surface is:

$$Y_{f,surf} = \frac{X_{f,surf}W_f}{X_{f,surf}W_f + (1 - X_{f,surf})W_{nonfuel,seen}}$$
(2.103)

where $W_{nonfuel,seen}$ is the molar mass of a mixture which has the composition of the seen gas excluding the fuel:

$$W_{nonfuel,seen} = (1 - Y_{f,seen}) \left(\sum_{k=1,k\neq k_f}^{S} \frac{Y_{k,seen}}{W_k}\right)^{-1}$$
(2.104)

The mass fraction of species other than fuel on the droplet surface is:

$$Y_{k,surf,k\neq k_f} = (1 - Y_{f,surf}) \frac{Y_{k,seen}}{1 - Y_{f,seen}}$$

$$(2.105)$$

As illustrated in Fig.2.9, in a typical case the seen gas temperature is higher than the droplet temperature, and the mass fraction of fuel is lower in the surrounding gas, thus the droplet is evaporating as heat is transferred from the gas to the droplet.

The Nusselt and Sherwood numbers determining heat and mass transfer in Eq.(2.99) and Eq.(2.98) are calculated using the Ranz-Marshall correlation:

$$Sh_m = 2 + 0.6Re_p^{1/2}Sc_m^{1/3}$$
 (2.106)

$$Nu_m = 2 + 0.6Re_p^{1/2}Pr_m^{1/3} \tag{2.107}$$

where Sc_m and Pr_m are the Schmidt and Prandtl numbers evaluated at the boundary layer conditions:

$$Pr_m = \frac{\mu_m c_{p,m}}{\lambda_m} \tag{2.108}$$

$$Sc_m = \frac{\mu_m}{\rho_m D_m} \tag{2.109}$$

Bird's correction is applied to the Nusselt number to account for the heat transfer reduction due to evaporation. (The Ranz-Marshall correlation is valid if there is no mass transfer.) The modified Nusselt number is:

$$Nu'_m = Nu_m \frac{\beta}{e^\beta - 1} \tag{2.110}$$

where β is the non-dimensional evaporation parameter:

$$\beta = -\left(\frac{3Pr_m\tau_p^{St}}{2}\right)\frac{\dot{m}_p}{m_p} \tag{2.111}$$

 Nu_m is replaced by Nu'_m in Eq.(2.98).

2.2.4 Gas properties in the boundary layer

The gas temperature and composition determines its properties around the droplet, which influence the momentum, heat, and mass transfer rates. The composition on the droplet surface is derived in subsection 2.2.3, and the composition of the surrounding gas is already known, however neither of these two states characterizes the boundary layer well. A reasonable compromise is reached by applying the so-called "1/3 rule". The boundary layer is characterized by the linear combination of the seen and surface states:

$$T_m = (1 - \alpha)T_p + \alpha T_{seen} \quad \text{and} \quad Y_{k,m} = (1 - \alpha)Y_{k,surf} + \alpha Y_{k,seen} \tag{2.112}$$

where $\alpha = 1/3$ is applied.

This method allows the calculation of density, viscosity, thermal conductivity, mass diffusivity, and specific heat in the boundary layer. However in the context of FGM this is illogical, since all the species mass fractions have to be retrieved from the FGM tables. The species tables are needed during runtime, thus all of them are stored in the memory (RAM.) The main disadvantages are the following:

- The available RAM limits the *size of the applicable reaction mechanism*, since the number of species cannot be arbitrary. This contradicts with the basic idea behind FGM: separation of species from the 3D solution.
- The available RAM also limits *parallelization*. Parallel computation in OpenFOAM is implemented by dividing the computational domain into multiple sub-domains. Each sub-domain is solved by a new instance of the solver. With this approach each new instance of the solver needs to store its own FGM tables in the RAM. If the necessary tables include all the species tables, then memory can be a bottleneck for parallelization.
- A substantial performance penalty is also associated with this method, as the species mass fractions are retrieved in every cell of the discretized domain, not just in the cells that contain parcels.

The main contribution of this graduation project is a solution to aforementioned problems. With the newly developed method the droplet surface is described by the FGM controlling variables $(Z_{surf}, Y_{c,surf}, \widetilde{Z''_{surf}}, \text{ and } \widetilde{Y''_{c,surf}})$ Thus there is no need for storing the species tables in the memory. The method is illustrated in Fig.2.11.



Figure 2.11: Boundary layer around droplet with FGM

Eq.(2.101) is used to determine the molar fraction of fuel on the surface, but in Eq.(2.103) the average molar mass of the non-fuel species ($W_{nonfuel,seen}$) is retrieved from an FGM table instead of being calculated.

The fuel vapour one-to-one contributes to the mixture fraction on the droplet surface, but the non-fuel components of the surrounding gas can also contain mass that originates from the fuel, thus the surface mixture fraction is calculated as:

$$Z_{surf} = Y_{f,surf} + (1 - Y_{f,surf})Z_{nonfuel,seen}$$
(2.113)

where $Z_{nonfuel,seen}$ is the mixture fraction of the seen gas mixture excluding the fuel, calculated as: $Z_{nonfuel,seen} = Z_{seen} - Y_{f,seen}$. The progress variable on the droplet surface is calculated similarly:

$$Y_{c,surf} = (1 - Y_{f,surf})Y_{c,nonfuel,seen}$$

$$(2.114)$$

where $Y_{c,nonfuel,seen}$ is the progress variable of the seen gas mixture excluding the fuel. This quantity is also tabulated during the FGM table generation just like $W_{nonfuel,seen}$. The mixture fraction and progress variable variances on the droplet surface are calculated similarly to the progress variable:

$$\widetilde{Z_{surf}^{\prime\prime2}} = (1 - Y_{f,surf})\widetilde{Z_{seen}^{\prime\prime2}}$$
(2.115)

$$\widetilde{Y_{c,surf}^{\prime\prime\prime2}} = (1 - Y_{f,surf})\widetilde{Y_{c,seen}^{\prime\prime2}}$$
(2.116)

If 4D FGM is used there is a possibility that the droplet temperature is different from the temperature corresponding to $\left(Z_{surf}, Y_{c,surf}, \widetilde{Z_{surf}''}, \widetilde{Y_{c,surf}''}\right)$. This inconsistency is one of the disadvantages of the new droplet model. It can only be resolved using 5D FGM, where Newton-Raphson method is used to find the enthalpy corresponding to the droplet temperature keeping the other control variables constant:

$$T\left(Z_{surf}, Y_{c,surf}, \widetilde{Z_{surf}'^{\prime 2}}, \widetilde{Y_{c,surf}'^{\prime 2}}, h_{surf}\right) = T_p$$
(2.117)

The "1/3 rule" is still applied but to the control variables:

$$Z_m = (1 - \alpha) Z_{surf} + \alpha Z_{seen} \tag{2.118}$$

$$Y_{c,m} = (1 - \alpha)Y_{c,surf} + \alpha Y_{c,seen}$$
(2.119)

$$\widetilde{Z_m'^2} = (1 - \alpha)\widetilde{Z_{surf}''^2} + \alpha \widetilde{Z_{seen}''^2}$$
(2.120)

$$\widetilde{Y_{c,m}^{\prime\prime 2}} = (1 - \alpha) Y_{c,surf}^{\prime\prime 2} + \alpha \widetilde{Y_{c,seen}^{\prime\prime 2}}$$
(2.121)

$$h_m = (1 - \alpha)h_{surf} + \alpha h_{seen} \tag{2.122}$$

The gas properties: μ_m , $c_{p,m}$, and λ_m are directly retrieved from the FGM tables. The density is calculated from the ideal gas law (Eq.(2.9)) using the resolved pressure and the tabulated compressibility: $\psi = W/(R_uT)$:

$$o_m = p_{seen}\psi_m \tag{2.123}$$

The mass diffusivity that is used to calculate the Schmidt number and the $\rho_m D_m$ mass transfer rate is the mass diffusivity of n-heptane at the boundary layer conditions.

