

CRANFIELD UNIVERSITY

School Of Mechanical Engineering

PhD THESIS

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Numerical Simulation of Spray Combustion using
Bio-mass Derived Liquid Fuels

PhD

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Abstract

The main objective of this work is to create a robust model for two-phase liquid spray combustion flow using vegetable oils, to investigate the flow structure generated by a swirler array with different fuels, and secondly to assess and optimise the capability of the CFD to predict accurately the results obtained experimentally and eventually enhance CFD model development and simulation. Validation is achieved by comparing the numerical results obtained with CFD with the experimental measurements.

The purpose of this research is to increase the scientific understanding of the fundamental mechanisms of the spray combustion process using a carbon neutral fuel such as ethanol and biodiesel. In fact, very few numerical simulations of liquid biomass fuels in gas turbine systems are available in the literature.

The flames are simulated using the commercial code FLUENT. The combustion/turbulence interaction is modelled using the laminar flamelet approach with detailed chemistry modelled using the OPPDIFF model from CHEMKIN.

While the experiments could be carried out only up to 3 atm, the simulations were further extended to a maximum pressure of 10 atm. The FLUENT results were assessed qualitatively and quantitatively between the experimental measurements and the simulation. The cold flow features have been captured by the present simulations with a good degree of accuracy. Effect of air preheating was investigated for the biodiesel, and sensitivity to droplet size and spray angles variation were analysed. Good agreement was obtained for ethanol except in the fuel lean region due to failure of the FLUENT laminar flamelet model to capture local flame extinction while biodiesel simulation resulted in a significant overprediction of the flame temperature especially in the downstream region and satisfactory results further upstream. The results show the importance of setting proper droplet initial conditions, since it will significantly affect the structure of the flame.

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ABBREVIATION

AFR: Air/Fuel ratio
AFTUR: Alternative Fuels for gas TURbines
CARM: Computer Assisted Reduction Method
CARS: Coherent Anti-Stokes Raman Spectroscopy
CO: Carbon monoxide
CO₂: Carbon dioxide
CTRZ: Central Toroidal Recirculation Zone
DLE: Dry Low Emission
DNS: Direct Numerical Simulation
DPM: Discrete Phase Model
DRW: Discrete Random Walk
DWFL: degenerate four wave mixing
EU: European Union
ERA: European Research Area
FAME: Fatty Acid Methyl Esters
GHG: Greenhouse Gas Protocol
H₂: Hydrogen
H₂O: water
HC: HydroCarbon
IEEE: Institute of Electrical and Electronics Engineers
LES: Large Eddy Simulation
LHF: Locally Homogeneous Flow
LIFS: laser induced fluorescence Spectroscopy
LPP: Lean-Premixed Prevaporized
LSV: Laser Speckle Velocimetry
MMD: Mass Mean Diameter
NASA: National Aeronautics and Space Administration
NO_x: Nitrogen Oxide
O₂: Oxygen
OPPDIF: OPPosed DIffusion Flame
PDPA: Phase DoPpler Anemometry
PDI: Phase Doppler Interferometry
PIV: Particle Image Velocimetry
PM: Particulate Matter
RANS: Reynolds-Averaged Navier-Stokes
RNG: ReNormalization Group
RSM: Reynolds Strees Model
SMD: Sauter Mean Diameter
SST: Shear Stress Transport
SF: Separated Flow
SPEED: Stochastic-Probabilistic Efficiency-Enhanced Dispersion

Nomenclature

Italic symbols

a: strain rate (s^{-1})
A, B, C: parameters determined by regression of experimental data to determine fuel viscosity
 A_{Ant} , B_{Ant} , C_{Ant} : Antoine constants
 A_p : droplet surface area (m^2)
 a_r : apparent slit length
 C_D : drag coefficient (adimensional)
 C_{ex} : coefficient of thermal expansion
 $C_{i,s}$: vapour concentration at the droplet surface ($kg.mol/m^3$)
 $C_{i,\infty}$: vapour concentration in the bulk gas ($kg.mol/m^3$)
 C_p : specific heat ($J.kg^{-1}.K^{-1}$)
 C_p^0 : specific heat capacity at 293.15 K ($J.kg^{-1}.K^{-1}$)
 C_x : constant
d: droplet diameter (m)
 $\bar{d}$: mean droplet diameter (μm)
 D_{30} : volume mean diameter
 D_{32} : Sauter mean diameter
 D_{hub} : hub diameter
 D_L : centre body diameter (m)
 d_{max} : maximum probe volume diameter
 D_{max} : maximum probe volume diameter
 D_o : swirler vane diameter (m)
 D_{sw} : swirler diameter
 F_c : correction factor
 F_x : additional acceleration
F: momentum source term
g: gravity
 G_{ij} : interaction parameter (Pa.s)
h: heat transfer coefficient ($W.m^{-2}.K$)
 h_{fg} : latent heat of vaporization ($J.kg^{-1}$)
 $h_{fg,b}$: latent heat of vaporization at the normal boiling point ($J.kg^{-1}$)
k: thermal conductivity ($W.m^{-1}.K^{-1}$)
 k_c : mass transfer coefficient (m/s)
 k_{turb} : turbulent kinetic energy (m^2/s^2)
L: distance between the tip of the liquid fuel cup and the tip of the oxidiser duct (m)
 l_k : Kolmogorov length scale
 l_0 : spatial scale of large eddies
M: mass source term
m: mass (kg)
m: number of carbon groups requiring an additional contribution, which are those that are joined by a single bond to a carbon group, which in turn is connected to a third

carbon group by a double or triple bound. If a carbon group meets this criterion in more than one way, m should be increased by one for each of the ways. Exceptions: $-\text{CH}_3$ groups or carbon groups in a ring never require an additional contribution; and the first addition contribution for a $-\text{CH}_2-$ group meets the criterion in a second way, the second additional contribution reverts to the 18.83 J/mol.K value.

$m_{p,0}$: initial mass of the particle (kg)

Δm_p : particle mass loss (kg)

$\dot{m}$: mass flow rate (kg.s^{-1})

MMD: mass mean diameter (m)

$\dot{m}_{p,0}$: initial mass flow rate of the particle injection tracked (kg/s)

$\overline{m}_p$: average mass of the particle in the control volume (kg)

MW: molecular weight

MW_k : species k molecular weight

n : spread parameter

n_C : number of carbon atoms

n_D : number of double bonds

N : ratio of droplet heating time to droplet lifetime

N_i : number of atomic groups i in the compound

N_{opt} : optimal number of droplets

N_{spe} : number of species

N_{tc} : corrected total number of droplets N_{tc}

Nu : Nusselt number (adimensional)

N_{vap} : molar flux of vapour ($\text{kgmol/m}^2.\text{s}$)

Oh : Ohnesorge number (adimensional)

P : pressure (Pa)

P_a : atmospheric pressure (Pa)

PA : probe area

P_C : critical pressure (bar)

P_{op} : operating pressure

Pr : Prandtl number (adimensional)

P_{sat} : saturation pressure (Pa)

P_{vi} : fatty acid vapour pressure

P_{vmix} : mixture vapour pressure

Q : heat source term

r : droplet radius

R : universal gas constant (kJ/kg.mol.K)

Re : Reynolds number (adimensional)

R_{rand} : uniform random number

R_t : turbulence Reynolds number

S : source term

Sc : Schmidt number (adimensional)

Sh : Sherwood number (adimensional)

SMD: Sauter Mean Diameter (m)

t : time (s)

Δt : time step

T : temperature (K)

T_{br} : reduced temperature at normal boiling point

T_C : critical temperature (K)

t_e : evaporation time (s)
 T_L : integral time scale
 T_r : reduced temperature
 T_r^R : reduced reference temperature
 t_{tot} : total acquisition time
 u : instantaneous fluid velocity ($m.s^{-1}$)
 $\bar{u}$: rms value of velocity fluctuation ($m.s^{-1}$)
 u' : velocity fluctuation ($m.s^{-1}$)
 V : velocity at injector exit ($m.s^{-1}$)
 V_1 : fuel velocity (m/s)
 V_2 : oxidiser velocity (m/s)
 V_C : critical volume, (mL/mol)
 VF : volume flux ($cm^3/s/cm^2$)
 Vol : volume (cm^3/g)
 Vol_l : total liquid volume (cm^3/g)
 Vol_{mix} : molar volume of mixture ($cm^3/g.mol$)
 Vol_R : experimental liquid molar volume at a reference reduced temperature T_R ($cm^3/g.mol$)
 X : mole fraction
 Y : mass fraction (adimensional)
 Z : mixture fraction (adimensional)
 Z_{RA} : constant for the Rackett equation

Greek symbols

α : swirl angle to the mainstream direction
 δ : mass diffusivity ($m^2.s^{-1}$)
 δ_{ij} : Kronecker delta
 Δm_p : change in the mass of the particle in the control volume (kg)
 δ_T : film thickness for heat transfer
 δ_T : film thickness for mass transfer
 $\Delta_T, \Delta_v, \Delta_p$: contribution constants for various atoms or groups of atoms used in the Lydersen method
 Γ : circulation
 Φ : equivalence ratio
 Φ_{conv} : convective heat flux
 Φ_{vap} : vaporization heat flux
 λ : dynamic viscosity ratio
 ε : turbulent dissipation rate (m^2/s^3)
 ρ : density ($kg.m^{-3}$)
 ρ_1 : fuel density ($kg.m^{-3}$)
 ρ_2 : oxidiser density ($kg.m^{-3}$)
 ρ_{Lb} : molal liquid density at the normal boiling point (gram.moles/ cm^3)
 ρ_{mol} : molar density ($kmol.m^{-3}$)
 ρ_R : experimental density at reference temperature T_R (kg/L)
 η : reaction progress variable
 η_Z : sample space variable corresponding to Z
 Ω_D : diffusion collision integral, dimensionless

σ : surface tension ($\text{kg}\cdot\text{s}^{-2}$ or N/m)
 σ_δ : characteristic length, $\text{\AA}$
 μ : dynamic viscosity ($\text{kg}\cdot\text{m}^{-1}\text{s}^{-1}$)
 θ : spray angle
 θ_{scatt} : scattered signal collection angle
 χ : scalar dissipation rate
 τ_a : characteristic aerodynamic time
 τ_e : characteristic eddy lifetime
 τ_H : liquid heating time
 τ_L : droplet lifetime
 τ_d : diffusion time
 τ_{ik} : viscous stress tensor
 ∞ : ambient environment
 ΔT_p : temperature change of the particle in the control volume
 A : underrelaxation factor
 x_k : spatial coordinate
 ω : production rate (mass/volume/time) by chemical reaction

Subscript

crit: critical
 c: critical
 d: droplet
 eff: effective
 f: fuel
 g: gas
 i, j: species, pure constituents
 inj: injection
 l: liquid
 m: mixture
 max: maximum
 o: oxidizer
 p: particle
 r: relative
 s: droplet surface
 st: stoichiometry
 atm: atmospheric

CHAPTER 1 - INTRODUCTION

1.1 Why biofuels?

The famous inventor Rudolph Diesel designed the original diesel engine to run on vegetable oil. He used peanut oil to run one of his engines at the Paris Exposition of 1900 and at the 1911 World's Fair in Paris, Dr Diesel ran his engine on peanut oil and declared 'the diesel engine can be fed with vegetable and will help considerably in the development of the agriculture of the countries which use it'. However, in the intervening years, readily available fossil fuels gave little incentive for encouraging environmental friendly renewable fuels. The energy crisis of the 1970s sparked a renewed interest in the use of vegetable oils and looking for alternative sources of energy now seems to be increasingly of vital importance albeit motivated by environmental considerations rather than fuel availability.

As part of a range of measures drawn up in response to international agreements to reduce greenhouse gas emissions, the EU is encouraging greater use of biofuels. Under the 2003 EU Biofuels Directive, a 2% share of the energy content of all petrol and diesel for transport must come from renewable sources, including both biodiesel and bioethanol. This must rise to 5.75% by the end of 2010. In order to meet this stringent environmental standard and reduce the amount of CO₂ emissions, a significant amount of research needs to be done into combustion properties of biomass derived fuels to assess the technological requirements.

Biomass derived fuels have been shown to be a promising alternative to fossil fuels, not only because they are renewable fuels, but also because they reduce also pollutant emissions substantially such as particulate matter (PM), unburned hydrocarbons (HC), carbon monoxide (CO) emissions (Haas et al., 2001), as well as carbon dioxide emissions by a substantial amount, comprised between 20 and 80% compared to conventional fossil fuels and hence produce environmental benefits. However, along with these advantages comes the fact that fuel properties are quite different from conventional fuels, with lower fuel volatility, high viscosity and surface tension and flame stability issues. Moreover, flames generated by vegetable oil derived fuels

generate soot, making the flame luminous, therefore influencing radiation which would affect the flame properties.

The broad objective of this project is to assess the ease with which biomass-derived liquid fuel might be used as fuel in gas turbines for heat and power generation as part of a sustainable energy production policy. The use of liquid fuels from biomass will help fulfil the Kyoto targets concerning Greenhouse Gas Protocol (GHG Protocol) emissions. The project aims to develop methodologies to assess the combustion performance of these fuels for clean and efficient energy production. Another objective is to extend the capability of dry low emission (DLE) gas turbine technologies based on lean premixed combustion to a wider range of potentially commercial fuels, including those of lower calorific value produced by gasification of biomass (Low Heating Value < 25% natural gas) and H₂ enriched fuels. The research forms part of a European Union funded project (AFTUR) with the global socio-economic objective of helping strengthen the technological infrastructure of the European Union (EU) and the European Research Area (ERA) through the established partnership in relation to renewable energy use.

1.2 Objectives

The main aim of the AFTUR project (2004) is to develop the modelling capability of spray flames related to biomass derived fuel in gas turbines environments. The results obtained will provide a measure of benchmarking for use in more complex combustors, such as lean-premixed prevaporized (LPP) combustion designs.

The main objective of this work is to create a robust model for two-phase liquid spray combustion flow using vegetable oils, to investigate the flow structure generated by a swirler array with different fuels, and secondly to assess and optimise the capability of the CFD to predict accurately the results obtained experimentally and eventually enhance CFD model development and simulation. Validation is achieved by comparing the numerical results obtained with CFD with the experimental measurements.

The purpose of this research is to increase the scientific understanding of the fundamental mechanisms of the spray combustion process using biodiesel. Very few numerical simulations of liquid biomass fuels in gas turbine systems are available in the literature. In fact, most of the work on biodiesel combustion has focused mainly on experimental studies, essentially in internal compression engines and mostly on assessing the fuel performance and auto-ignition phenomena. The rare detailed numerical studies available related to the field of liquid combustion using vegetable oils have been carried out by Griend et al. (1990), Choi and Reitz (1999), Yuan et al. (2002). Choi and Reitz (1999) conducted computer simulations to study the combined effects of methyl soyate with diesel. However, this study has been limited to a 20% and 40% biodiesel blend in diesel engines whereas the present study focused on pure biodiesel combustion simulations for industrial gas turbines. Additionally, their study sought to acquire a better understanding of the factors controlling the formation of NO_x, which is not in the scope of this work. Yuan et al. (2002; 2003; Yuan et al, 2003) limited their work on the soybean-based biodiesel to comparison of ignition delay with diesel and the reduction of NO_x emissions.

1.3 Challenges

Numerical prediction of two phase reacting flow in gas turbine engines is a very complicated and challenging task, involving numerical models for the combined chemical, thermodynamic and aerodynamic processes. The task is formidable since the equations satisfied by the species mass fraction and the temperature are strongly coupled with the three-dimensional Navier-Stokes equations. The development of liquid fuel spray, break-up phenomenon, evaporation processes and finally mixing with air govern the combustion and are dependent on one another, further increasing the complexity of the problem. These processes which are already significantly difficult to predict, need to be thoroughly addressed and investigated since they will affect pollutant emission formation. A satisfactory prediction of the two phase flow inside gas turbines is one of the most important issues to be addressed in order to have a thorough understanding of the chemical and physical processes involved and consequently improve gas turbine combustion and pollutant emissions predictions. Moreover, a better understanding of the chemical and physical processes will lead to more accurate numerical submodels.

Particular importance has been given to the estimation of the fuel physical and thermodynamic properties necessary for the combustion modelling. Predicting the physical properties of the vegetable oils and biofuels is a crucial step in the accurate prediction of the spray atomisation and combustion processes especially since the biomass derived fuels have significantly different properties from conventional fuels (diesel or kerosene), such as high viscosity and surface tension, low latent heat of vaporization and low volatility.

1.4 Thesis layout

The thesis is divided in 7 chapters. After this brief introduction in chapter 1, chapter 2 is mainly a literature review related to the different spray combustion submodels used for turbulent reacting sprays such as turbulence models, multiphase flow, evaporation and combustion models as well as a description of diffusion flames and their extinction behaviour. Chapter 3 gives a description of the fuel properties which need to be calculated, especially for biodiesel based on their fuel fatty acid composition before being implemented into the CFD code. Chapter 4 reports the results of the experimental study for the ethanol and biodiesel spray flames, at pressures ranging from 1 to 3 atm, which is necessary to gain both some physical insight and for the inputs to be defined in the computational model. Droplet size and velocity measurements, as well as gas temperature are reported in this section. In chapter 5 the specific modelling strategies available at the present time for the spray flame configuration are described including the different submodels for turbulence modelling, multiphase flow, droplet evaporation, breakup and combustion models and their advantages as well as drawbacks are assessed and choice of model justified. Chapter 6 describes the cold swirling flow and reacting spray results and numerical results are compared with the experimental data for validation. Then a discussion on the suitability of the FLUENT submodels ensues and a set of recommendations is also presented. Chapter 7 concludes the thesis by summarising the main conclusions and important aspects of the work, with some future recommendations for future work.

CHAPTER 2 – LITERATURE REVIEW

This section provides an overview of the different submodels used, which account for the numerical method, turbulence model, multiphase model, evaporation, combustion model, and breakup model. Spray wall interaction is not considered to be significant in the present study and hence will not be treated in this study.

Spray flames relevant to gas turbine combustion embraces a number of complicated processes involving strongly coupled areas of fluid mechanics such as turbulence, heat and mass transfer due to mixing between the fuel and oxidiser, chemical reactions with the associated kinetics and thermodynamics, multiphase flow, droplet evaporation and breakup, all parameters which are influenced by fuel type, ambient gas composition, temperature and pressure, droplet initial size distribution as well as relative velocity between the droplets and the surrounding gas. It is further complicated by the complex geometry used for the combustion chambers nowadays. Hence a basic understanding of the physical and chemical processes is needed for reliable combustion predictions. CFD simulation must be taking into account all these parameters in order to provide accurate predictions, introducing turbulence, droplet dispersion and evaporation, gaseous mixing, combustion chemistry, radiation and soot production.

The ultimate goal is a general prediction procedure enabling the performance of a combustor to be accurately described even beyond the costly experimental arrangements. Hence it is of prime importance to be able to solve the partial differential equation which describes the convective heat and mass transfer, evaporation and combustion process accurately and within reasonable time. However, thermal radiation will not be included in this study, to limit the scope of this study. Secondly, it is important to have good physical models for the various phenomenon described above in order to capture the good physics and chemistry. All these features are present in the FLUENT commercial package, and this code has been judged a tool sophisticated enough for this study. The FLUENT programs covers all the aspects needed to carry out a turbulent spray reacting flow simulation, which are required features to carry out this investigation.

2.1 Turbulence models

Turbulent flows continue to provide a challenge to engineers and physicists to provide an accurate description of reacting flows. The importance of turbulence is underlined by the fact that it will strongly influence the rate of mixing of the reactants in a combustion system. Indeed, in order to achieve complete combustion, the rate of mixing must occur at the smallest scale of turbulence, known as Kolmogorov scale. Hence to compute combusting flows, the different turbulence parameters must be accurately modelled.

The literature of turbulence modelling is very rich in single-phase flows with predictive schemes that are mostly based on Reynolds average numerical simulation (RANS), the favoured application for engineering purposes and there is a rich choice of turbulence models to be chosen from.

Among the RANS turbulence models, the standard k - ϵ , RNG k - ϵ , realizable k - ϵ and Reynolds stress models (RSM) are the most commonly used. k and ϵ refer respectively to the turbulence kinetic energy and its dissipation rate. The results show that for weakly swirling flow reasonable results are obtained with the different k - ϵ models. RNG k - ϵ is better than the other k - ϵ models in predicting the basic flow fields but the RSM must be used for strongly swirling flows. The standard k - ϵ is a semi-empirical model that has become the most popular for practical engineering applications since it has been proposed by Jones and Launder (1972) due to its robustness, simplicity and reasonable accuracy.

However, Chambers and Wilcox (1976) demonstrated that the k - ϵ turbulence model possessed some serious flaws in accurately predicting adverse pressure gradients flows and later on, Wilcox (1993) explained this serious deficiency. In order to improve the performance of the standard k - ϵ model, some variants have been put forward. Yakhot et al (1986) developed the RNG k - ϵ model and Shih et al (1995) the realizable k - ϵ model. Wilcox (1974a) demonstrated that the k - ϵ model was not adapted for low Reynolds number cases and as a result developed the k - ω model free of the deficiencies from the widely used standard k - ϵ Jones and Launder (1972)

turbulence model. Nearly simultaneously, Yang and Shih (1998) developed a new time scale k - ϵ model optimised for near wall turbulence eliminating the previous drawbacks of the new wall turbulence predictions of the standard k - ϵ Jones and Launder (1972) model. Menter (1984a) reviewed the performance of some eddy-viscosity turbulence models, between the standard k - ϵ model, the RNG k - ϵ and the Shear Stress Transport (SST) model against a number of attached and separated adverse pressure gradient flows and he concluded that the SST model gave the best agreement for the adverse pressure gradient cases, since it was optimised for this kind of application. In general, the k - ϵ models can give sufficiently accurate results for engineering purposes if a qualitative trend is needed rather than accurate values.

The Reynolds stress model (Daly and Harlow, 1970; Launder et al. 1975; Gibson and Launder, 1978; Launder, 1989) involves calculation of the individual Reynolds stresses, $\overline{u_i' u_j'}$, using differential transport equations. The individual Reynolds stresses are then used to obtain closure of the Reynolds-averaged momentum equation. The RSM is the most elaborate of the RANS turbulence models accounting for the isotropic viscosity effect and is especially designed for highly swirling flows, considered in this study, and as a result provide more accurate solution than the k - ϵ turbulence model. Its disadvantage is the more expensive computational time required to solve the additional transport equations. The Reynolds Stress Model (RSM) closes the Reynolds-averaged Navier-Stokes equation via solving transport equations for the Reynolds stresses and an equation for the dissipation rate.

Alternatively, large eddy simulations (LES) is particularly promising and represents an attractive solution as it provides a compromise between accuracy and cost, and is increasingly becoming a practical tool for engineering applications. The philosophy behind LES is to offer a solution for larger scales of turbulence while the smaller scales are modelled, including the interaction between the flow and the combustion processes (Grinstein and Fureby, 2005). The flame is usually thinner than the affordable grid size, and thus subgrid combustion models must be used (Seshadri and Trevnino, 1989). Very few studies have been performed on LES of reacting gaseous flows on unstructured meshes but Selle et al. (2004) have demonstrated the capability of LES to handle such meshes, as well as investigated the capabilities of LES in a

realistic configuration, and comparison of the LES results with experimental data was very satisfactory. Grinstein and Fureby (2005) have also carried out a study of non-reacting and reacting flows in a lean premixed gas turbine combustor using LES to determine its potential for design studies of engineering applications and a reasonable agreement was found with experimental data.

Since it does not attempt to resolve the smallest scales by numerical integration, the computational resources can be manageable even for large values of the Reynolds number as found in practice (Sirignano, 2003). In the foreseeable future, LES will be able to replace RANS models as a way of simulation engineering applications of turbulent flows. However, the LES calculations have not yet incorporated the most advanced droplet heating and evaporation models. The theoretical and numerical aspects of LES are further discussed in recent reviews published by Lesieur and Métais (1996), and Meneveau and Katz (2000).

In the long term, DNS is expected to play a leading role in treating multiphase turbulence, but at this stage is out of reach of the capability of supercomputers for engineering solutions and is mostly used for academic purposes, since its applicability will remain limited to simple flow geometries and to Reynolds numbers which are low compared to industrial applications (Libby and Williams, 1994), but it still can be a powerful tool for benchmarking RANS or LES simulations and great insight for the description for the fluid mechanical and chemical aspects of fundamental flows. In fact, although its range of applicability has been demonstrated to be quite limited, DNS calculations will extract information which are impossible to be obtained through experimental measurements, such as pressure fluctuations, the rate of strain tensor and the three vorticity components for example (Libby and Williams, 1994).

The main limitation related to the applicability of DNS for non reacting flows resides in the fact that it requires grid size which must be prohibitively large in order to capture the small scales. This limitation is enough to restrict the use of the DNS to simple flows with a sufficiently low Reynolds number.

2.2 *Multiphase flow modelling*

Two-phase flow consists of any moving mixture of gas, liquid or solid. The various phases are constituted of interfaces and may take the form of discrete particles (bubbles, solid particles, droplets), geometrically random formed entities (slurries, clobs, slugs) or a liquid or gas carrier fluid. A spray is one type of two-phase flow and a particle will be defined as an unattached body whose motion is primarily controlled by convection and/or gravity forces. It involves the liquid as the dispersed or discrete phase in the form of droplets and the surrounding gas as the continuous phase. Bubbly flow is the opposite as the gas is the discrete phase and the liquid is the continuous phase. A very complex issue consists in the theoretical description of the discrete phase. To describe the combustion process, conservation equations are needed for each phase separately.

Basically, there are two approaches commonly used to predict particulate two-phase flow: the Euler/Euler and Euler/Lagrange method, respectively frequently called Eulerian and Lagrangian method. In both Euler/Lagrange and Euler/Euler method, the continuous phase is treated with the Eulerian method. For the dispersed phase the Eulerian (quasi continuous) or the Lagrangian approach (tracking of particle trajectories) are used and these formulations are examined. Both approaches have been studied extensively and excellent reviews (Crowe, 1982; Faeth, 1995) in both modelling schemes have been introduced in the past.

2.2.1 Lagrangian approach

Spray Lagrangian models can be divided into two categories: locally homogeneous flow (LHF) models and separated flow (SF) models. Shuen (1987) mentioned that LHF models represent the simplest treatment of a multiphase flow and have been widely used to analyse sprays. The key assumption of the LHF is that interphase transport rates are fast in comparison to the rate of development of the flow. This implies that all phases have identical properties at each point in the flow. LHF are correct only for flows containing infinitely small droplets. Faeth (1983) demonstrated that, while LHF models provide a reasonable qualitative description of the flow

structure, they generally overestimate the rate of development of the flow and yields unrealistically high evaporation rates.

Dukowicz (1980) and Gosman and Ioannides (1983) have adopted stochastic methods to study droplet dispersion by turbulence. Faeth (1983) and co workers (Shuen et al., 1986; Shuen et al., 1985; Solomon et al., 1985a; Solomon et al., 1985b; Solomon et al., 1985c) extended the analysis by Gosman et al. (1983) to include the effects of turbulence on interphase heat and mass transport. Their stochastic separated flow (SSF) model has been evaluated in a wide variety of flows with encouraging results. Shuen (1986) and Aggarwal and Chitre (1991) extended their analysis by considering swirling and recirculating flows. The stochastic separated flow (SSF) model is employed to represent the effect of gas-phase turbulence on droplet trajectories and transport rates.

Duckowicz (1980) mentioned that the main aspect and first important issue in the Lagrangian treatment of the dispersed phase is to introduce a large number of particles in order to generate accurate statistics. However, this method is costly in terms of computer time and storage requirement therefore it is not always possible to represent this large number of particles so various strategies have been suggested to alleviate this problem and reduce the total number of particles that must be tracked. Duckowicz (1980) proposed in his stochastic approach to consider the use of relatively small number of ‘computational’ particles, called parcels, which groups the real particles into numerical parcels treated as discrete entities, consisting of a large number of physical droplets having the same properties (size, velocity, trajectory) but this may result in significant errors if the ratio of the computational to real particles is too small.

Zhou and Yao (Zhou and Yao, 1992) developed a group modelling method where only the centre of a group of particles is tracked in the Lagrangian equation of motion, which resulted using only 20 times less computational time needed for generating similar results than via the traditional stochastic approach. Chen and Pereira (1997) also proposed a method called stochastic-probabilistic efficiency-enhanced dispersion

(SPEED) model to decrease the number of particle trajectories required for accurate calculation of statistics, hence improving computational efficiency.

The Lagrangian method is usually applied to describe dilute flows which are characterised by a relatively small local dispersed phase volume fraction ($<10\sim12\%$) and where particle interactions are not significant hence no influence is expected from neighbouring droplets and collisions are infrequent. This allows droplets to be tracked separately, i.e. the effect of adjacent droplets is ignored in a Lagrangian approach, since it is difficult and costly to include. Information is transmitted only along droplet trajectories.

The liquid phase properties are obtained by solving Lagrangian ordinary differential equations for the trajectory, velocity, temperature and size of each statistically significant sample of individual droplets and the gas phase equations must be solved simultaneously with the droplet equations. Individual trajectories are predicted as a result of the forces on the droplet from the existing solution of the gaseous phase equations. The Lagrangian path is the trajectory of an average droplet present in the neighbourhood and by doing so, synthetic turbulence is obtained, which is the physical representation of real turbulence. The effect of the droplet on the gaseous phase is taken into account by calculating the particles' contribution to the continuous phase source term for each computational cell visited through full interphase coupling due to mass, momentum and energy is taken into account. Instantaneous gas phase properties crossed by the droplets are taken into account in a Lagrangian approach

The stochastic particle method accounts for two-way turbulence coupling between the dispersed and the continuous phase, which needs to be considered when the mass loading ratio is high. With two-way coupling, sprays are injected into the flow with sufficient momentum to have a substantial effect on the continuous phase, then afterwards the gas controls the motion of particles and as a result turbulence coupling needs to be taken into account.

Previously, Rudinger (1965) introduced a one way coupling approach, which only considered the influence of gas to particles, while the gas flow field characteristics was assumed to be unaffected by the presence of particles. The one way coupling

approach is proper only for low particle mass loading (Boyson and Swithenbank, 1979).

Later on, Melville and Bray (1979), and Michaelides (1984) studied the influence of dispersed particles on the turbulence structure of the carrier phase and as a result two-way coupling was introduced. Another Lagrangian approach that does take into account the particles' effect on the fluid turbulence is that of Gosman and Ioannides (1981; 1983). More recently, general mathematical models for turbulent two phase flows have been proposed with some success by Chen and Wood (1985) for Eulerian approach and by Mostafa and Mongia (1988) for Lagrangian approach.