Without this development the applied hardware cannot handle the Lu and Law mechanism, as it incorporates 188 species. The viscosity, specific heat, thermal conductivity and compressibility are necessary for the solution of the gas phase equations. Two new tables are generated in the preprocessing phase $(Z_{nonfuel} \text{ and } Y_{c,nonfuel})$, these and the fuel mass fraction table Y_f are still necessary for the simulation. However the rest of the species mass fractions are not needed, thus S - 3 lookup tables¹ become unnecessary. In the 4D FGM cases each lookup table contains $101 \times 101 \times 11 \times 11 = 1234321$ double precision numbers (8 B), which is approximately 9.42 MB. Thus in case of Lu and Law mechanism this improvement omits the usage of 185×9.42 MB ≈ 1.7 GB RAM for each parallel thread.

Note that although the new droplet model appears to be quite similar to the old one, the necessary modifications of the OpenFOAM source code are not trivial. In the old solver the FGM lookup is only used once in every time step to retrieve gas properties, thus a loosely integrated code is adequate. In the new approach the FGM lookup has to be included in the thermodynamic model, thus it is accessible for both the droplet model and the gas phase equations.

2.2.5 Coupling to gas phase equations

The ODEs describing the state of the parcels (Eq.(2.89), Eq.(2.90), Eq.(2.98), and Eq.(2.99)) couple the parcel with the gas phase properties. In this study two way coupling is realised. I.e.: not only the droplets are affected by the gas phase, but the effect of droplets is represented in the gas phase governing equations too.

This is implemented through source terms in Eq.(2.74), Eq.(2.75), Eq.(2.76), Eq.(2.77), and Eq.(2.80). The source terms are presented in Table 2.2 where the number of droplets represented by a parcel is N_p , the volume of the computational cell containing the parcel is V_{cell} , the t_n and $t_n + \Delta t$ superscripts mark the old and new time steps, and $h_{f,vapour}(T_p)$ is the specific enthalpy of the evaporated fuel.

The evaporating fuel increases the mass contained in the cell, similarly the mixture fraction increases too. The vapour added to the gas is pure fuel, thus the mass and mixture fraction sources are the same. The change in gas phase momentum due to drag is equal to the drag acting on the droplets but has opposite sign. The gas phase momentum also changes due to the added vapour which moves with the same velocity as the droplet. The progress variable decreases as the evaporating fuel dilutes the gas mixture, although according to Ma and Roekaerts (2017) this effect is negligible. The gas phase enthalpy is changed by heat transfer between the gas and the droplets, and by the mixed in vapour which generally has a lower enthalpy than the surrounding gas. Note that \dot{m}_p is negative if the droplet is evaporating. The source terms in the $k - \epsilon$ model are neglected. (Ma, 2016)

 Table 2.2:
 Source terms due to the presence of parcels

Source term	Discretized expression
$\overline{S^e_{ ho}}$	$-\frac{1}{V_{cell}}\sum_p \dot{m}_p N_p$
$\overline{S^e_{u_i}}$	$-\frac{1}{V_{cell}}\sum_p m_p N_p \left[\left(U_{p,i}^{t_n + \Delta t} - U_{p,i}^{t_n} \right) / \Delta t - g_i \right] - \frac{1}{V_{cell}}\sum_p \dot{m}_p N_p U_{p,i}^{t_n}$
$\overline{S_Z^e}$	$-rac{1}{V_{cell}}\sum_p \dot{m}_p N_p$
$\overline{S^e_{Y_c}}$	$-\widetilde{Y_{c,seen}}\overline{S^e_{ ho}}$
$\overline{S_{H}^{e}}$	$\frac{1}{V_{cell}}\sum_{p}N_p\left(T_p - T_{seen}\right)\pi D_p\lambda_m N u_m - \frac{1}{V_{cell}}\sum_{p}\dot{m}_p N_p h_{f,vapour}(T_p)$

¹Each lookup table is stored in a separate file, and loaded to the RAM during runtime if necessary.

Chapter 3

Application

The CORIA Jet Spray Flame introduced in section 1.1 is used to validate the simulation approach. The case specific settings are elaborated below.

3.1 Geometry and Mesh

The domain consists of a cylinder downstream the injection plane, with a diameter of 400 mm and a height of 300 mm. Shum-Kivan et al. (2017) use a cylinder with the same parameters to model the atmosphere, however the upstream geometry (injection system) is also included in their domain. With these parameters the boundaries are assumed to be far enough not to affect the region of interest ($z \in [0 \text{ mm}, 80 \text{ mm}]$ and $x \in [-40 \text{ mm}, 40 \text{ mm}]$.)



Figure 3.1: Simulation domain (blue: air inlet, red: burner wall, grey: atmosphere)

Fig.3.1 shows the domain, marking the different boundaries:

- The air inlet is an annulus at z = 0 mm with inner and outer radii of 5 mm and 10 mm.
- The burner wall is considered at z = 0 mm for radii below 5 mm and for an annulus of inner and outer radii of 10 mm and 70 mm.
- All other boundaries are representing the atmosphere.

3.1.1 Mesh

OpenFOAM's blockMesh utility is used to create the mesh. Fig.3.2 and Fig.3.3 show the structure of the mesh along the axis of the cylindrical domain and perpendicular to it.



Figure 3.2: Cross section of mesh along the axis (a: cross section of the whole domain, b: refinement around air inlet annulus)

A structured mesh is used with hexahedral cells. The axial (z) and radial (x and y) distribution of nodes is independent. The cells near the fuel nozzle have a characteristic size of 0.66 mm. In the axial direction the mesh is coarsened with an expansion ration of 1.01 for $z \in [0 \text{ mm}, 100 \text{ mm}]$. Further downstream the expansion ration is increased to 1.03.

The grid is more complex in the x - y plane, so it can accommodate the air inlet and the cylindrical nature of the geometry. The details are illustrated in Fig.3.3. In the centre of the domain is covered by a 4 mm × 4mm block to avoid unnecessarily small wedge shaped cells along the axis. The cells surrounding this central block are stretched such that at r = 5 mm the cell edges are aligned with the tangential direction. For r > 5 mm the mesh is axisymmetric. The characteristic cell size and the size of the central block together define the circumferential discretization of the outer parts of the domain.



Figure 3.3: Cross section of mesh perpendicular to axis
(a: cross section of the whole domain, b: refinement around air inlet annulus)

The radial spacing of nodes is refined around the air inlet and coarsened towards the outer radii. The radial size of cells decrease to 0.2 mm around the edges of the inlet annulus. The radial cell size is restored to 0.66 mm at r = 12.5 mm. Outside this region the radial expansion ratio is 1.01, it is increased to 1.03 for r > 70 mm. The radial refinement around the air inlet is only implemented below z = 100 mm, where the refinement is suddenly discontinued. (See Fig.3.2b)

The mesh consists of 459264 cells, divided by 1383692 faces out of which 1373924 are internal. The cells are fairly orthogonal on most part of the domain. The maximal aspect ratio is 32.9, which is caused by the independent radial and axial meshing (i.e.: in some locations the radial and axial cell size is significantly different.)