2.2.2 Eulerian approach

Eulerian formulations treat the particles as a continuous phase, intermixed with the fluid phase. The motion is predicted by solving a set of continuum equations representing the fluid and the particles. Two-way coupling is accounted for as extra source terms in the equations for both phases. Eulerian approach is usually applied and particular suited to dense flows, i.e. regions of high dispersed phase volume fraction as it is the case near a fuel injector, where particle collisions dominate the droplet motion. A major problem lies in the fact that the droplet size distribution, however, can not be predicted with the Euler/Euler method (Platzer and Sommerfeld, 2002).

Eulerian methods for the prediction of turbulent two-phase flows have been used by various groups of researchers (Melville and Bray, 1979; Elgobashi et al. 1984), (Chen and Wood, 1986), however most of the investigations relate mostly to the response of the particles to the fluid turbulence and the momentum transfer between the primary fluid phase and the secondary phase made of particles but neglected the heat and mass transfer between the two phases.

However, more recently Hallmann et al. (1995) introduced an Eulerian model for the computations of fuel spray characteristics including droplet heating and evaporation and excellent agreement with the Lagrangian calculations in terms of droplet velocities and diameter was obtained. More work on an Eulerian model involving

spray evaporation and combustion has been carried out by Truchot et al. (2004a; 2005; Truchot et al. 2004b). In their study, the spray was assumed to be initially monodispersed.

2.2.3 Eulerian versus Lagrangian

Lagrangian and Eulerian approaches both have advantages and disadvantages. The Lagrangian approach ensures that there is no numerical diffusion in the droplet equations. However, there can be interpolation problems between the two methods for the dispersed and continuous phase when calculating the source terms for the gaseous phase, because droplet time scale may be much smaller than for the gaseous phase, which can make the solution difficult to converge. This problem does not exist for the Eulerian approach, since the same computational approach is employed for each phase and all the equations are solved on the same mesh which becomes a distinct accuracy advantage in two-way coupling (Loth, 2000). On the other hand, the dispersed phase will be subject to the same numerical diffusion as that of the gaseous phase.

The Lagrangian approach allows to deal accurately with the most complex configuration of collision, coalescence, counter flowing particles, heat and mass transfer can be handled in this approach without substantial complication or loss of physical representation and it is not limited by a lack of knowledge of the governing equations of the droplet phase when treated as a continuum as for the Eulerian approach. But the Lagrangian approach is computationally more expensive than the Eulerian method since Eulerian approaches are typically more node wise efficient when dealing with a very large number of particles. In fact, the computation of Eulerian equations does not depend on the number of particles, avoiding further computational complications.

2.3 *Spray Evaporation*

Droplet heating and vaporization must be described in a sufficiently accurate and simple manner to be implemented in a CFD code representing spray combustion. Indeed, the concentration of fuel vapour in the combustion chamber is determined by

the evaporation rate, which affects the performance of the combustor significantly and will have a knock-on effect on the simulation of the combustion process. However, as it is a multidisciplinary issue, droplet heating and evaporation becomes even more complex and challenging. In fact, spray evaporation and combustion involves heat and mass transfer, multiphase flow, fluid dynamics, and chemistry. Also evaporation is further complicated by the fact that the droplet diameter is in constant regression, involving a moving boundary.

Introduction description of droplet evaporation has been introduced by the works of Kuo (1986), Kanury (1975), Glassman (1987), Clift et al (1978), Williams (1985), Lefebvre (1989) and useful research reviews have been written by Williams (1973), Faeth (1983), Law (1982) and Sirignano (1982, 1993a) which tend to show that spray evaporation and combustion is reasonably understood under the spherically symmetric configuration first introduced by Godsave (1953) and Spalding (1953). Indeed, because of the importance of fundamentals and application to spray combustion, droplet evaporation has been extensively investigated.

2.3.1 Droplet Vaporization Models

Sirignano (1999) divided the droplet heating and evaporation models into six groups of increasing complexity:

- constant droplet temperature models such as the d^2 -law with uniform and constant droplet temperature;
- infinite conductivity model with uniform (no temperature gradient inside the droplet) but time varying droplet temperature;
- conduction limit model, which takes into account the finite liquid thermal conductivity but not the droplet internal circulation;
- effective conductivity model, which takes into account both the finite liquid thermal conductivity and the droplet internal recirculation via the introduction of a correction factor to the liquid thermal conductivity;
- vortex model which account for the droplet internal circulation via the vortex dynamics;
- models based on the solutions of the Navier-Stokes equations.

The two last groups are not expected to be implemented into CFD codes in the foreseeable future due to their complexity (Sazhin, 2006). These models are widely used for a better understanding of the droplet heating and evaporation process as well as a tool of validation of the simpler models (Sirignano, 1999). A correction factor is required to take into account the convective heat transfer from the gas to the liquid for the first three models, while internal circulation and liquid model is added in the three remaining models. Models such as the infinite conductivity, conduction limit, and effective conductivity models would rather be implemented in CFD codes. In fact, a major concern for implementation is to find a reasonable balance between results accuracy and computing time, without sacrificing too much on either side, which is a condition satisfied by these models.

For all the models presented a complete list of assumptions is as follows:

- quasi-steady gas film around the droplet
- uniform physical properties of the surrounding fluid
- the equation of state is based on the ideal gas law
- the air is insoluble in the liquid phase
- uniform pressure around the droplet
- liquid/vapour thermal equilibrium on the droplet surface
- radiation and gravity effects are not considered
- liquid phase viscosity is generally taken as variable but density and other properties are typically taken as constant (Sirignano, 1999).

One of the first theoretical and simplest approaches to the problem of droplet evaporation of historical significance was made by Godsave (1953) and Spalding(1953). The model has been termed the d^2 -law because they experimentally found that it predicts that the square of the droplet diameter decreases linearly with time. It should be noted that the d^2 -law neglects the liquid-phase heat and mass transfer and is basically a gas-phase model (Aggarwal et al. 1984). Also it assumes quasi-steadiness in terms of droplet temperature, spatially and temporally. The change of droplet diameter with the d^2 -law is represented as follows:

$$d^2 = d_0^2 - \lambda t$$

Equation 2.1

with

$$\lambda = \frac{8k_g}{\rho_l c_{p,g}} \ln(1+B) \quad \text{Equation 2.2}$$

where

$$\lambda = -d(d)^2 / dt \quad \text{Equation 2.3}$$

λ characterises the rate of decrease in size of the initial drop, which is called the evaporation constant. λ depends linearly on the transport properties, through either $k_g/c_{p,g}$ or $\rho_g \delta_g$ therefore the evaporation constant can also be written

$$\lambda = \frac{8\rho_g \delta_g \ln(1+B)}{\rho_l} \quad \text{Equation 2.4}$$

The d^2 -law is based on the main assumption of unitary Lewis number, hence the species mass and thermal diffusivity are equal. Furthermore, when $Le = 1$, $Sh = Nu$ and this results in:

$$Nu = Sh = 2 \frac{\log(1+B)}{B} \quad \text{Equation 2.5}$$

The resulting relationship for fuel evaporation rate for a spherically symmetric droplet - where the heat and mass transfer are expected to occur in a spherically symmetrical manner between the droplet surface and the gas phase- is written as below:

$$\dot{m} = 2\pi d \delta \rho_g \ln(1+B) \quad \text{Equation 2.6}$$

B is the mass transfer number such as $B_v = C_p(T_g - T_s)/L_s$ for pure vaporization and $B_c = [C_p(T_g - T_s) + qY_o/\nu]/L_s$ for combustion with ν the stoichiometric oxygen to

fuel mass ratio and q the chemical heat release per unit mass of fuel burned. Typical values of B_v and B_c range from 0.1 to 1 and 1 to 10, respectively.

The d^2 law appears to be too simplistic for applications in most CFD codes (Sazhin, 2006) and is not appropriate for high boiling point droplets lifetime predictions (Sirignano, 1983) such as vegetable oils.

Since the classical d^2 law, many significant advances in the modelling of droplet vaporization have been reported. Law (1976) developed the infinite conductivity model or rapid mixing limit model where it is assumed that rapid internal circulation occurs within the droplet and the droplet temperature is uniform but time varying. By assuming that the droplet temperature is spatially uniform, the challenging task of describing the droplet internal circulation is avoided, although its effects are still included in his analysis. The gas phase model remains spherically symmetric and quasi-steady.

Compared to the d^2 law, L is replaced by

$$L + \frac{1}{m} \left(\frac{4}{3} \pi \rho_l C_{p_l} \right) \frac{dT_l}{dt} \quad \text{Equation 2.7}$$

The infinite conductivity model is relaxed with the conduction limit model developed by Law et al. (1977), where the internal liquid motion is assumed negligible, heat transfer inside the droplet will be controlled by thermal conduction only and droplet temperature quasi-steadiness can be achieved after a certain portion (between 10 to 40 %) of the droplet lifetime. With the d^2 law (no transient droplet heating), the droplet vaporizes much faster than with the conduction limit model. For the conduction limit model, L is replaced by:

$$L + \frac{1}{m} 4\pi r^2 k_l \left. \frac{dT_l}{dt} \right|_{r_s} \quad \text{Equation 2.8}$$

The conduction limit model is essentially a spherically symmetric, low-pressure model for monocomponent fuels such as the ones investigated in this study.

Prakash and Sirignano (1980) developed a gas phase analysis coupled with a modified liquid phase analysis from a previous paper (Prakash and Sirignano, 1978) this time accounting for the changing droplet size due to evaporation as well as the internal liquid motion within the droplet. This droplet heating model is named the vortex model due to the explicit identification of a spherical vortex in the liquid as illustrated in figure 2.1.

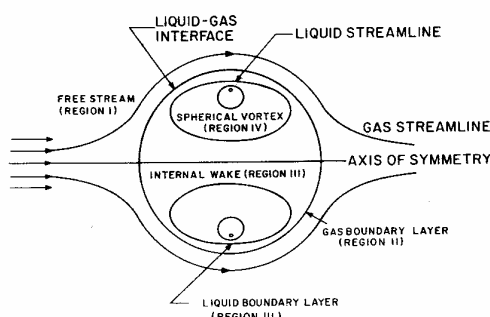


Figure 2.1 Schematic of droplet with internal circulation (Sirignano, 1983)

However their analysis is too complicated to be implemented for spray calculations. Tong and Sirignano (1982) strived to present a simplified model without sacrificing accuracy, however it is only valid when the Reynolds number is large compared to unity.

More recently, Abramzon and Sirignano (1989) provided a relatively ‘inexpensive’ vaporization model of a moving fuel droplet, particularly suitable for the spray combustion calculation, which includes all the effect of variable thermophysical properties, non unity Lewis number (in the range 1-4) in the gas, the effect of transient liquid heating, droplet internal circulation and the effect of the Stefan flow on heat and mass transfer between the droplet and the gas. This model possess such advantages as simplicity, application to a wide range of parameters (Re , B , etc.) making it a more robust model, and necessitating low amount of computational time.

The liquid phase portion of this model is often branded the ‘effective conductivity model’ since it implicitly represents the effect of the liquid vortex through an effective conductivity larger than the actual conductivity. The liquid finite thermal conductivity models could be generalised to take into account the internal recirculation inside droplets and correctly predict the heat transfer to moving droplet.

On the basis of the simplifications made in the classical models, the ‘exact solution’ based on the resolution of the Navier-Stokes equations is highly desirable. Exact analysis for gaseous flow over vaporizing liquid droplets have been performed by several researchers (Renksizbulut and Haywood, 1988; Haywood et al. 1989; Chiang et al. 1992) and can serve several purposes. First, they yield detailed insight to the heat and mass transfer as well as momentum between the droplet and the gas phase. Second, they offer a basis of comparison with the other simplified models.

2.3.2 Convective Effects

Convection greatly affects the heat and mass transfer at the droplet surface and as a consequence, the gasification process. Indeed, where relative motion exists between the droplets and the surrounding gas, the rate of evaporation is enhanced by forced convection, but it also generates liquid circulation inside the droplet which increases the liquid heat transfer and evaporation rate.

In the case of stagnant droplets, there is no relative motion between the droplet and the ambient gas, and convection is hence inexistent, reducing the heat transfer to a conduction problem. Based on equation 2.5, $Nu = 2 \frac{\log(1+B)}{B}$ in absence of convection. As B tends toward zero, $\ln(1+B)/B$ approaches unity and $Nu = 2$. Therefore, for constant fluid properties, in the absence of convection, the Nusselt number describes a non dimensional heat transfer rate to the droplet is:

$$Nu = hD/k = 2$$

Equation 2.9

The effect of forced or natural convection is then treated by an additional empirical correlation due to Ranz and Marshall (1952).

$$Nu = hD/k = 2 + 0.6 Re^{1/2} Pr^{1/3} \quad \text{Equation 2.10}$$

The Reynolds number, based on the relative velocity between the droplet and the surrounding gas, and described as $Re = \frac{\rho_{\infty} |U_{\infty} - U_{droplet}| d}{\mu_g}$, can be as high as 100 (Law et al. 1977) in a typical spray application, especially for large droplets where the convective transport processes are dominant.

Hence the convection correction for the heat transfer rate calculated in the absence of convection is written as follows:

$$h/h_{Re=0} = 1 + 0.3 Re^{1/2} Pr^{1/3} \quad \text{Equation 2.11}$$

$$\text{Hence } \dot{m} = \dot{m}_0 (1 + 0.3 Re^{1/2} Pr^{1/3})$$

Sometimes, the power 1/3 of the Prandtl number is replaced by 0.4 (Sazhin, 2006) and instead of a factor of 0.3, Frossling (1938) suggested a value of 0.276. For Reynolds numbers that are very large compared to unity, the Reynolds number is the dominant effect and the Nusselt number as well as the vaporization rate will be directly proportional to the square root of the Reynolds number. This correlation is commonly used for the d^2 -law, conduction limit and infinite conductivity models.

Other correlation, valid for wide range of Reynolds number, have been provided by Renksizbulut-Yuen (1983) and Abramzon and Sirignano (1989) have been demonstrated to accurately predict experimental data and numerical results written in other publications..

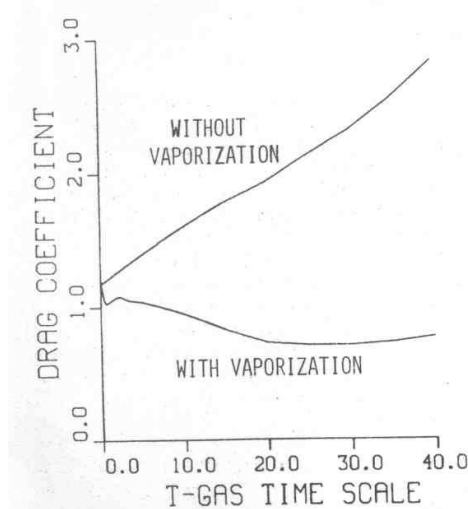
2.3.3 Droplet drag coefficients

Droplet drag coefficients is crucial to determine the dynamics of the evaporating droplet and its penetration into the combustor apparatus, since the momentum exchange between the droplets and the gaseous phase is assumed to be governed by a drag law.

Bolt and Saad (1957) in agreement with Spalding (1955) remarked that the existence of the flame around and in the wake of the droplet tends to decrease the drag force. Eisenklam et al. (1967) showed that the drag coefficient is reduced due to the blowing effect of evaporation by a factor $(1+B_M)$ where B_M is the mass transfer number. Yuen and Chen (1976) extended the work of Eisenklam et al. (1967) to higher Reynolds number and found that the droplet drag coefficient is close to that for a solid sphere of the same diameter.