3.2 Boundary conditions

3.2.1 Gas phase boundary conditions

As mentioned before, there are three different boundaries in this model: the air inlet, the burner wall, and the atmosphere. The modelling approach applied in each case is described below. Boundary conditions are needed for pressure, velocity, turbulent kinetic energy and dissipation rate, and the FGM controlling variables: mixture fraction, progress variable, their variances, and enthalpy (in case of 5D FGM).

Air inlet 6 g/s air is supplied through the inlet annulus. Since the injection system (see Fig.1.1) is not included in the domain, the air inlet velocity profile is modelled. The model profile is based on fully developed flow in annuli. (Brighton and Jones, 1964) The hydraulic diameter of an annulus is:

$$D_{hyd,ann} = D_{outter} - D_{inner} = 10 \text{ mm}$$
(3.1)

where $D_{inner} = 10$ mm and $D_{outter} = 20$ mm. The Reynolds number of the annulus is:

$$Re_{ann} = \frac{u_{mean} D_{hyd,ann} \rho_{ann}}{\mu_{ann}} = 13731 \tag{3.2}$$

where $u_{mean} = 21.58$ m/s is the mean inlet velocity, $\rho_{ann} = 1.180 \text{ kg/m}^3$ is the density at the inlet conditions, and $\mu_{ann} = 1.85448 \ 10^{-5}$ Pa s is the viscosity at the inlet conditions. The friction factor definition and a proposed correlation according to Brighton and Jones (1964) is:

$$f = -\frac{D_{hyd,ann}}{2\rho_{ann}u_{mean}^2}\frac{\partial p}{\partial x} = 0.087Re_{ann}^{-0.25} = 0.008037$$
(3.3)

for $Re_{ann} > 4000$. Based on the momentum balance of unit length of annular pipe, the wall shear stress is:

$$\tau_w = \frac{A}{P} \frac{\partial p}{\partial x} = 0.5 \rho_{ann} u_{mean}^2 f = 2.208 \text{ Pa}$$
(3.4)

where A is the cross section area, and P is the perimeter of the pipe. The friction velocity (Pope, 2000) is defined as:

$$u_{\tau} = \sqrt{\frac{\tau_w}{\rho_{ann}}} = u_{mean}\sqrt{0.5f} = 1.368 \ \frac{\mathrm{m}}{\mathrm{s}}$$
 (3.5)

Brighton and Jones (1964) conclude, that the boundary layers near the inner and outer wall are well represented by fully developed channel flow for the given geometry. The profiles join at the location of velocity maximum (r_{max}) . Croop and Rothfus (1962) suggests that r_{max} is such, that:

$$\xi = \frac{r_{max} - r_{inner}}{r_{outer} - r_{inner}} = 0.47 \tag{3.6}$$

However in this study, the location of velocity maximum is shifted inwards ($\xi = 0.3$), considering the inertia of airflow in the curved inlet geometry. The local wall distance is defined as:

$$y = y(r) = \begin{cases} r - r_{inner}, & r < r_{max} \\ r_{outer} - r, & r \ge r_{max} \end{cases}$$
(3.7)

or in dimensionless form (in *wall units* (Pope, 2000)):

$$y^{+} = \frac{\rho_{ann} u_{\tau} y}{\mu_{ann}} \tag{3.8}$$

According to Pope (2000) the boundary layer is divided into 4 regions:

- 1. Viscous sub-layer $y^+ \leq 5$
- 2. Buffer layer $5 < y^+ \le 30$
- 3. log-law region $30 < y^+$ and $y/y(r_{max}) \le 0.3$
- 4. Core region $0.3 < y/y(r_{max})$

where the axial velocity in the viscous sub-layer is:

$$u_{ax} = u_{\tau} y^+ \tag{3.9}$$

and in the log-law region is:

$$u_{ax} = u_{\tau} \left(5.2 + \frac{1}{0.41} \ln(y^+) \right) \tag{3.10}$$

The buffer layer is modelled with a 4th order polynomial with coefficients such that it is 2nd order continuous on both sides. The core region is modelled similarly, using the assumed maximum location. The maximum velocity value is obtained, by extrapolating the two log-layer profiles to the maximum location, and selecting the lower value. (The way of this extrapolation does not have a strong effect on the profile, since the velocity gradient is fairly low in the core region.)



Figure 3.4: Cross section of KIAI burner inlet Cordier et al. (2013)

To accommodate the complex inlet geometry, a radial velocity component is added. The magnitude of the radial component is defined such, that the velocity vector is tilted with a prescribed angle, which is a linear function of the radius. Thus the tilting is characterised by the angles at the inner and outer edge of the annulus. So the radial velocity is:

$$u_{rad} = \tan(\alpha)u_{ax} \tag{3.11}$$

where α is the angle between the axial direction and the real velocity vector:

$$\alpha = \alpha_{inner} + \frac{\alpha_{outer} - \alpha_{inner}}{r_{outer} - r_{inner}} \left(r - r_{inner} \right)$$
(3.12)

where $\alpha_{inner} = -18^{\circ}$ and $\alpha_{outer} = -13^{\circ}$ is applied. Fig.3.1 justifies the selection of α_{inner} , while α_{outer} is not rationalised here. A sensitivity study showed the benefit of not imposing

fully axial velocity at the outer perimeter. The velocity profile presumed at the air inlet annulus is illustrated in Fig.3.5. A novel OpenFOAM utility is introduced to set the annular velocity profile parametrized by the diameters, inlet angles, mass flow, density, viscosity, and the location of velocity maximum. The pressure is treated with zero-gradient boundary condition.



Figure 3.5: Inlet velocity profile

Dirichlet boundary conditions are imposed for the turbulent kinetic energy (k) and its dissipation rate (ϵ) . The turbulent kinetic energy is set to $15 \text{ m}^2/\text{s}^2$. The turbulence intensity is defined as the ratio of turbulent and mean velocity scales. (Pope, 2000) The prescribed turbulent kinetic energy corresponds to a turbulent intensity of:

$$I = \frac{\sqrt{\frac{2}{3}k}}{u_{mean}} = 14.7\%$$
(3.13)

based on the average inlet velocity. The dissipation rate of turbulent kinetic energy is determined based on an assumed turbulent mixing length at the inlet l = 0.7 mm:

$$\epsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{l} = 13637 \text{ m}^2/\text{s}^3 \tag{3.14}$$

where $C_{\mu} = 0.09$ is a model constant of the $k - \epsilon$ model. This is set using the OpenFOAM boundary condition: compressible::turbulentMixingLengthDissipationRateInlet. Note that the mixing length (l) applied here is different from the turbulent length scale (l_t) of the $k - \epsilon$ model.

The inlet is pure air, at room temperature, thus the FGM control variables are trivial: $Z = 0, Y_c = 0, \widetilde{Z''^2} = 0, \widetilde{Y_c''^2} = 0$, and if 5D FGM is used $h = h_{ad}$. These boundary conditions define the inlet temperature and gas properties.