Renksizbulut and Yuen (1983) developed the following correlation based on experimental data, for a intermediate Reynolds number between 10 and 260:

$$C_D(1+B)^{0.2} = 24\text{Re}_m^{-1} + 4.8\text{Re}_m^{0.63}$$



Drag coefficient variation (Dwyer and Sanders, 1984)

Chiang et al. (1992) proposed the following correlation:

$$C_D = \frac{24}{\text{Re}} \left(1 + 0.325 \text{Re}_m^{0.474} \right) (1 + B)^{-0.32} \quad \text{Equation 2.12}$$

for $0.4 \leq B_T \leq 13$; $30 \leq \text{Re} \leq 200$

Liu et al. (1993) expressed the drag coefficient as a function of the droplet Reynolds number:

$$C_D = \frac{24}{\text{Re}_d} \left(1 + \frac{1}{6} \text{Re}_d^{2/3} \right) \text{ if } \text{Re} < 1000 \quad \text{Equation 2.13}$$

$C_D = 0.424$ if $\text{Re}_d > 1000$

Where Re_d is the droplet Reynolds number

2.3.4 Droplet Evaporation at elevated pressures

The trend toward higher combustion chamber pressures driven by the requirement of increased mixing rates has led to a need to get a clear understanding of the evaporation process under super critical conditions and the literature on droplet evaporation under higher pressure has become quite extensive in the past decade with reviews by Givler and Abraham (1996) and Bellan (2000).

Theoretical studies have shown that the quasi-steady approximation is no longer valid when the droplet approaches its critical temperature and when the ambient pressure increases beyond the fuel supercritical pressure (Rosner and Chang, 1973; Givler and Abraham, 1996). Lazar and Faeth (Lazar and Faeth, 1971) and Matolsz et al. (1972) have experimentally demonstrated that the portion of droplet lifetime spent in the quasi-steady state decreases as the ambient pressure increases and that none of the droplet reached the fuel critical temperature.

Once the critical temperature is reached and the droplet changes into gaseous phase, the ambient gas is soluble into the liquid phase and as a consequence solubility effects should be taken into account under high pressures (Jia and Gogos, 1993). In most models of droplet evaporation, it is assumed that the ambient gas is ideal but several researchers (Matlosz et al. 1972; Delplanque and Sirignano, 1996; Givler and

Abraham, 1996; Holmann and Renz, 2003; Sazhin, 2006; Sazhin, 2006) mentioned that for high pressure this assumption is no longer valid and the Raoult law has to be replaced by the equation of state proposed by Peng and Robinson (1976).

Matolsz et al (1972) and Kim and Sung (2003) demonstrated that the evaporation rate was enhanced for sub and supercritical pressure conditions but high ambient temperature contributes more significantly to the evaporation rates than increase in pressure, as shown in the figure 2.2.

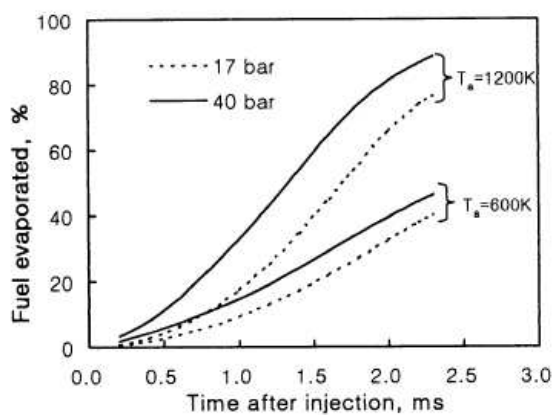


Figure 2.2 Effect of ambient pressure on the fraction of fuel evaporated (Kim and Sung, 2003)

2.4 Droplet interactions

2.4.1 Droplets collision and coalescence

Because of the dense nature of the droplet concentration in the region immediately downstream of the injector, droplet collision and coalescence is a frequent event. The collision and coalescence of fuel engine sprays and gas turbines is of great interest since it will affect the droplet size, number density and velocity of the droplet, essentially influencing the structure of the spray and altering engine performance and as a consequence fuel emissions. Depending on the drops velocity and configuration of the spray, as well as the physical properties of the fluid, collision can lead to various outcomes, such as bouncing collision, due to the presence of an intervening air film, permanent or temporary coalescence, which occurs when the kinetic energy exceeds the value for stable coalescence, followed by disruption or fragmentation

(Brenn and Frohn, 1989b; Orme, 1997). The number of droplets resulting from disruption remains the same whereas fragmentation is the outcome of catastrophic breakup into numerous small droplets. Droplet coalescence is the phenomenon where two droplets combine and generate one single droplet and it is expected to occur when droplets can approach each other with a distance smaller than a critical value depending on the droplet properties and its environment. The different collision outcomes are illustrated in the figure 2.3.

There are few significant studies in which droplet collision and coalescence is directly related to spray combustion applications such as the experimentations carried out by Benn and Frohn (1989b; 1989a), on propanol and hexadecane liquids, however these were mainly observational studies. Jiang et al. (1992) carried out the most detailed investigation of collision behaviour involving hydrocarbon droplets, with studies involving fuels from heptane to hexadecane. Orme (Orme, 1997) demonstrated that collision dynamics and outcome for the hydrocarbon droplets for the hydrocarbon droplet can be significantly different and much more complex than collision of water droplets (Brenn and Frohn, 1989b), due to the difference in physical properties.

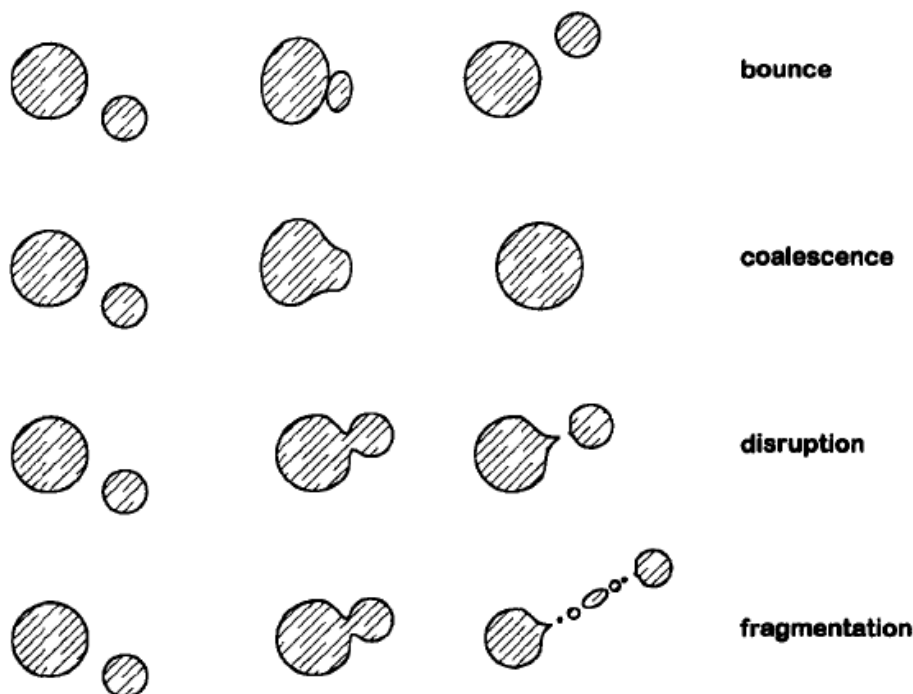


Figure 2.3 Possible outcomes of droplet collisions (Orme, 1997)

Generally collision needs to be incorporated in the numerical description of dense spray configurations. Indeed the numerical results of Martinelli et al. (1984b) predicted a much smaller mean droplet diameter of $7\mu\text{m}$ than the $42\mu\text{m}$ measured experimentally by Hiroyasu and Kadota (1974b) and he explained that the main reason for this major discrepancy was because droplet coalescence was neglected. This also demonstrates that in the presence of collision and coalescence phenomena, the droplet size is less dependent on the initial conditions.

2.4.2 Droplet breakup

The atomization of liquids has many important applications such as internal combustion engines, gas turbine and agricultural sprays among others and atomization quality is crucial to ensure good combustion efficiency and low emissions of pollutants. As a result, numerous interesting studies on droplet breakup phenomena from Lee (1932), Lane (1951), Giffen (1953), Krzeczkowski (1980a), Lefebvre(1989), Faeth (1991), Hinze (1995), Hsiang and Faeth (1995), Gelfand (1996) have been reported for several decades and literature on this physical process is quite abundant.

The atomization process is generally divided into two stages. First, primary droplet breakup process defines the initial conditions for the spray, affecting mixing rates, secondary breakup and collisions. Early observation (Lee and Spencer, 1932) showed that liquid fuel leaving the nozzle is broken up into shreds and small ligaments by aerodynamic forces and instabilities developing at the liquid/gas interface as illustrated in figure 2.4. These ligaments are quickly broken up into drops by the surface tension of the fuel.

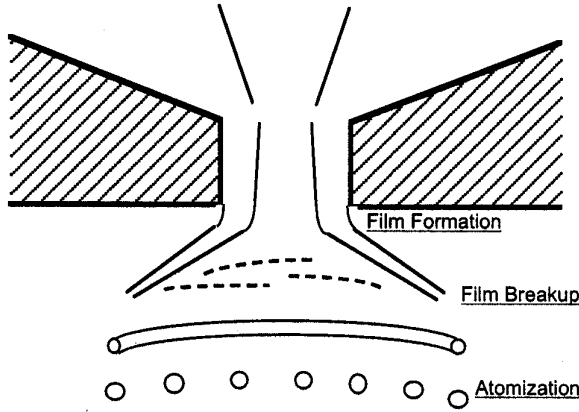


Figure 2.4 Sheet disintegration(Dombrowski and Johns, 1963)

Then the secondary breakup where the large drops produced in primary atomization are further disintegrated into smaller droplets due to the strong shear forces imposed on the droplets, due to high relative velocities between the gas and the spray phase. Primary followed by secondary breakup is likely to be a phenomenon occurring in dense sprays. The transformation of an initial liquid jet into a multitude of small liquid droplets will increase the surface area per unit volume of liquid and as a result the evaporation rate and it will lead to a significant shortening of the droplet lifetime (Chin, 1995). The relative velocities of the droplet are significantly reduced during secondary breakup (between 30 and 70% deceleration, depending on droplet size) due to large drag coefficients due to the droplet deformation (Hsiang and Faeth, 1993) significantly reducing droplet penetration and hence avoiding the issue of wall wetting and carbon deposits.

Breakup regime transitions depend largely on the ratio of disruptive aerodynamic force to surface tension forces, represented by the Weber number,

$$We = \frac{\rho_d |u - u_d|^2}{\sigma} \text{ and the ratio between the liquid viscous and the surface tension}$$

forces, represented by a dimensionless group known as Ohnesorge number defined

$$\text{by Hinze (1995), } Oh = \frac{\mu_l}{(\rho_l d \sigma)^{1/2}} \text{ or } Oh = We^{0.5} / Re \text{ with } Re = \rho_g |u - u_d| D / \mu_g .$$

The higher the Weber number, the larger the deforming external pressure forces are, compared with the restoring surface tension forces. In the absence of such disruptive forces, surface tension tends to pull the liquid into the form of a sphere. The

Ohnesorge number accounts for the influence of liquid viscosity on droplet breakup. At low Oh, droplet deformation becomes significant at We of roughly 1, and droplet breakup occurs at We of around 10-12, with a critical Weber number taken to be generally of 12, with bag, multimode, and shear breakup regimes observed progressively at larger Weber number, as illustrated in the figures 2.5 to 2.8. With increasing Oh, however, higher values of We are needed in order to trigger breakup, as illustrated figure 2.10, because the high viscous forces hinder droplet deformation, which are the first stage towards the breakup process.

**Figure 2.5**

Typical pictures of bag breakup for water droplets, $We = 13.5$ (Krzczkowski, 1980)

**Figure 2.6**

Typical pictures of bag-jet breakup for glycerine droplets, $We = 36.0$ (Krzczkowski, 1980)

**Figure 2.7**

Typical pictures of transition breakup for butanol droplets, $We = 48.1$ (Krzczkowski, 1980)

**Figure 2.8**

Typical pictures of shear breakup for ethanol droplets, $We = 162$ (Krzczkowski, 1980)

The resulting deformation and breakup regime map, showing transitions between different breakup regimes such as those described in figure 2.5 to 2.9 as a function of the Weber number and Ohnesorge number have been identified and illustrated in the figure 2.10.

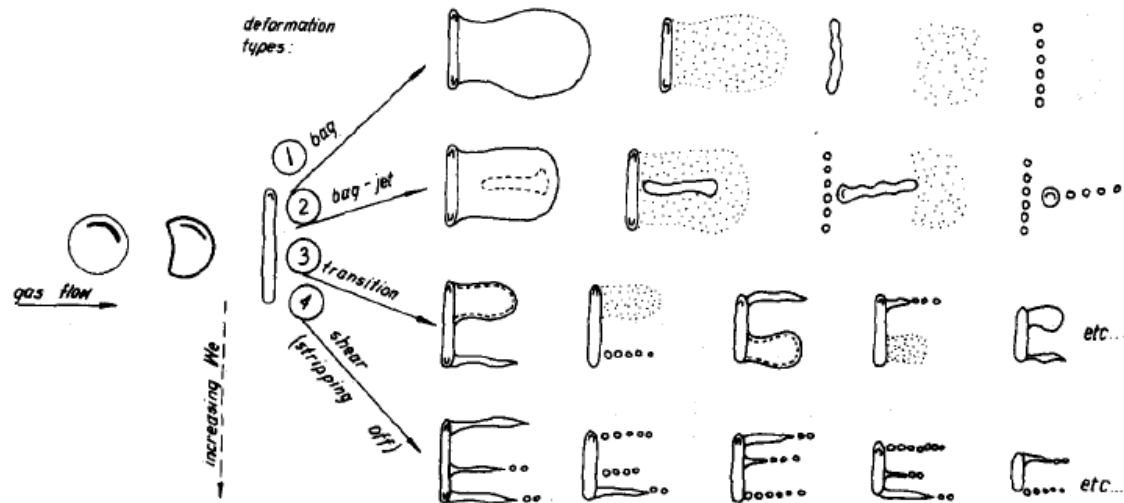


Figure 2.9 Sketch of droplet deformation development (Krzeczkowski, 1980a)

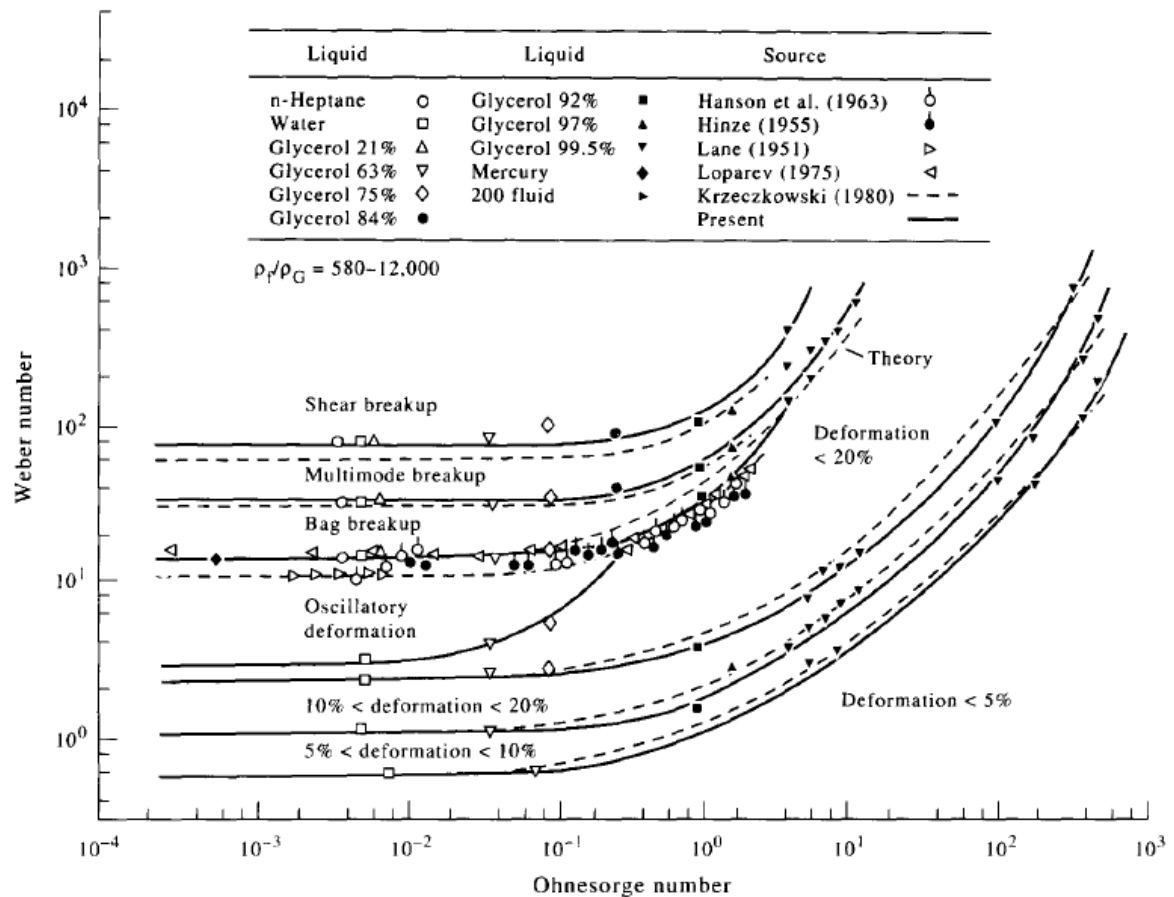


Figure 2.10 Drop deformation and breakup regime map as a function of We and Oh(Hsiang and Faeth, 1995)

2.4.3 Breakup models

Despite being the subject of numerous investigations, breakup models remain imperfect, which explains why several breakup models exist in the literature.

Reitz and Diwakar (1987; 1988) proposed a method called WAVE method for calculating droplet breakup and found that the droplet size downstream of the injector were influenced by the competition between collision and coalescence. They had some success in predicting the experimental measurements made notably by Hiroyasu and Kadota (1974).

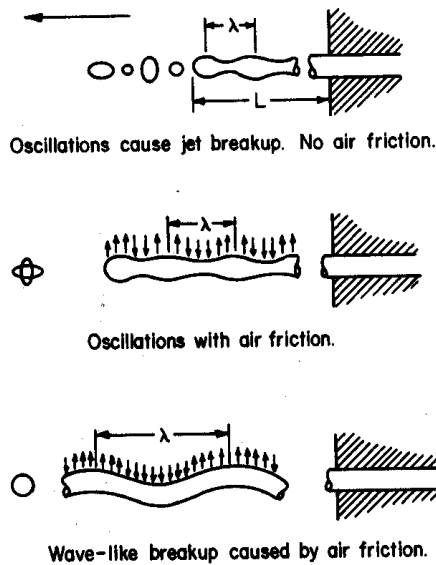


Figure 2.11 Schematic drawings of pressure-swirl atomizers (Senecal et al., 1999)

O'Rourke and Amsden (1987) presented an alternative model for droplet breakup, the so called TAB model. This model is based on an analogy, suggested by Taylor, between an oscillating and distorting droplet and a spring mass system. The TAB model is mostly valid at low drop Weber numbers and possesses several advantages over the Reitz and Diwakar (1988) breakup model, enumerated by O'Rourke and Amsden (1987), such that there is not a unique critical Weber number for breakup, the effects of liquid viscosity are included, which can significantly affect the oscillations of the small droplets. Also, the model predicts the state of oscillation and distortion of the droplets and gives drop sizes that are more in agreement with experimental data of liquid jet breakup (Reitz and Bracco, 1979). Finally, the model does not need to input the spray angle since the spray angle is automatically calculated by the TAB method, unlike the Reitz and Diwakar model (1988), but on the other hand, the TAB models needs more constants. O'Rourke and Amsden (1987) demonstrated that one major limitation of the TAB model is that only one oscillation mode can be kept tracked of, while many such modes exist in reality.

Some improvements were also introduced concerning the atomization process introducing a 'hybrid' model (Beatrice et al. 1995), based on the TAB (O'Rourke and Amsden (O'Rourke and Amsden, 1987) and the WAVE Reitz and Diwakar model (Reitz and Diwakar, 1987; Reitz and Diwakar, 1988). Indeed, it has been established that the TAB model underestimates the tip penetration, resulting in fast evaporation

and fuel rich regions close to the nozzle while the WAVE model overestimates it (Bertoli and Migliaccio, 1999) and the simultaneous choice of both models has a physical meaning since for large diameter drops, near the nozzle exit, the model of unstable wave propagation on a liquid surface may be more relevant, while in the later stages of the injection process, the computation of break-up with the TAB analogy seems to be more appropriate for smaller drops (Bertoli and Migliaccio, 1999). The WAVE and TAB models are the most used secondary breakup models in CFD simulations.

Ibrahim et al. (1993) introduced the droplet deformation and breakup model (DDB) which provided a better agreement with experimental data compared with the TAB model since the breakup criteria has been modified. Indeed, the assumption in the TAB model that the breakup criterion is the amplitude of oscillations of the drops equals the drop radius has been proven to be unrealistic following Krzeczowski's (1980) publication, who suggested that breakup occurs at different sizes for different Weber numbers. The model suggested by Ibrahim et al. (Ibrahim et al. 1993) is applicable for breakup regimes whose $We > 20$.

Alloga et al. (1994) assessed the capabilities of the TAB, WAVE and DDB breakup models by comparing their results with experimental measurements of tip penetration, spray cone angle and Sauter mean diameter. The DDB models match well the experimental penetration data at low temperature, while the three models underpredict the droplet size and, at high temperature, the DDB model shows the highest penetration rate suggesting that it is more appropriate for simulating the spray dynamics for small engine like conditions and the WB model is more suitable for large engines, while the TAB model is estimated to be completely inadequate. The TAB and WB models underestimate the spray cone angle at low temperature, whereas the DDB overestimates it, but at higher temperature it gives accurate predictions, whereas WB and TAB calculate lower values.

2.5 Combustion models

The complex turbulence-chemistry interaction can be modelled by the laminar flamelet modeling, probability density function and conditional moment closure. The different combustion methods for turbulent non premixed combustion are outlined and their success in predicting temperature and species concentration in turbulent jet diffusion flame is reviewed. The limitations of the modelling assumptions made and the advantages of the methods are discussed.

2.5.1 Laminar diffusion flamelet models

The chemical equilibrium assumption may not be sufficient in turbulent flows where local diffusion time scales vary considerably and non-equilibrium effect must be taken into account. The deviation from chemical equilibrium is based on the assumption that a turbulent nonpremixed flame can be viewed as consisting of locally thin, one-dimensional reaction zones that are continually displaced and stretched within a turbulent medium as illustrated in the figure 2.12. This picture of a turbulent flame as a statistical ensemble of laminar flames has been termed the laminar diffusion flamelet model (Peters, 1984). As shown by Bilger (1976) the formulation of diffusion flamelet structure is introduced through a coordinate system where the physical space x is suppressed in favour of the mixture fraction Z , itself transported by convection and diffusion in the flame, which means the temperature, species mass fraction and all thermochemical variables will be expressed as function of the mixture fraction Z , key to the simplification introduced by flamelet modelling (Moss, 1995) illustrated figure 2.13. The mixture fraction is bounded between values of zero and unity. An advantage of the transformation is that in the Z coordinate the profiles are much less strongly dependent on the flow configuration than they are in the original spatial coordinate. These relationships are then averaged, for the turbulent flame, using an assumed pdf – clipped Gaussian form or Beta function - for the mixture fraction (Liew et al. 1981).

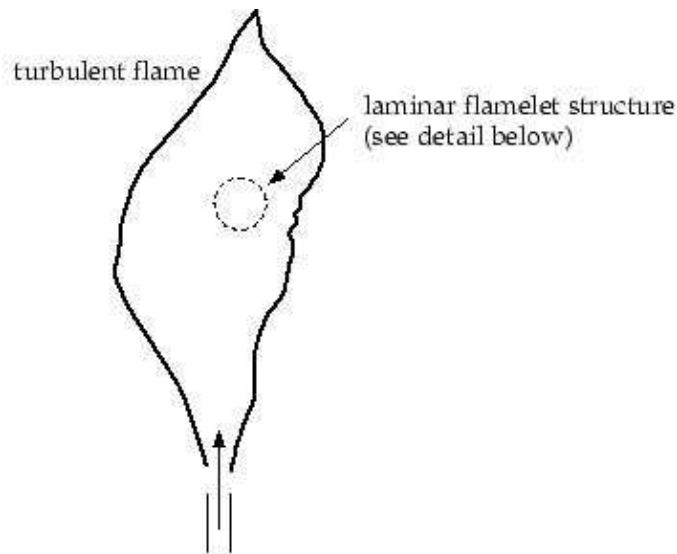


Figure 2.12 Flamelet illustration (Fluent documentation)

In figure 2.12, Z_c is the stoichiometric mixture fraction; the mixture is fuel-lean for $Z < Z_c$ and rich for $Z > Z_c$. Thus there are two separate zones, one ($Z < Z_c$) in which oxygen diffuses into the flame and the other $Z > Z_c$ where the fuel diffuses into the flame (hence the name diffusion flame).

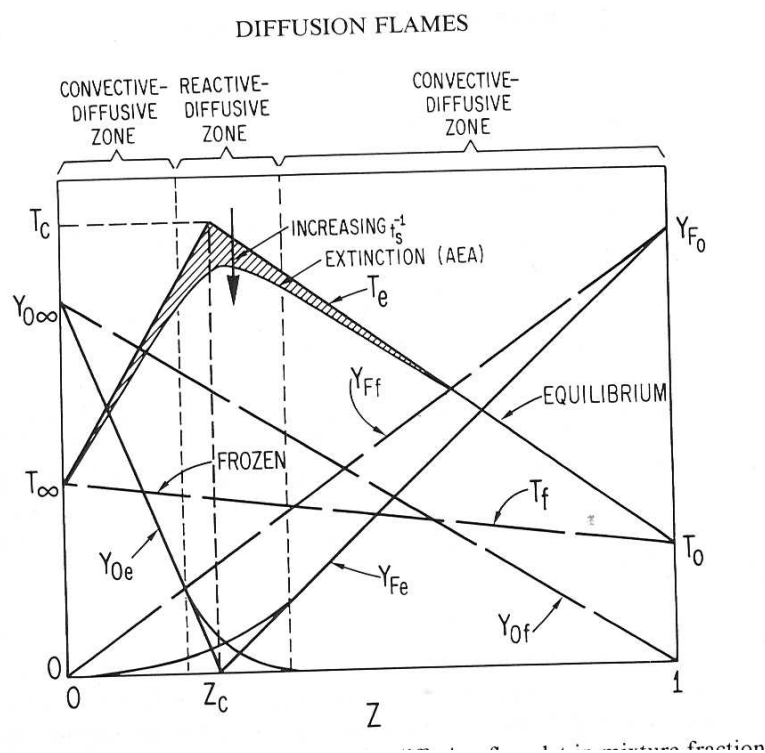


Figure 2.13 Illustration of the structure of a diffusion flamelet in mixture fraction space (Liñán and Williams, 1993)

An essential objective of the flamelet formulation is to simplify the coupling between chemical kinetics and turbulence. It should therefore be possible to evaluate the scalar profiles from a laminar flow configuration and to use them in a turbulent flow. This requires that the Z dependence of $\chi(Z,t)$ agrees sufficiently well for the laminar and turbulent flows considered (Peters, 1984). In the laminar flamelet model, it is assumed that the structure of the turbulent diffusion flame is locally that of a laminar diffusion flame at the same instantaneous value of the mixture fraction Z and scalar dissipation, χ (Tsuji and Yamaoka, 1966; Peters, 1984). The scalar dissipation rate is defined by:

$$\chi = 2\delta \left[\left(\frac{\partial Z}{\partial x} \right)^2 + \left(\frac{\partial Z}{\partial y} \right)^2 + \left(\frac{\partial Z}{\partial z} \right)^2 \right] \quad \text{Equation 2.14}$$

With δ the diffusion coefficient.

The coupling between non-equilibrium effects and turbulence is ascribed to the instantaneous scalar dissipation rate, χ_{st} , which quantifies the amount of flame stretch. At low value of stretch, laminar flamelet profiles approach the equilibrium structure, and at very high stretch, extinction can occur. The introduction of laminar flamelet into a turbulent flow is performed by considering the joint statistics of the mixture fraction Z and the scalar dissipation rate χ_{st} (Liew et al. 1984).

For the counterflow geometry, the scalar dissipation rate at the location where the mixture is stoichiometric may be approximated, assuming constant density and diffusivity, by

$$\begin{aligned} \chi_{st} &= (a/\pi) \exp \left\{ -2 \left[\text{erfc}^{-1}(2Z_{st}) \right]^2 \right\} \\ &\approx 4aZ_{st}^2 \left[\text{erfc}^{-1}(2Z_{st}) \right]^2 \end{aligned} \quad \text{Equation 2.15}$$

where a is the velocity gradient and erfc^{-1} the inverse of the complementary error function.

The formulation of diffusion flamelet allows the use of complicate chemistry including pollutant formation and soot. An accurate prediction of the species concentration to determine the flamelet structure will depend on the selection of a detailed enough reaction mechanism (Peters, 1984). Compared to the assumption of chemical equilibrium, substantial improvement in the prediction of mean CO and CO₂ concentration in the fuel rich region is obtained in a laminar diffusion flame.

For diffusion flames in the extreme flamelet limit ($Da \gg 1$), flamelet models treat the coupling between reaction and diffusion accurately and elegantly. But, flamelet models have quite limited applicability since, in practice Da spans, typically, four orders of magnitude (Pope, 1990) and is suited to predict moderate chemical non-equilibrium in turbulent flames but not slow-chemistry flames such as NO_x formation. Discussion of the laminar flamelet validity has been initiated by Bilger (1988) who suggests that the condition for flamelet concepts that the reaction zone be thinner than the smallest scales of turbulence will be violated in most non-premixed flames of practical interest. Nevertheless, calculations accounting for transient behaviour in flamelets have countered criticism (Peters, 1991; Buriko et al. 1994) of the basic concept with capabilities of the model extending beyond the range of flamelet behaviour (Desjardin and Franel, 1996).

In summary, the flamelet concept has proven to be useful for non-premixed combustion because it is a straight forward extension of the local equilibrium model, the turbulent flow and finite rate chemistry and a two-variable formulation appears to be introduced with a reasonable physical approximation.

2.5.2 Joint PDF methods

Probability density functions have been used in the study of turbulent reactive flows for nearly 60 years (Hawthorne et al., 1949) and the PDF methods described below, employ joint pdf of reactive scalars and conserved scalars in modelling scalar transport and production (Smith et al., 1995). With the pdf approach, the effects of convection and chemical reaction can be accommodated without approximation, avoiding modelling problems and, no assumption is needed about the shape of the

joint pdf of Z since the joint pdf is calculated and not an assumed form (Pope and Correa, 1986), therefore providing a more accurate closure than the assumed-pdf method (Pope, 1990). A modelled procedure is only necessary for molecular transport.