Burner wall No-slip boundary condition is applied for the velocity. The built-in OpenFOAM wall functions (compressible::kqRWallFunction and compressible::epsilonWallFunction) were used to characterise the turbulence properties at the wall. OpenFOAM's wall function for the turbulent kinetic energy (k) is a simple zero-gradient boundary condition, while the dissipation rate (ϵ) boundary condition overwrites the dissipation and production terms of the $k - \epsilon$ model in the boundary cell:

$$\epsilon = C_{\mu}^{3/4} \frac{k^{3/2}}{0.41\Delta s} \tag{3.15}$$

$$P_k = \mu_t \left| \frac{\partial \widetilde{\mathbf{u}}}{\partial s} \right| C_{\mu}^{1/4} \frac{k^{1/2}}{0.41\Delta s}$$
(3.16)

where s is the coordinate perpendicular to the wall, Δs is the distance of the wall from the cell centroid. The FGM control variables (including the enthalpy in case of 5D FGM) are treated with zero-gradient boundary conditions.

Atmosphere The velocity and pressure boundary conditions are coupled on the boundaries representing the atmosphere. For this OpenFOAM's pressureInletOutletVelocity and totalPressure boundary conditions are applied. Using the totalPressure boundary condition, the pressure at the boundary is calculated as:

$$p = p_0 - 0.5\rho |\tilde{\mathbf{u}}|^2 \tag{3.17}$$

where p_0 is the total pressure, ρ is the density obtained from the internal field, $\tilde{\mathbf{u}}$ is the velocity vector on the boundary. A new OpenFOAM preprocessing utility is developed to set non-uniform total pressure on the boundary that includes the hydrostatic pressure:

$$p_0 = p_{0,ref} + \rho \mathbf{g} \cdot (\mathbf{x} - \mathbf{x_{ref}}) \tag{3.18}$$

where $p_{0,ref} = 101325$ Pa is the total pressure at the reference point: $\mathbf{x_{ref}} = [0, 0, 300]$ mm. (Without including the gravity effects on the boundary, there would be a downward flow along the outer edge of the domain.)

The pressureInletOutletVelocity boundary condition sets the velocity boundary condition such that, for outflows it is a zero-gradient boundary condition. For inflows the velocity on the boundary is determined from the internal velocity field. The two boundary conditions are coupled through the momentum governing equations (Eq.(2.75).) An increasing inflow velocity decreases the boundary pressure (Eq.(3.17)), thus modifying the pressure gradient. This two changes have opposing effect on the momentum equation, thus a steady solution is possible.

For outflow both the turbulence variables and the FGM control variables are modelled with a zero-gradient boundary condition. For inflow the turbulent kinetic energy and its dissipation rate are treated with turbulentIntensityKineticEnergyInlet and compressible::turbulentMixingLengthDissipationRateInlet respectively. The turbulent kinetic energy is:

$$k = 1.5(I|\widetilde{\mathbf{u}}|)^2 \tag{3.19}$$

where a turbulence intensity of I = 0.5% is applied. The dissipation rate is determined using Eq.(3.14) with a turbulent mixing length of l = 5 mm. These values correspond to a very low level of turbulence which represent the quiescent air of the laboratory. The FGM control variables are set similarly to the air inlet $(Z = 0, Y_c = 0, \widetilde{Z''^2} = 0, \widetilde{Y''^2} = 0, h = h_{ad})$

3.2.2 Droplet boundary conditions

The parcels are introduced on a disk centred at [0, 0, 0] mm with a diameter of 0.2 mm which corresponds to the real injector orifice. Each parcel has the same initial mass, 2.2 10^6 parcels are introduced in each second, thus the initial parcel mass is:

$$m_{parcel,ini} = \frac{0.28 \ 10^{-3} \ \text{kg/s}}{2.2 \ 10^6 \ 1/\text{s}} = 1.273 \ 10^{-10} \ \text{kg}$$
 (3.20)

The initial droplet temperature is set to $T_{p,ini} = 298$ K in accordance with the measurements. The temperature is limited to the [270 K, 371.55 K] interval. OpenFOAM's default functions are used to calculate the density, and specific heat of the liquid, and the heat of vaporisation for n-heptane. (Daubert and Danner, 1985) The liquid density is calculated as:

$$\rho_{p,liquid}(T_p) = \frac{61.38396836 \text{ kg/m}^3}{0.26211 \left[1 + \left(1 - \frac{T_p}{540.2 \text{ K}} \right)^{0.28141} \right]}$$
(3.21)

which means an initial density of $\rho_{p,liquid}(T_{p,ini}) = 681.7 \text{ kg/m}^3$. This way one parcel corresponds to N_p droplets:

$$N_p = \frac{6m_{parcel,ini}}{D_p^3 \pi \rho_{p,liquid}(T_{p,ini})} = \left(\frac{70.99 \ \mu m}{D_p}\right)^3$$
(3.22)

The specific heat of the droplets is calculated as:

$$c_{p,liquid}(T_p) = \frac{a^2}{\eta} + b - 2ac\eta - \eta^2 ad - \eta^3 c^2/3 - \eta^4 cd/2 - \eta^5 d^2/5$$
(3.23)

$$\eta = 1 - T_p/T_c, \ T_c = 540.2 \text{ K},$$

$$a = 6.11976102401216 \ \sqrt{J/(\text{kg K})}, \ b = 3137.69909384855 \text{ J/(kg K)}$$

$$c = 182.274175063868 \ \sqrt{J/(\text{kg K})}, \ d = -254.530511150515 \ \sqrt{J/(\text{kg K})}$$

The heat of vaporization is:

$$L_v(T_p) = 499121.791545248 \frac{\mathrm{J}}{\mathrm{kg}} \left(1 - \frac{T_p}{T_c}\right)^{0.38795}$$
(3.24)

The average magnitude of the initial droplet velocity is set to $|\mathbf{U}_{\mathbf{p},\mathbf{mean}}| = 32.88 \text{ m/s}$. The conditional droplet injection model proposed by Ma (2016) is used for scaling the velocity magnitude and introducing a random component in the initial direction. Fig.3.6 illustrates a general case of the conditional droplet injection model.



Figure 3.6: Conditional droplet injection model (Ma, 2016)

The direction is varied around the nominal spray angle ($\theta_{mid} = 40^\circ$), but the range depends on the droplet diameter and is not necessarily symmetric. The direction of injection is determined as:

$$\theta_p = \begin{cases} \theta_{min}(D_p) + 2\Lambda \left[\theta_{mid} - \theta_{min}(D_p)\right], & 0 \le \Lambda < 0.5\\ \theta_{mid} + (2\Lambda - 1) \left[\theta_{max}(D_p) - \theta_{mid}\right], & 0.5 \le \Lambda \le 1 \end{cases}$$
(3.25)

where $\Lambda \in [0, 1]$ is a random number, θ_{min} and θ_{max} are the minimum and maximum injection angles associated with the droplet diameter. The limiting angles are determined for two diameters and interpolated in-between:

$$\theta_{min}(D_p) = \begin{cases} \theta_{min,S}, & D_p < D_S \\ \theta_{min,S} + \frac{\theta_{min,L} - \theta_{min,S}}{D_L - D_S} \left(D_p - D_S \right), & D_S \le D_p \le D_L \\ \theta_{min,L}, & D_L < D_p \end{cases}$$
(3.26)

$$\theta_{max}(D_p) = \begin{cases} \theta_{max,S}, & D_p < D_S \\ \theta_{max,S} + \frac{\theta_{max,L} - \theta_{max,S}}{D_L - D_S} \left(D_p - D_S \right), & D_S \le D_p \le D_L \\ \theta_{max,L}, & D_L < D_p \end{cases}$$
(3.27)

where $D_S = 20 \ \mu \text{m}$ and $D_L = 70 \ \mu \text{m}$ are the two droplet diameters ("small" and "large") where the limiting angles are defined: $\theta_{min,S} = 20^\circ$, $\theta_{max,S} = 60^\circ$, $\theta_{min,L} = 35^\circ$, and $\theta_{max,L} = 42^\circ$.