The instantaneous reaction rate for fuel disappearance, is a complex representation of the composition, Y_f and Y_o , the mixture density, ρ and the temperature T , whence

$$\overline{S_Z} = \int S_Z(Y_f, Y_o, \rho, T) p(Y_f, Y_o, \rho, T) dY_f dY_o d\rho dT \quad \text{Equation 2.16}$$

where $p(Y_f, Y_o, \rho, T)$ is a joint probability density function for these scalar variables.

The joint pdf contains all statistical informations to determine mean reaction rate. All the thermochemical variables are tabulated as functions of Z for use in the Monte Carlo procedure. The variables tabulated are: the species mass fraction, the density and the temperature (Pope and Correa, 1986).

Pope (1985) demonstrates that the transport equation for the joint pdf can be solved using a Monte Carlo method in flows of practical interest. Indeed, finite difference methods have difficulty in coping with the large dimensionality of the pdf's and the integro-differential nature of the equations. This method has been replaced in favour of the Monte Carlo method, which makes possible the solution of the pdf equation for the general case (Pope, 1981).

PDF methods have been successfully employed to calculate laboratory turbulent flames. They can predict phenomena such as super equilibrium levels, and local extinction (Norris and Pope, 1995). Because of these advantages, PDF methods are becoming used increasingly in industrial combustor code but coupling the detailed description of the turbulent combustion flow field provided by PDF methods with detailed chemical kinetic mechanisms (Yang and Pope, 1998) remains a challenge. Indeed, the PDF calculations are very computationally expensive. Also, despite its more accurate closure compared with an assumed pdf method, the weakest component

of pdf method is the modelling of molecular diffusion, especially in the presence of reaction.

2.5.3 Conditional Moment Closure Modelling

The modelling of turbulent reactive flow is significantly more difficult than modelling laminar flames and reactive systems, due to the need to consider the highly non-linear processes associated with high levels of fluctuations of species concentrations and temperature. The unconditional average approach commonly employed is of little use in turbulent combustion modelling because it does not provide a mean of closure for the non-linear chemical production terms present in the reactive species balance equation (Pope, 1990). Using moment conditional on a stoichiometric variable, such as the mixture fraction, eliminates this major source of nonlinearity and more accurate closure for the reaction rate becomes available, hence conditional averaging reduced the problem considerably (Bilger, 1993; Bilger, 1997).

This alternative method pioneered and proposed by Bilger (1993) and Klimenko (1990) is called the CMC (Conditional Moment Closure) method, and makes extensive use of conditional averages of reactive scalar values to close the chemical reaction terms in the governing equations. By conditioning on conserved scalar values, the effect of turbulent fluctuations in conserved scalar space on the chemical system is accounted for, and instantaneous chemical reaction expressions can be evaluated in terms of these conditionally averaged scalar values to give conditionally averaged mean reaction rates. Solution of the system is then achieved via a conventional solver (Smith et al. 1995).

In the CMC method, the instantaneous equations governing reactive scalar transport and production in a statistically turbulent reactive flow are averaged, on the condition that mixture fraction $Z(x,t) = \eta_Z$ in the sample range $0 \leq \eta_Z \leq 1$, that is, only those members of the whole ensemble that meet this condition are included in the average in order to close the chemical reaction terms.

The equations governing the behaviour of the conditional moments of the individual species mass fractions in a homogeneous turbulent flow are:

$$\frac{\partial Q_i(\eta_z, t)}{\partial t} = \frac{1}{2} \langle \chi | \eta_z \rangle_t \frac{\partial^2 Q_i(\eta_z, t)}{\partial \eta_z^2} + \langle \omega_i | \eta_z \rangle \quad \text{Equation 2.17}$$

where closure is obtained in terms of the conditional average

$$\langle Y_i | \eta_z \rangle = Q_i(\underline{x}, \eta_z) \equiv \langle Y_i(\underline{x}, t) | Z(\underline{x}, t) = \eta_z \rangle \equiv \langle Y | \eta_z \rangle \quad \text{Equation 2.18}$$

Where the angled brackets denote ensemble (or here, where stationary turbulent flow is assumed, time) averaging of the i th species mass fraction and the vertical bar denotes that this is done only for those members of the ensemble satisfying the conditions to the right of the bar (Bilger, 1993).

Due to the lack of significant variation of the conditional moment with cross-stream coordinates, the cross-stream dependence of the conditional means is eliminated therefore reducing the dimensionality of the problem (Bilger, 1993). It is worth noting that the method is applicable to systems of arbitrary complex chemistry within reasonable computational cost compared to stochastic approaches such as the Monte Carlo methods (Pope, 1990), allowing more complete chemical mechanisms to be considered without detracting from the viability of solving the combustion problem.

However, the closure used for the conditional chemical rate term is only valid for low values of fluctuations about the conditional mean closures as most of the fluctuations in species and temperature are associated with fluctuations in the mixture fraction (Bilger, 1997). For unconditional averaging such approximation leads to very large errors in combustion system (Bilger, 1993).

The CMC approach is considered to provide a novel framework for the theory of reacting turbulent flows, particularly in non-premixed systems, predicting temperature and mass fraction fields of major species and radicals quite accurately (Smith et al. 1992; Bilger, 1997). The main idea behind the CMC approach is the assumption that,

while the quantities of interest (species mole fractions, etc.) scatter significantly around their unconditional average, the scatter, for a given mixture fraction is small enough for the approximations discussed above to hold.

2.6 Diffusion flames

Flames of gaseous fuels are commonly divided into two categories, the premixed flame and the diffusion flame. In the diffusion flame, the fuel and the oxidiser are initially separated and the reactants mix in the same region that reaction takes place and are also called non premixed flames. Tsuji (1982) asserted that the diffusion flame differs from the premixed flame in that combustion occurs at the interface between the fuel gas and the oxidant gas, and the burning process depends more upon the rate of mixing than on the rates of the chemical processes involved. In fact, the original paradigm for turbulent non-premixed combustion has the viewpoint that such combustion is basically mixing controlled as illustrated by the reference paper from Hawthorne et al. (1949), where they discussed the flame length and diffusion flame structure which are found to correlate well with the mixing laws presented in their study. For this reason, the characteristics of diffusion flames are markedly dependent on the aerodynamics of the particular flow situation, and diffusion flame behaviour cannot be discussed without invoking aerodynamic considerations. A diffusion flame does not propagate and therefore, burning velocity cannot be defined. The characteristic chemical time is much smaller than the characteristic diffusion time, hence the chemical reaction occurs in a very narrow region between the fuel and the oxidiser.

Candles, matches, and wood fires are familiar examples of diffusion flame. The Diesel engine employs diffusion flames that ignite and burn around droplets or sprays. Liñán (1993) also mentions that in many liquid propellant rocket engines diffusion flames occurs around individual fuels or oxidizer droplets, and some application of solid propellant rockets as well as supersonic combustion, considered for hypersonic propulsion also involves diffusion flames.

Processes involved in a representative example of diffusion-flame combustion can be addressed by considering spray combustion into an oxidising gas (Liñán and

Williams, 1993). Indeed, Onuma and Ogasawara (1974) made a direct comparison between the structures of a spray combustion flame and a turbulent gas diffusion flame and they concluded that the flames are similar in structure since they observed that most of the droplets do not burn individually, rather forming a vapour cloud due to droplet evaporation. The process can be decomposed into several stages: atomization of the liquid fuel, spray vaporization, mixing of the droplets with the oxidizing environment, mixing of the fuel vapour with the oxidiser, diffusion flames around the droplets or a cloud of droplets, possibly some regions of premixed-flame propagation, production of air pollutants, and possibly the extinction of burning around fuel droplets as they reach cold gas, leaving unburnt fuel that can represent additional pollutants and diminish combustion efficiency. Several experimental studies (Presser et al., 1993; Goix et al. 1994; Abduljalil et al. 2004) show that droplets are strongly interacting with the flame structure, especially because of the concentration fluctuation due to droplet evaporation, and this will lead to a flame shape different from purely gaseous flames. Compared to gaseous fuels, comparatively fewer studies have been undertaken related to the determination of flame properties of practical liquid fuels, as a result of the complexities that the liquid phase introduces into the experimentation and also the fact that the chemical kinetics of liquid fuels are far more complex and less understood than those for gaseous fuels (Holley et al. 2006).

To investigate diffusion-flame structures, it is desirable to establish a simple configuration that can be probed in detail. The counterflow diffusion flame illustrated figure 2.14, represents such a configuration where these flames have been demonstrated as being suitable for a fundamental study of diffusion flames and its combustion characteristics (Dixon-Lewis, 1991). Major advantages of this setup are the steadiness of the flow, a well-defined flow field, and the ease to vary experimental boundary conditions such as strain rate, temperatures and composition of the feed streams. Counterflow diffusion flames, illustrated by the broad review of experimental studies of these counterflow diffusion flames carried out by Tsuji (1982), is now well documented, and has been used extensively to study diffusion flames and their structures. Opposing jets of fuel and oxidizer are directed toward

each other, and after ignition, a planar diffusion flame is established normal to the axis of the jets.

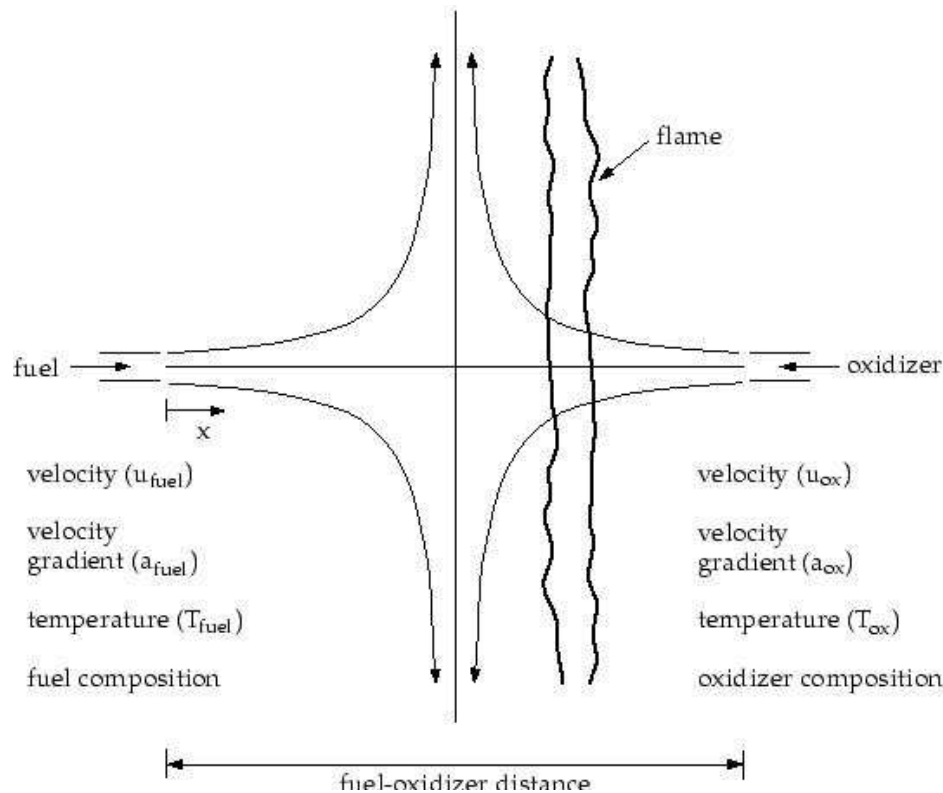


Figure 2.14 Laminar Opposed Flow Diffusion Flamelet (Fluent documentation)

Turbulent combustion regimes may be classified by Damköhler number. The Damköhler number is the ratio of the diffusion time to reaction time:

$$Da = \frac{\text{characteristic diffusion time}}{\text{characteristic reaction time}} \quad \text{Equation 2.19}$$

For sufficiently small Damköhler numbers, the fluid dynamics is rapid compared to the chemistry process, and the turbulent mixing tends to smooth out the concentration fluctuations before the combustion occurs. The reaction then occurs slowly in large regions of the flow. On the other hand, for sufficiently large Damköhler numbers, the reaction occurs very rapidly compared with turbulence, and the combustion occurs in thin sheets, where the fuel and the oxidiser diffuse into each other.

For a counterflow diffusion flame stabilized in a counterflow geometry, there are two independent parameters by which one may control the Damköhler number and thereby the structure of the flame. One parameter is the mass fraction of oxygen in the oxidiser stream, which determines the maximum flame temperature and thereby the chemical reaction time, and the other parameter is the velocity of the oxidiser jet at the injection plane, which determines the strain rate.

The value of the strain rate, on the oxidizer side of the stagnation plane is presumed to be given by (Seshadri and Williams, 1978):

$$a = \frac{2V_2}{L} \left(1 + \frac{|V_1|\sqrt{\rho_1}}{|V_2|\sqrt{\rho_2}} \right) \quad \text{Equation 2.20}$$

where V_2 is the velocity of the oxidiser stream near the injection plane and L is the distance between the tip of the liquid fuel cup and the tip of the oxidiser duct. At a fixed nozzle separation distance, increasing the exit velocities of either or both fuel and oxidizer increases the gradient of axial velocity –the strain rate–, as well as the gradient of fuel and oxidizer in the mixing layer, hence decreasing the local diffusion time in the vicinity of the flame. The jet flows are tailored to exhibit uniform exit velocity profiles and the velocities are large enough to make buoyancy effects negligible (Froude number large enough), but small enough to prevent flow instabilities and turbulence from developing (Reynolds number not too large)(Liñán and Williams, 1993). Since the characteristic chemical reaction time does not change, the Damköhler will also decrease. This decrease subjects the flame to non-equilibrium effects and eventually results to flame extinction. The flame is extinguished by increasing either the velocity or the dilution of the gas.

2.6.1 Extinction of turbulent counterflow non-premixed flames

The extinction mechanism is a fundamental issue. Pioneering work on extinction of counterflow diffusion flames was first done by Norris and Pope (1995) who conducted experiments testing the maximum air velocity a flame can persist using kerosene as fuel. Tsuji (1982) mentioned that in the diffusion flame, the combustion

rate is controlled by the rate at which fuel and oxidiser diffuse to the reaction zone, and this combustion rate increases with the diffusion rate, which is strongly dependent on the aerodynamics of the flow, particularly with convection. But, as the flow velocity is increased, the characteristic aerodynamic time τ_a and as a consequence the diffusion time τ_d become shorter. If the flow of fuel and oxidant into the reaction zone increases, and exceed a critical value, the chemical reaction cannot keep pace with the supply of fuel and oxidant and the reaction ceases, and as a result the Damkhöler number goes below a critical value provoking the extinction of the diffusion flame. In fact, there is a critical stagnation velocity gradient beyond which a flame can never be stabilized (Tsuji and Yamaoka, 1966a) and this is defined as the extinction mechanism.

Hence the flame structure is influenced not only by molecular diffusion but also by turbulence effect, rendering analysis even more difficult. Kitajima et al. (1996) investigated the effects of difference between the turbulence of the fuel stream and the air stream for the structure and extinction of counter-flow non premixed flames. They concluded from their experimental results that for methane-air non-premixed turbulent flames, extinction limits are mostly influence by air stream turbulence rather than the turbulence provided by the fuel stream. They explained it by the fact that the methane-air flames were established in the air stream flow.

2.7 Reaction mechanisms

Detailed reaction mechanisms are widely used to describe the transformation of reactants into products, through a large number of elementary steps. Previous reviews on detailed kinetics models for hydrocarbons include a comprehensive review by Westbrook and Dryer (1984) and a progress report of the last 25 years including a forward looking projection by Cathonnet (1983). Cathonnet (1983) mentioned that most of the results available from kinetic modelling studies in literature concern small molecules (hydrocarbons up to C₄, methanol and ethanol, formaldehyde and acetaldehyde, nitrogen oxides and their byproducts: cyano and amine compounds). For molecules with more than 4 carbon atoms, the most advanced oxidation mechanisms is for alkanes, and it has been applied for the modelling of a wide variety of application. However, there exist relatively few computational or experimental

studies of the combustion of high hydrocarbon under non-premixed conditions. Cathonnet (1983) also mentioned that the laminar flamelet concept used by Peters (1984) would be able to include detailed chemical kinetics into the calculation of turbulent flames in order to accurately predict pollutant emissions. Simmie (2003) published a thorough and detailed review of the post 1994 progress in the modelling of detailed chemical kinetics for the combustion of hydrocarbon fuels. Hydrocarbon is by far the best studied class of compounds for which reliable and detailed kinetic models exists.

The main purpose of this study is to investigate the spray combustion using biomass derived fuels and the accurate prediction of biofuels combustion performance and emission characteristics necessitates a good knowledge of their combustion kinetics. Due to the complexity of biofuels, which is a mixture of fatty acids methyl esters (C_8 to C_{24}), it is difficult to propose a detailed reaction mechanism for its oxidation and a better knowledge of vegetable oil and oxygenated fuels kinetics is necessary for modelling its combustion in gas turbine engines. Consequently, the literature regarding the burning of higher hydrocarbon fuels, especially liquid biofuels is relatively sparse and the development of accurate surrogate fuel models for use in computational models is a critical steps towards enabling the accurate simulation of biofuels combustion characteristics. Reaction Design (2007) has been selected by the NASA to develop fuel models for simulating the operation of jet engines with biofuels with experimental support from researchers at the University of Southern California. Recently, Zhao et al. (2005) presented a detailed decane reaction mechanism but it does not posses the oxygenated structure representative of biofuels. The known published reaction mechanism for which the highest hydrocarbon is investigated is the oxidation of hexadecane $C_{16}H_{34}$, reported by Ristori et al. (2001). Sahasrabudhe et al. (2005) proposed n-hexadecane as an appropriate surrogate for rapeseed oil methyl ester and the reactivity of rapeseed oil methyl ester was well predicted by the kinetic model. Hexadecane molecular weight is close to that of biodiesels and good agreement between the experimental data and the model was obtained, confirming the effectiveness of using surrogate fuels for modelling the combustion of complex commercial fuels. However this was not applied to diffusion

flames where transport data are needed and too many were missing to be able to use this mechanism.

Therefore, the development of a detailed kinetic model for methylbutanoate could be considered as a possible alternative as a surrogate for biodiesel fuel (Fisher E.M. et al. 2000). Although methyl butanoate does not have the high molecular weight of a biodiesel fuel or of vegetable oil, it has the essential chemical structural features, namely the $RC(=O)OCH_3$ structure (where R is an alkyl or 4 alkenyl radical) that might emulate the effects of oxygen that is found in biodiesel molecular structures. The paper from Fisher et al. (2000) strives to fill some information on the thermodynamics and kinetics of $RC(=O)OCH_3$ and species derivated. However, it has been recently demonstrated that methyl butanoate is probably not the ideal biodiesel surrogate.

Westbrook and Dryer (1984) mentioned that the word detailed is used to describe the elementary steps illustrating the process of fuel oxidation into final products at a molecular level, which is essential for tracing species. The hydrocarbon fuel is fragmented into smaller intermediate species which are ultimately converted into final products, made of in majority of water vapour (H_2O) and carbon dioxide (CO_2). Carbon monoxide (CO) and hydrogen (H_2) are also common species observed during hydrocarbon oxidation as well as some radicals, such as OH . From these observations, a reaction mechanism can be constructed systematically, beginning with the simplest species and then adding new species by order of complexity. Each reaction has to be thoroughly validated against experimental results. However, this is not sufficient to ensure that the reaction mechanism is valid for a whole class of operating conditions. Indeed reaction mechanisms are usually valid only for a set range of temperature and pressures

However, as the number of species and reactions becomes too great, a reduced mechanism is needed as the numerical solution of the conservation equations including detailed kinetics is computationally too demanding, especially for engineering applications. Thus it is highly recommended to use reduced mechanism without sacrificing accuracy, by identifying non-contributing reactions. Conventional

numerical solution techniques for the differential equations encountered in both detailed and simplified kinetics schemes indicate that the computer time requirements are roughly proportional to N_{spe}^2 , where N_{spe} is the number of species (Westbrook and Dryer, 1981). There is a rapidly growing useful literature on reduced kinetics for combustion and different approaches have been taken. Chen (1988) has developed a systematic procedure in constructing reduced mechanisms based on matrix operations called Computer Assisted Reduction Method, (CARM) and further created a computer algorithm for automatic generation of reduced chemistry (Chen, 1997) which can be applied for small (Sung et al., 1998) and large hydrocarbon fuels (Sung et al. 1998). Wang and Frenklach (1991), Frenklach et al. (1986) and (1984) introduced a method where two criteria were defined which tests the contribution of a given reaction to the main reaction and to the heat released and removes the least-contributing species. Tomlin et al. (1992) and Turányi (1989; 1990a; 1990b) illustrated an approach where rate sensitivity and temperature sensitivity analysis as well as quasi-steady state analysis are employed, method which Rabitz et al. (1983) has been one of the first to link to chemical kinetics. Other methods based on intrinsic low-dimensional manifolds by Mass and Pope (1992), species lumping (Li and Rabitz, 1989; Li and Rabitz, 1990), computational singular perturbation (CSP) (Lam, 1993; Lu et al. 2001; Massias et al. 1999; Ristori et al. 2001) and more recently new strategies such as adaptive chemistry method (Schwer et al. 2003), linear integer programming (Bhattacharjee et al. 2003) and genetic algorithm (Elliott et al. 2005) are amongst the most significant effort produced in this research area. Cathonnet (1983) prophesied that in the next 10 to 15 years, efficient computer codes for the automatic reduction of large reaction mechanisms will be systematically used for modelling practical combustion systems.

2.8 Concluding remarks

A vast body of work related to the different processes involved in turbulent reacting spray flows has been written, from turbulence to combustion models, including multiphase flow methods and spray evaporation models and has been reviewed in this chapter. Radiation and soot modelling has not been incorporated in this study, to limit

the already vast scope of this study. Indeed, complex issues such as turbulence, droplet interactions, spray evaporation and combustion already play a significant part in the prediction of the numerical simulation.

Throughout this review, it appears that each physical process can be represented by sophisticated numerical models and although it would be preferred to obtain as accurate results as possible, a compromise has to be found between computational time and accuracy, by eventually using simple approaches. Chapter 5 will describe the models of choice for the present study.

CHAPTER 3 – FUEL PROPERTIES

As the use of alternative fuels becomes more widespread, researchers have shown a growing interest in modelling combustion processes in order to understand the fundamental combustion characteristics of fuels which are renewable, biodegradable and oxygenated such as vegetable oils, their derivative and mixtures. To faithfully predict alternative fuel combustion, accurate prediction of the physical properties of alternative fuels is critical in the representation of spray, atomization, and combustion process in the combustion chamber (Yuan et al. 2003b). Lefebvre (1984) has proven that physical properties can directly affect combustion performance and CO₂ emissions. Atomization quality is influenced by the physical properties of the fuel, such as density, surface tension and viscosity. Therefore, predicting the physical properties of the vegetables oils and biofuels is a crucial step in the accurate prediction of the spray atomisation and combustion processes. Most computational softwares (KIVA, FLUENT) used to model atomization and combustion includes the effects of the different fuel properties. Key properties such as viscosity, surface tension, which intervene in the spray breakup process, density, vapour pressure, latent heat of vaporisation are needed on a temperature range representative of the droplet vaporisation and combustion in order to obtain accurate numerical results for combustion modelling.

Different models have been developed to predict the properties of biodiesel based on their fatty acid composition (Allen et al. 1999a; Allen et al. 1999b; Allen and Watts, 2000). However, their predictions are either for a specific fuel, or for a single point of temperature, limiting the usefulness of the information (Tat and Van Gerpen, 1999; Tat and Van Gerpen, 2000b; Tate et al. 2006b; Tate et al. 2006a) . Allen et al. (Allen et al. 1999b; Allen et al. 1999a) predicted the surface tension and viscosity of 15 different biofuels but at a single point of temperature. Yuan et. al (2005) presented a method aimed at calculating the physical properties of the biodiesels based on their fatty acid composition over a wide range of temperature, so that it can be used in combustion modelling. However, the properties were validated for a temperature of up to 373 K, as no published experimental data for higher temperatures were available. Added to the difficulty in obtaining the biofuels physical properties, biodiesel even from the same

source may have a different structure and consequently different properties (Yuan et al. 2003b). However, spray secondary breakup is not occurring in the experiments carried out for this study, therefore calculation of fuel viscosity and surface tension will not be presented here, since they are not needed in the numerical model.

The fuels which have been considered in this study are ethanol and rix biodiesel. Biodiesel fuels are the fatty acid methyl or ethyl esters (FAME) derived from vegetable or animal fats and oils. In the European Union, FAMES are mostly vegetable oil methyl esters from rapeseed and sunflower oils (Gökalp and Lebas, 2004). Ethanol is produced by alcoholic fermentation of sugar plants (beets, sugar cane) or of cellulose material (straw, wood). Biodiesels and ethanol present the possibility of being directly used in a gas turbine and can also be blended in various proportions with Diesel fuel.

3.1 Biodiesel properties

3.1.1 Fatty acid methyl ester chemical structure

Table 3.1 lists the chemical structure of fatty acid methyl esters. Biodiesels have a different structure from conventional petroleum-based fuels which contain only carbon and hydrogen atoms, whereas vegetable oil, biodiesels and alcohol are oxygenated hydrocarbons.

Number of carbons	Fatty acid methyl ester	Chemical structure
8	Caprylic (carboxylic acid C ₈)	CH ₃ (CH ₂) ₆ COOCH ₃
10	Capric (carboxylic acid C ₁₀)	CH ₃ (CH ₂) ₈ COOCH ₃
12	Lauric (carboxylic acid C ₁₂)	CH ₃ (CH ₂) ₁₀ COOCH ₃
14	Myristic (carboxylic acid C ₁₄)	CH ₃ (CH ₂) ₁₂ COOCH ₃
16	Palmitic (carboxylic acid C ₁₆)	CH ₃ (CH ₂) ₁₄ COOCH ₃
16	Palmitoleic (cis-9-Hexadecanoic acid)	CH ₃ (CH ₂) ₅ CH=CH(CH ₂) ₇ COOCH ₃
17	Heptadecanoic (carboxylic acid C ₁₇)	CH ₃ (CH ₂) ₁₅ COOCH ₃
17	Heptadecenoic (cis-9-Heptadecanoic acid)	CH ₃ (CH ₂) ₆ CH=CH(CH ₂) ₇ COOCH ₃
18	Stearic (carboxylic acid C ₁₈)	CH ₃ (CH ₂) ₁₆ COOCH ₃
18	Oleic (cis-9-Octadecenoic acid)	CH ₃ (CH ₂) ₇ CH=CH(CH ₂) ₇ COOCH ₃
18	Linoleic (cis, cis-9-12-Octadecadienoic acid)	CH ₃ (CH ₂) ₃ (CH ₂ CH=CH) ₂ (CH ₂) ₇
18	Linolenic (cis, cis, cis-9,12,15-Octadecatrienoic acid)	CH ₃ (CH ₂ CH=CH) ₃ (CH ₂) ₇ COOCH ₃
18	Elaidic (trans-9-Octadecenoic acid)	CH ₃ (CH ₂) ₇ CH=CH(CH ₂) ₇ COOCH ₃
18	C18:2 (trans, trans- 9,12-	CH ₃ (CH ₂) ₃ (CH ₂ CH=CH) ₂ (CH ₂) ₇ COOCH ₃

18	Octadecadienoic acid) C18:3 (trans, trans, trans-9,12,15- Octadecadienoic acid)	$\text{CH}_3(\text{CH}_2\text{CH}=\text{CH})_3(\text{CH}_2)_7\text{COOCH}_3$
20	Eicosanoic (carboxylic acid C_{20})	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$
20	Eicosenoic (cis-10-eisenoic acid)	$\text{CH}_3(\text{CH}_2)_8\text{CH}=\text{CH}(\text{CH}_2)_8\text{COOCH}_3$
22	Behenic (carboxylic acid C_{22})	$\text{CH}_3(\text{CH}_2)_{20}\text{COOCH}_3$
22	Eruric (cis-13-docosanoic acid)	$\text{CH}_3(\text{CH}_2)_7\text{CH}=\text{CH}(\text{CH}_2)_{11}\text{COOCH}_3$
24	Lignoceric (carboxylic acid C_{24})	$\text{CH}_3(\text{CH}_2)_{22}\text{COOCH}_3$

Table 3. 1 Chemical structure of fatty acid (Giannelos et al. 2002)

3.1.2 Volatility and boiling points

Volatility is a fuel tendency to vaporize and the vapour pressure curve helps to determine the level of volatility. Rix biodiesel is a mixture of fatty acid methyl esters (FAME) and can be regarded as a near ideal solution (Swern,1979; Goodrum, 2002).Therefore, the total vapour pressure is based on the mixture of the vapour pressure of the different fatty acids composing the biodiesel and can be calculated following Raoult's law:

$$P_{\text{vmix}} = \sum_i P_{\text{vi}} x_i \quad \text{Equation 3. 1}$$

where P_{vi} and P_{vmix} are respectively the fatty acid and the mixture vapour pressure.

The Rix biodiesel FAME mass fraction is given in table 3.2.