The scaling of the velocity magnitude is coupled to the variation of the injection angle by applying the same random variable. A is rescaled such that it increases from 0 to 1 as the spray angle ranges from θ_{mid} to the limiting angles. The rescaled random variable is:

$$\eta = |2\Lambda - 1| \tag{3.28}$$

The droplet velocity ranges from $|\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1+\alpha_p)$ at the middle to $|\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1-\alpha_p)$ at the edges, where $\alpha_p = 0.05$ is applied:

$$|\mathbf{U}_{\mathbf{p}}| = |\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1+\alpha_p) + \eta [|\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1-\alpha_p) - |\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1+\alpha_p)] = (3.29)$$
$$= |\mathbf{U}_{\mathbf{p},\mathbf{mean}}|(1+\alpha_p - 2\alpha_p\eta)$$

Fig.3.7 shows the trajectory of the droplets based on the PDA data measured at z = 7 mm in the non-reacting case. Due to the high velocities at the air inlet only the largest droplets $(D_p > 40 \ \mu\text{m})$ can maintain the nominal spray angle. The velocity of droplets below 15 μm relaxes to the gas phase flow fast, thus these follow the air jet which is inclined towards the axis.

Ma (2016) justifies the choice of parameters for the conditional droplet injection model using a plot similar to Fig.3.7, however the flow characteristic is entirely different in this work. Ma (2016) studied the Delft Spray-in-Hot-Coflow flame, where a generally axial and low velocity co-flow is applied. Whereas in the CORIA Jet Spray Flame the air inlet annulus is characterised by high inlet velocity concentrated in a small region. The incoming air jet acts as a filter separating the small droplets which are carried towards the axis by the air jet, but leaving larger droplets to maintain quasi-ballistic trajectory.

Fig.3.8 underlines this phenomena. The individual droplet PDA data is provided for 6 radial locations. The droplet size PDF is reconstructed for all 6 locations. The PDFs show, that for locations inside the nominal spray angle ($x \in [0 \text{ mm}, 4 \text{ mm}]$) the droplets are predominantly



Figure 3.7: Measured droplet trajectory angle at z = 7 mm (non-reacting case, plotted from the individual droplet PDA data for all radial measurement locations.) $\theta_{mid} = 40^\circ, \ \theta_{min} \text{ and } \theta_{max} \text{ are determined using Eq. (3.26) and Eq. (3.27) respectively.}$ Note that a negative θ denotes the droplets moving towards the axis.

small and rather mono-disperse. While for $x \in [6 \text{ mm}, 10 \text{ mm}]$ all droplet sizes are present and the mode is located at a larger diameter.

The initial parcel size PDF is modelled with Rosin-Rammler distribution. Note that in accordance with Eq.(3.22) a parcel of larger diameter represents fewer droplets. Thus the parcel size PDF has to be weighted with D_p^{-3} to obtain the droplet size PDF. Using Rosin-Rammler distribution the diameter associated with a parcel is calculated as:

$$D_p = D_{p,min} + \overline{D_p} \left[-\ln\left(1 - \Lambda K\right) \right]^{\frac{1}{n}}$$
(3.30)

where $D_{p,min} = 3.5 \ \mu\text{m}$ is the minimal diameter, $\overline{D_p} = 35.062 \ \mu\text{m}$ is such, that the average diameter is $(D_{p,min} + \overline{D_p})$, Λ is a random variable, n = 3.45 is a parameter expressing the dispersion (as *n* increases the distribution approaches a Dirac δ around the average diameter), and *K* is defined as:

$$K = 1 - e^{-\left(\frac{D_{p,max} - D_{p,min}}{\overline{D_p}}\right)^n}$$
(3.31)

where $D_{p,max} = 70 \ \mu \text{m}$ is the maximum diameter. The parcel size probability density function imposed at the injection disk is presented in Fig.3.9. The D_p^{-3} weighting shifts the PDF towards smaller diameters. The mode of the *droplet* PDF is located at 16.25 μ m. Note that the measurement data presented in Fig.3.9 combines the measurements at all 6 radial locations. At each location the measurements are conducted either for 30 s or the first 40000 samples. (Verdier et al., 2017) At most locations (except x = 8 mm and 10 mm) the 40000 limit is reached, so the measurement time frame varies from location to location, thus PDFs are not comparable. Nevertheless Fig.3.9 gives insight of the relation between the measured and the modelled PDFs.



Figure 3.8: Droplet size PDF at z = 7 mm (non-reacting case, plotted from the individual droplet PDA data, bin size: 0.5 μ m)



Figure 3.9: Imposed droplet and parcel PDF at z = 0 mm and the measured PDF at z = 7 mm for all x

3.3 Base case results

This section presents the base case results of 4D and 5D FGM simulations. The base case mesh and boundary conditions are the ones presented in sections 3.1 and 3.2. Lu and Law mechanism (188 species) is used to generate the manifold. The 4D and 5D FGM cases are named "FIN01" and "FIN02" respectively.



Figure 3.10: Gas temperature contour plot in base cases $(z \in [0 \text{ mm}, 80 \text{ mm}] \text{ and } x \in [0 \text{ mm}, 40 \text{ mm}])$

Fig.3.10 and Fig.3.11 show the flame structure. These figures also illustrate the position of the air inlet, and the nominal spray half-angle. The source term of the progress variable (Eq.(2.81)) reveals the double flame structure, while the temperature contour shows that there is hot flue gas between the inner and outer flames.

The flame lift-off height is affected by multiple interacting phenomena. The cold droplets cross the high velocity air jet, where the evaporation is negligible since the air jet is cool. As the droplets reach the edge of the air jet, they cross the flame front. Evaporation is significantly faster as the droplets are surrounded by the mixture of hot flue gasses and fuel which is low in oxygen. The fuel mixes with the air jet (inner flame), and the quiescent air of the environment (outer flame) to reach stoichiometric mixture fraction, where the progress variable source term is the highest (Fig.2.7.)

Fig.3.12a, Fig.3.12b, and Fig.3.12c provide a comparison for the measured and simulated OH profiles. This underlines one of the limitations of RANS simulation: an average flame front



Figure 3.11: Progress variable source term contour plot in base cases ($z \in [0 \text{ mm}, 80 \text{ mm}]$ and $x \in [0 \text{ mm}, 40 \text{ mm}]$)



Figure 3.12: OH contour comparison

location is reproduced, while in reality both the inner and outer flame fronts are unsteady. The higher frequency fluctuations (inner flame) can be partially captured by the turbulence-chemistry interaction model: the assumed PDF method. However the low frequency movement of the upper part ($z \ge 50$ mm) of the outer flame is harder to represent.

Fig.3.13 shows the mixture fraction and its source term (see $\overline{S_Z^e}$ in Tab2.2.) The source term contour confirms that intensive evaporation happens between the two flame fronts. The large droplets approximately maintain their original trajectory, and enter the burnt region at



(a) Mixture fraction

(**b**) Mixture fraction source term

Figure 3.13: Contour plot of mixture fraction mean field and source term in base cases $(z \in [0 \text{ mm}, 80 \text{ mm}] \text{ and } x \in [0 \text{ mm}, 40 \text{ mm}])$



Figure 3.14: Contour plot of control variable variances in base cases ($z \in [0 \text{ mm}, 80 \text{ mm}]$ and $x \in [0 \text{ mm}, 40 \text{ mm}]$)

the flame base. The smaller droplets reach higher axial locations before crossing the inner flame front. Overall the droplets are concentrated in the lower 25 mm of the flame. The mixture fraction source term has another peak near the injector, where the spray is dense. Since the primary atomization is not modelled, the parcels already represent a fine spray cloud $(D_p \in [3.5 \ \mu\text{m}, 70 \ \mu\text{m}])$ at the injection plane. Consequently the interface density is overestimated, which causes significant evaporation even in cold gasses.

Fig.3.14 shows the variances of progress variable and mixture fraction. Both variances have their peak values in the inner flame front, which indicates the turbulent, corrugated nature of this part (see Fig.3.12c.) The fluctuations of the outer flame front are represented by lower variances. Note that high variances can inhibit the reactions. As Fig.2.6 illustrates a high variance turns the β -function bimodal with the two modes at 0 and 1. For mixture fraction this implies alternating between lean and rich states, while for scaled progress variable the two states

are unburnt and fully burnt. Fig.2.7 indicates that high progress variable source terms occur at intermediate mixture fractions $(Z \approx Z_{st})$ and intermediate progress variables (high strain rate flamelets.) Thus high variances decrease the progress variable source term.



Figure 3.15: Axial gas phase velocity in base cases

Fig.3.15 and Fig.3.16 show the mean velocity field at different axial locations. The simulation matches the measured values quite well. The notable discrepancies are the following:

- At z = 5 mm and 7 mm the velocity along the axis is too high. The negative velocities are not observed in the simulation. This is most probably caused by the poor performance of the standard $k \epsilon$ model.
- For $z \ge 35$ mm the velocity field is affected by the presence of the flame. Since the outer flame location is not predicted perfectly:
 - a) the axial velocity is under-predicted for $x \ge 10 \text{ mm}$,
 - b) the radial spreading is not reproduced.

The velocity comparison at z = 5 mm suggests that the inlet velocity boundary condition presented in subsection 3.2.1 performs considerably well.



Figure 3.16: Radial gas phase velocity in in base cases

The turbulent kinetic energy profiles are presented in Fig.3.17. To construct the turbulent kinetic energy from the measurement data, isotropy is assumed in the radial and circumferential direction. Thus the measured turbulent kinetic energy is:

$$k_{measurment} = \frac{1}{2} \left(\widetilde{u_z''^2} + 2 \ \widetilde{u_x''^2} \right) \tag{3.32}$$

Verdier et al. (2017) use the same assumption.

The measurements show, that a turbulent kinetic energy peak develops at a radial location of 10 mm. This peak reaches its maximum at z = 30 mm, for higher axial locations the peak declines. This characteristic change in behaviour coincides with the flame lift-off height. The simulations reproduce the profile adequately for $z \leq 16$ mm. However in the simulation, the peak value does not rise and fall between z = 20 mm and z = 50 mm. The poor performance of the standard $k - \epsilon$ model can explain the discrepancies at intermediate heights.



Figure 3.17: Turbulent kinetic energy in base cases



Figure 3.18: Axial droplet velocity in base cases

Fig.3.18 and Fig.3.19 show the mean axial and radial droplet velocities. The measured gas velocity is also presented in these plots which indicate that the droplets move together with the gas phase for $z \ge 30$ mm.

The simulated velocity profiles are characteristically similar to the measurements, however the following phenomena are observed:

- 1. The radial velocities are overestimated for $z \leq 20$ mm.
- 2. The overestimated radial velocity causes the droplets with high axial velocity to move to outer radii. This causes higher and higher over-predictions of axial droplet velocity for radii over 10 mm.
- 3. The discrepancy in the axial droplet velocity only decreases for high axial locations, because here the axial gas velocity is under-predicted.



Figure 3.19: Radial droplet velocity in base cases

The D_{10} average of droplet size is presented in Fig.3.20. The measurement data is the average of characteristic diameters constructed from measurements in two orthogonal directions. (Verdier et al., 2017) In the simulation the parcels are assumed to be spherical, thus simple arithmetic average is used. The droplet size is generally lower near the axis and increases outwards. Hollow cone sprays show such behaviour even in more homogeneous, low velocity co-flow. (Ma, 2016) The presence of the high velocity annular air inlet further increases the inequality of droplet diameters between different radial locations.

Below the flame lift-off height (z = 25 mm) the simulated droplet size matches quite well, however when the droplets enter the flame region, evaporation becomes too fast and the droplet size rapidly drops.



Figure 3.20: Mean droplet diameter in base cases

The profiles of mean droplet temperature are presented in Fig.3.21. The simulated droplet temperature is also weighted according to Eq.(1.5), so it is comparable with the measurements. The liquid temperature drops below the inlet value at z = 20 mm due to evaporation. In the measurements the droplets reach an equilibrium temperature (~ 331 K) as they cross the flame front. According to Verdier et al. (2017) this corresponds to the wet-bulb temperature of n-heptane in the flue-gas conditions.

The simulation shows similar behaviour, however the typical temperatures inside and outside the flame are different. In the central air jet the parcel temperatures drop to the limiting value set in the model: 270 K. The parcels surrounded by the hot flue gasses are heated to ~ 365 K. This temperature is significantly different from the measured one, although it is below boiling temperature.





Figure 3.21: Mean droplet temperature in base cases

The equilibrium between heat loss due to evaporation and heat gain due to convective heat transfer defines the wet bulb temperature. In the 4D FGM the evaporative cooling of the cells cannot be accounted for. The simulated gas mixture in the cell stays hot even though evaporation happens, thus the droplet temperatures will be over-predicted. It could be expected that introducing the enthalpy loss as a 5^{th} control variable can decrease the discrepancies of droplet temperature. However as Fig.3.22 illustrates, even if the heat loss is significant the decrease in the flame temperature is not more than 200 K.

> sim.FIN01 4D base case R _____ sim.FIN02 5D base case R _____



Figure 3.22: Gas temperature in base cases



Figure 3.23: Axial droplet velocity of different droplet groups in base cases

Fig.3.23 and Fig.3.24 shows the size classified velocity of droplets. The discrepancies are higher for larger diameters. The small droplets relax to the gas phase flow field faster, thus the corresponding errors would originate from the error in the gas flow.

The cause of the discrepancy in the axial velocities of the large droplets appears to be similar to the mechanism described before for the mean droplet velocities. The radial velocities are overestimated, thus parcels with high axial velocity are transported to a too high radius. E.g.: in Fig.3.23 at z = 30 mm and $D_p \in [40 \ \mu\text{m}, 50 \ \mu\text{m}]$ the magnitude of the axial velocity is captured well, however the corresponding radial location is too high.

It is suspected that the high air inlet velocities around the fuel injector affect the primary atomization in a way, that cannot be captured by the conditional droplet injection model.



Figure 3.24: Radial droplet velocity of different droplet groups in base cases

Overall, the simulation results are reproduce some phenomena quite well. The double flame shape is present even though the location of the outer flame front is not perfect. Knowing the limited capabilities of RANS simulation the results are satisfactory.

The differences between 4D and 5D FGM are very limited. The inclusion of enthalpy loss only affects the flame shape and the gas phase temperature. The progress variable source term in Fin.3.11 shows how the flame becomes more narrow due to the cooler outer flame front (Fig.3.22.) Otherwise the two solvers provide te same results.

3.4 Sensitivity study

To explain the selection procedure of the boundary conditions, and to underline the developments introduced in this work, a detailed sensitivity study is presented below. Only the differences are emphasized, if the alteration of the base case does not change specific properties, then those properties are not illustrated.

3.4.1 Chemical mechanism

In this study, the main development added to the work of Ma (2016) is the new droplet model, which is capable of describing the film around the droplet with the FGM control variables (mixture fraction, progress variable and their variances.) This development allows the usage of the skeletal reaction mechanism developed by Lu and Law (188 species and 939 elementary reactions.)

The 4D FGM base case presented in section 3.3 ("FIN01") is compared to a case where Patel et al. mechanism (29 species and 52 reactions) is used for the FGM table generation ("FIN03"), all other settings are equal. Fig.3.25 shows the comparison of gas temperature and OH concentration contours plots. There are notable differences especially in the OH mass fraction field.

Such details are important in the prediction of emissions (CO, NO_x) Note that the applied mechanisms do not contain reactions describing NO_x production. With the original solver the finite available RAM could prevent the inclusion of these mechanisms, while with the new development the size of the chemical mechanisms is unlimited.



Figure 3.25: Comparison of skeletal and reduced reaction mechanisms Contour plot of temperature and OH mass fraction ($z \in [0 \text{ mm}, 80 \text{ mm}]$ and $x \in [0 \text{ mm}, 40 \text{ mm}]$)
3.4.2 Effect of new development

The old and new software is compared using the Patel et al. mechanism (29 species and 52 reactions) since the usage of larger mechanisms is prevented by the memory requirements of the old solver. Using 4D FGM the new developments are already used in the case: "FIN03". The case "FIN04" is calculated using the original software of Ma (2016), otherwise it is the same as the case "FIN03".

Both models are over-predicting the rate of evaporation, as illustrated by Fig.3.26. The same pattern is observed: as the parcels cross the flame front their size decreases significantly. The slight differences are caused by the different flame shape.



Figure 3.26: Comparison of the new and the original solver, mean droplet diameter

Fig.3.27 illustrates, that in case of the old solver the simulated droplet temperatures are even less accurate than with the new solver. Using the original software of Ma (2016), the droplet temperatures are confined by the manually set limits ($T_p \in [270 \text{ K}, 371.55 \text{ K}]$) on both sides: the droplets surrounded by hot flue gas are heated to the boiling temperature. In the new solver the droplet temperature is stabilised at a lower temperature in the flame, hence it is closer to the measurements.



Figure 3.27: Comparison of the new and the original solver, mean droplet temperature

Fig.3.28 illustrates, that the flame shape is drastically different for the new and old solvers. The two shapes mainly diverge in the shape of the flame base. As Fig.3.28a indicates, the parcels of the old solver evaporate faster, thus the mixture fraction source term is concentrated in a smaller area. Using the new solver the flame base is widened, because the parcels evaporate over a longer path.



(a) Mixture fraction source term

(b) OH mass fraction

Figure 3.28: Comparison of the new and the original solver Contour plot of mixture fraction source term and OH mass fraction ($z \in [0 \text{ mm}, 80 \text{ mm}]$ and $x \in [0 \text{ mm}, 40 \text{ mm}]$)

3.4.3 Air inlet conditions

The boundary conditions of the air inlet annulus introduced in subsection 3.2.1 are somewhat arbitrary. The sensitivity of the simulation results to the inlet parameters is examined to determine the parameters validity.

Inlet angle The inlet angle is varied $\pm 5^{\circ}$ across the whole annulus. In the case "FIN05" the inlet angles are increased by 5°, thus the air jet is less inclined: $\alpha_{inner} = -13^{\circ}$ and $\alpha_{outer} = -8^{\circ}$. In "FIN06" the angles are decreased, so: $\alpha_{inner} = -23^{\circ}$ and $\alpha_{outer} = -18^{\circ}$. (See Eq.(3.12).)

Interestingly the varying inlet angle has more effect on the axial velocity then on the radial (the latter not shown here.) As Fig.3.29 presents, the axial velocity near the axis increases with more inclined ("FIN06" -5°) inlet profile, since the annular inflow is more focused.

There is a trade-off between accuracy on high and low axial locations. The less inclined inlet velocity ("FIN05" +5°) performs better at low axial locations ($z \leq 10 \text{ mm.}$) The recirculation zone at the axis is reproduced well. The more inclined inlet velocity ("FIN06" -5°) approximates the axial velocity better at high axial locations ($z \geq 35 \text{ mm.}$) The angles applied in the base case are a compromise between the two. The different axial gas velocities cause different axial droplet velocities, otherwise the varying inlet angle does not change the simulation results.



Figure 3.29: Effect of air inlet angle, axial gas phase velocity

Inlet turbulent kinetic energy In the base cases a constant turbulent kinetic energy of $15 \text{ m}^2/\text{s}^2$ is set across the whole inlet. This value is varied by $\pm 10\%$ in the cases "FIN08" and "FIN09". It is concluded, that the turbulent kinetic energy field is *not* sensitive to the inlet value.

Turbulence intensity boundary condition for inlet One can object to the selection of constant turbulent kinetic energy inlet, as it does not consider the effect of the boundary layers in the injector system. In case "FIN07" the turbulent kinetic energy at the edge of the inlet annulus is lowered by applying OpenFOAM's turbulentIntensityKineticEnergyInlet boundary condition. (See. Eq.(3.19)) Otherwise it is equivalent to the 4D FGM base case ("FIN01".) The applied turbulence intensity is I = 14.7%. The differences are negligible, thus the results are not shown here. In conclusion, the internal turbulent kinetic energy field is insensitive to both the inlet value and the shape of the inlet profile.



Figure 3.30: Effect of inlet mass flow, axial gas phase velocity

Inlet mass flow The inlet velocity magnitude is varied by varying the inlet mass flow rate. In cases "FIN10" and "FIN11" $\pm 10\%$ change in the inlet mass flow is applied, thus the velocity profile is different in the inlet annulus. (See subsection 3.2.1.) Its effect on the gas phase axial velocity is illustrated in Fig.3.30. The region around the axis is the most affected, the spreading of the jet is not modified. The axial droplet velocity changes together with the gas phase velocity (not shown here.)

The turbulent kinetic energy is significantly modified by the varying axial velocity as shown in Fig.3.31. The higher velocity gradients increase the turbulent kinetic energy production term (Eq.(2.29)), thus the steady state value of turbulent kinetic energy is higher.

The flame shape is presented in Fig.3.32. The lift-off height is quite insensitive to the inlet mass flow, which confirms the hypothesis presented in section 3.3: the location of the flame base is for the most part determined by the spray angle, since the flame will stabilize where the droplets leave the air jet.



Figure 3.31: Effect of inlet mass flow, turbulent kinetic energy



Figure 3.32: Effect of inlet mass flow, OH mass fraction

3.4.4 Mesh

The simulation is run on a mesh with 50% smaller cells to confirm mesh independence. The cell size at the injection is decreased to 0.33 mm while the smallest cells around the air inlet annulus have a radial size of 0.01 mm. The differences are insignificant for all properties.

Fig.3.33 shows the flame shape in the base case and with the refined mesh. The refined mesh allows a more elaborate flame structure. One example is the transient disturbance caused by parcels piercing through the lower part of the outer flame front. Otherwise the flame shape is essentially the same in the two cases.



Figure 3.33: Effect of mesh refinement, OH mass fraction

3.4.5 Droplet film properties

As proposed by Ma (2016), the properties in the boundary layer around the droplet are calculated using the "1/3 rule". In the new droplet model the same averaging is applied, but for the FGM control variables and their variances in Eq.(2.118)-(2.121). (4D FGM) The coefficient α expresses the contribution of the seen gas properties in the average quantities describing the boundary layer. Three values are examined: $\alpha \in \{0, \frac{2}{3}, 1\}$ in cases "FIN13", "FIN14", and "FIN15" respectively. Otherwise the cases are the same as "FIN01".

Fig.3.34 shows how the droplet temperature is affected by the weighting. By only considering the droplet surface properties ($\alpha = 0$) the discrepancies decrease notably. (Compared to the base case where $\alpha = \frac{1}{3}$.) In this case the equilibrium temperature of droplets immersed in the flame decreases to ~ 355 K.

The flame shape is presented in Fig.3.35. The OH mass fraction differs from case to case in the region where the droplets interact with the flame fronts. Otherwise changing the "1/3 rule" does no affect the flame shape.



Figure 3.34: Effect of droplet boundary layer properties, mean droplet temperature



Figure 3.35: Effect of droplet boundary layer properties, OH mass fraction

3.4.6 Modelling coefficients in variance equations

In Eq.(2.78) and Eq.(2.79) the modelling constants describing the dissipation of mixture fraction and progress variable variances, are chosen as: $C_{d,Zv} = C_{d,Y_cv} = 2$ based on the recommendation of Ma (2016). However the most adequate value of these constants can vary from case to case. Here the sensitivity to these parameters is examined.

Mixture fraction variance dissipation $C_{d,Zv}$ is set to 1 and 3 in cases "FIN16" and "FIN18" respectively, otherwise they are the same as "FIN01" Fig.3.36 and Fig.3.37 show, that even though the higher dissipation decreases the mixture fraction variance, this has limited effect on the flame shape.



Figure 3.36: Effect of $C_{d,Zv}$, OH mass fraction



Figure 3.37: Effect of $C_{d,Zv}$, mixture fraction variance

Progress variable variance dissipation The progress variable variance is examined more comprehensively. $C_{d,Y_{c}v} \in \{1,3,5,10\}$ is studied in cases "FIN17", "FIN19", "FIN20", and "FIN21" respectively, otherwise they are the same as "FIN01". The sensitivity study reveals, that the RANS simulations are heavily affected by the choice of $C_{d,Y_{c}v}$. Fig.3.38 and Fig.3.39a show the OH mass fraction contours. As $C_{d,Y_{c}v}$ increases, the radial location of the outer flame agrees better with the OH-PLIF measurements.



Figure 3.38: Effect of C_{d,Y_cv} , OH mass fraction



Figure 3.39: Effect of C_{d,Y_cv} , OH contour comparison

Fig.3.40 shows that indeed as the modelling coefficient of progress variable variance dissipation increases, the steady state values of progress variable variance are lower and lower. As mentioned in section 3.3, high progress variable variances decrease the progress variable source term, thus inhibiting the reactions. By decreasing the variance the reaction zone can shift to an outer radial location.



Figure 3.40: Effect of C_{d,Y_cv} , progress variable variance



Figure 3.41: Axial gas phase velocity in reacting case

Some of the discrepancies in the base cases are related to the poorly predicted flame shape. As Fig.3.41 indicates, by widening the flame, the discrepancies of the axial gas velocity decrease at high axial locations in the flame ($x \ge 10 \text{ mm.}$) The high temperature flue gas between the two flame fronts has low density, thus to transport the same mass flow, higher axial velocities are reached. The effect of buoyancy also increases the axial velocity.

With the better flame shape, the radial spreading inside the flame also appears in the simulation results. Even though the radial velocities (Fig.3.42) are still underestimated at $z \ge$ 35 mm, the characteristics are well captured.



Figure 3.42: Radial gas phase velocity in reacting case

Chapter 4

Conclusion

The RANS-FGM spray combustion solver originally implemented by Ma (2016) and further developed in this work, is a very adequate tool for the simulation of spray flames. Although, considering the limitations of RANS simulations, the results need to be treated with caution.

The software was successfully tested on an n-heptane flame in cold co-flow: the CORIA Jet Spray Flame. (Verdier et al., 2017) This proves the universal applicability of the model, as Ma (2016) concentrated mostly on ethanol flames.

The novel droplet model introduced in section 2.2, is capable of describing the droplet surface properties in the context of the flamelet generated manifold. It acts similarly to the original model, however it does not limit the size of the applicable chemical mechanism.

Altogether the accuracy of the RANS-FGM results presented in 3.3 are fairly good. The flame shape and the axial gas phase velocity predictions are significantly improved by tuning the modelling coefficient of progress variable variance dissipation: $C_{d,Y_cv} = 5$ is proposed as the best scenario. The poorly predicted droplet size and temperature are the two main shortcomings of the RANS-FGM model, which remain unresolved in this study.

Ma (2016) uses FGM with both RANS and LES simulation. Similarly to this work, the rate of droplet evaporation is over-predicted inside the flamelet, thus the droplet size is below the measured values. Note that Ma (2016) reconstructs the gas phase flow field of the Delft Spray-in-Hot-Coflow flame perfectly using RANS simulation. This underlines the difficulty caused by the complex inlet geometry of the CORIA Jet Spray Flame. Shum-Kivan et al. (2017) use LES with Lagrangian droplet treatment to simulate the CORIA Jet Spray Flame. Their published results match the measurements well, the sudden drop in diameter as the droplets enter the flame is not present. (There is no published data on the droplet temperature.)

The modelling approach presented in subsection 3.2.1 reconstructs the annular air inlet conditions quite well.

This research contributes to a comparative study of simulation approaches that will be presented in the 6th Workshop on Measurement and Computation of Turbulent Spray Combustion (September 17, 2017, Naples.)

4.1 Recommendations

The application of Large Eddy Simulation (LES) could radically improve the turbulent and mean velocity fields as demonstrated by Shum-Kivan et al. (2017).

The sensitivity study reveals the importance of good turbulence-chemistry interaction models. To correctly resolve the FGM control variable variances, Ma (2016) applies an adaptive method to dynamically determine the local values of the modelling constants in LES. This is not an option in RANS simulation, so a study is necessary on how to choose adequate modelling coefficients.

The size classified droplet velocity (presented in Fig.3.23 and Fig.3.24) suggests that the conditional droplet injection model could be further improved by introducing size dependency in the selection of velocity magnitude at the injection plane.

A more detailed heat and mass transfer model is necessary to correctly capture the droplet temperature. The effects of non-equilibrium thermodynamics and the interaction between heat and mass transfer can be included.

It is challenging to simulate the complex injector applied for the CORIA Jet Spray Flame. A simpler burner geometry would allow easier validation of the spray flame models.

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