Fatty acid methyl ester	FAME mass fraction
Palmitic 16:0	13.73
Stearic 18:0	5.33
Oleic 18:1	50.96
Linoleic 18:2	19.93
Linolenic 18:3	4.2
Eruric 22:1	5.85

Table 3.2 Rix biodiesel fatty acid composition

The vapour pressure of all the FAME present in rix biodiesel are commonly calculated based on the Antoine equation.

$$P_{\text{vi}} = A_{\text{Ant}} - \frac{B_{\text{Ant}}}{T + C_{\text{Ant}}} \quad \text{Equation 3. 2}$$

	A	B	C
C16:0	9.5714	2229.94	-111.01
C18:0	9.3746	2174.39	-131.23
C18:1	9.9155	2583.52	-96.15
C18:2	8.2175	1450.62	-188.03
C18:3	8.1397	1387.93	-196.16
C20:0	10.3112	2987.15	-84.56
C20:1	10.3525	3009.62	-81.66
C22:0	10.6867	3380.86	-73.20
C22:1	10.7518	3423.99	-69.43
C24:0	11.0539	3776.89	-62.90

Table 3. 3 Antoine equation constants of pure FAMES (Yuan et al. 2005)

Based on the Antoine constants and equation 3.2, the vapour pressure for biodiesel can be plotted figure 3.1:

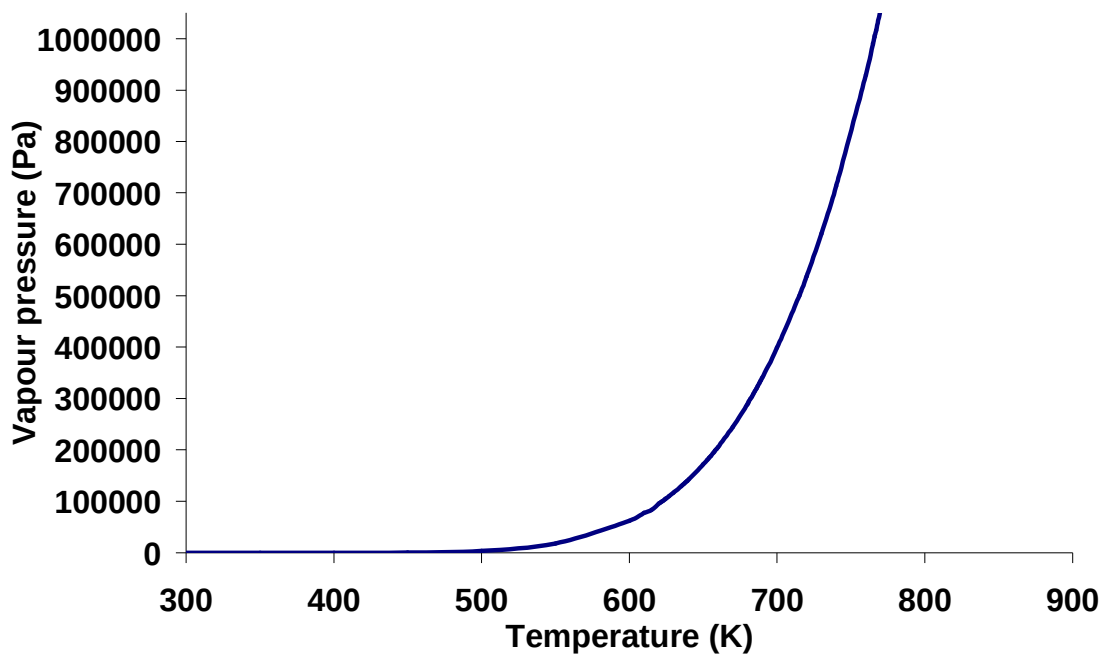


Figure 3. 1 Rix biodiesel vapour pressure

The normal boiling point of biodiesel is determined by the location where the curves reached 1 atm and it can be found that it is 623 K. Its high boiling point is an indication of its low volatility.

Pressure	1 atm	2 atm	3 atm	5 atm	10 atm
Boiling point (K)	623	659	683	715	767

Table 3. 4 Rix biodiesel boiling point at different pressures

3.1.3 Critical properties

The critical properties are used to estimate the properties such as liquid density, viscosity, surface tension, heat capacity, diffusion coefficient, heat of vaporization and thermal conductivity. The critical properties are also used to estimate the fuel boiling point and establish a correlation for vapour pressure. Hence it is particularly important to accurately predict the fuel critical properties, as they will influence the prediction of the other fuel properties.

The Lydersen's method recommended by Reid (1977) was a group contribution method, which employs structural contribution to estimate the critical pressure P_c , the critical temperature T_c and the critical volume V_c of the different groups, which are described as follows:

$$T_c = \frac{T_b}{0.567} + \sum \Delta_T - \left(\sum \Delta_T \right)^2 \quad \text{Equation 3. 3}$$

$$P_c = \frac{MW}{\left(0.34 + \sum \Delta_p \right)^2} \quad \text{Equation 3. 4}$$

$$V_c = 40 + \sum \Delta_v \quad \text{Equation 3. 5}$$

Δ_T , Δ_v and Δ_p are the contribution constants used for various atoms or groups of atoms.

The critical properties of the different fatty acids have been incorporated in the mixing rules using the Lee-Kesler equation (Reid et al.,1977):

$$T_{cij} = \left(T_{ci} T_{cj} \right)^{1/2} \quad \text{Equation 3. 6}$$

$$T_{cm} = \frac{1}{V_{cm}^{1/4}} \sum_i \sum_j x_i x_j V_{cij}^{1/4} T_{cij} \quad \text{Equation 3. 7}$$

$$V_{cij} = \frac{1}{8} \left(V_{ci}^{1/3} + V_{cj}^{1/3} \right)^3 \quad \text{Equation 3. 8}$$

$$V_{cm} = \sum_i \sum_j x_i x_j V_{cij} \quad \text{Equation 3. 9}$$

$$\omega_m = \sum_i x_i \omega_i \quad \text{Equation 3. 10}$$

$$P_{cm} = \frac{(0.2905 - 0.085\omega_m)RT_{cm}}{V_{cm}} \quad \text{Equation 3. 11}$$

Where m refers to the mixture, i and j refer to the pure constituents and x to the mole fraction of the pure constituent i or j. The pure component acentric factor (ω_i) was computed as follows:

$$\omega_i = \frac{\alpha}{\beta} \quad \text{Equation 3. 12}$$

Where

$$\alpha = -\ln P_{ci} - 5.97214 + 6.09648\theta^{-1} + 1.28862 \ln \theta - 0.169347\theta^6 \quad \text{Equation 3. 13}$$

$$\beta = 15.2518 - 15.6875\theta^{-1} - 13.4721 \ln \theta + 0.43577\theta^6 \quad \text{Equation 3. 14}$$

With

$$\theta = \frac{T_{br}}{T_{ci}} \quad \text{Equation 3. 15}$$

with T_{bi} : normal boiling point of the pure constituent i (K) and
 T_{br} : reduced temperature at normal boiling point

The normal boiling point of some fatty acid methyl esters which compose the biodiesel have been published by several authors (Graboski and McCormick, 1998; Weast and Melvin, 1982; Swern, 1979).

Fatty acid methyl esters	T_{nb} (K)
C16:0	623
C18:0	625
C18:1	622
C18:2	639
C18:3	642
C22:1	654

Table 3. 5 Normal boiling points for common pure methyl esters

The critical properties can then be calculated for the fatty acids composing the mix biodiesel and consequently for the biodiesel and are displayed table 3.5.

Property	C16:0	C18:0	C18:1	C18:2	C18:3	C22:1	Rix biodiesel
Critical temperature (K)	779	773	770	792	796	802	788
Critical pressure (bar)	13.70	12.45	12.66	12.86	13.11	10.67	12.15
Critical volume (mL/mole)	1000	1110	1090	1070	1050	1310	1068

Table 3. 6 Estimated critical properties for the FAME and rix biodiesel

3.1.4 Density

Various methods for estimating densities have been described by Kurtz and Sankin (1954), Li et al. (1956), Reid et al. (1977). Spencer and Danner (1972) have conducted an extensive evaluation of the available methods for predicting the saturated liquid density of pure hydrocarbons as a function of temperature. They concluded that the most accurate mean of predicting the effect of temperature on the saturated liquid densities is by the modified Racket equation. The Rackett's equation (Rackett, 1970) has been slightly modified by Spencer and Danner (Spencer and Danner, 1972) (Reid et al., 1977) to predict the saturated liquid density as a function of temperature:

$$Vol = \left(\frac{RT_c}{P_c} \right) Z_{RA}^{\phi} \quad \text{Equation 3. 16}$$

hence

$$Vol = Vol_R Z_{RA}^{\phi} \quad \text{Equation 3. 17}$$

Vol_R is an experimental liquid molar volume at a reference reduced temperature T_R where

$$\phi = (1 - T_r)^{2/7} - (1 - T_r^R)^{2/7} \quad \text{Equation 3. 18}$$

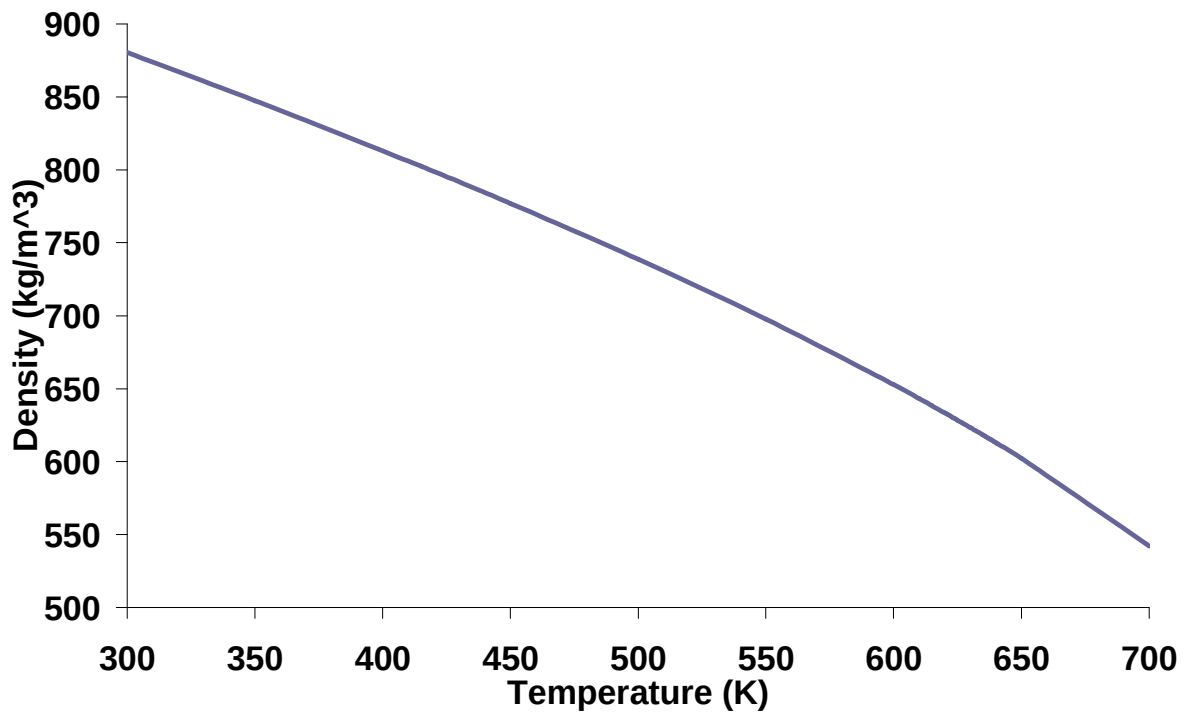
Yuan (2003a) employed the experimental data obtained by Tat and Van Gerpen (2000a) using densities measured at 0 °C and 100 °C to determine a constant Z_{RA} used to calculate biodiesel density. The Rackett parameter, Z_{RA} , is a unique correlating parameter for each compound. The following relationship is derived from equation 3.16:

$$\rho = \frac{\rho_R}{Z_{RA}^\phi}$$

Equation 3. 19

By selecting $T_R=0$ °C, Tat and Van Gerpen (2000a) obtained an experimental value of 0.8976 kg/L and equation 3.33 becomes:

$$\rho = 0.8976 * 0.237^{-\phi}$$

Equation 3. 20**Figure 3. 2** Predicted density of rix biodiesel vs. temperature (Yuan et al. 2003a)

The predicted density of rix biodiesel is shown figure 3.2. The rix biodiesel liquid density seems to be decreasing at a linear rate up to the boiling point and from then, decreases at a slightly higher rate, which could be attributed to an increasing liquid expansion rate.

Temperature (K)	300	350	400	450	500	550	600	650	700	750
Rix biodiesel density (kg/m ³)	880	847	813	777	738	697	652	602	542	460

Table 3. 7 Predicted density of rix biodiesel vs. temperature (Halvorsen et al. 1993)

Biodiesel density is moderately higher than conventional fuels at 300 K (880 kg/m³ versus 790 kg/m³ for kerosene). An increase in fuel density will have a slight direct effect on spray compactness and penetration, resulting in less air resistance, since for the same volume, the fuel mass flow will be increased. At the pressures investigated in this study, the variation of density as a function of pressure is negligible.

3.1.5 Enthalpy of vaporisation

The enthalpy of vaporization also called the latent heat of vaporization, is the difference between the enthalpy of the saturated vapour and the enthalpy of the saturated liquid at the same temperature. The higher the enthalpy of vaporization, the more energy is required to obtain fuel vaporization.

The Pitzer acentric factor correlation (Reid et al.,1977; Pitzer et al. 1955) was used to determine the latent heat of vaporization h_{fg} up to the biodiesel critical temperature. An analytical representation of this correlation for $0.6 < T_r \leq 1.0$ is given below:

$$\frac{h_{fg}}{RT_c} = 7.08(1 - T_r)^{0.354} + 10.95\omega(1 - T_r)^{0.456} \quad \text{Equation 3. 21}$$

The enthalpy of vaporization will be determined at the fuel boiling point. To determine the latent heat of evaporation at low temperatures ($T_r < 0.6$) the following relationships suggested by Fish and Lielmezs (1975) were used:

$$h_{fg} = h_{fgb} \frac{T_r}{T_{br}} \frac{\chi + \chi^q}{1 + \chi^p} \quad \text{Equation 3. 22}$$

where

$$\chi = \frac{T_b}{T_r} \frac{1 - T_r}{1 - T_{br}} \quad \text{Equation 3. 23}$$

With $q = 0.3598$ and $p = 0.13856$ for organic liquids (Reid et al.,1977)

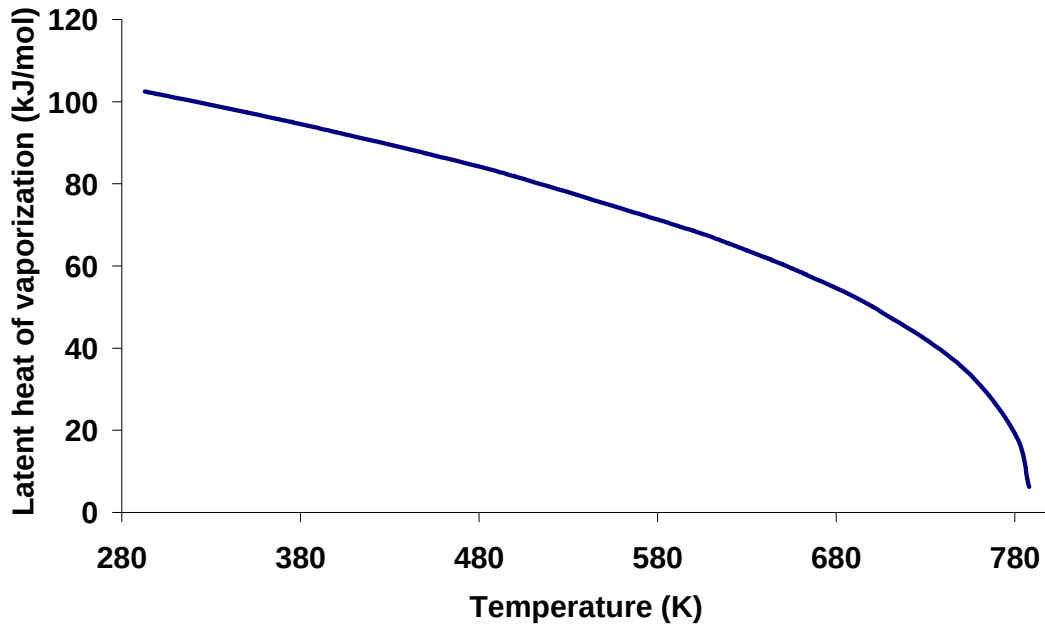


Figure 3. 3 Latent heat of vaporization of rix biodiesel versus temperature based on the Pitzer and Fish and Lielmezs method (Pitzer et al. 1955; Fish and Lielmezs, 1975)

The latent heat of vaporization of the Rix biodiesel is much lower than fossil fuels and ethanol, which means that much less energy is needed to vaporize Rix biodiesel than ethanol.

3.1.6 Specific heat capacity

Liquid heat capacities are not strong function of temperature except above $T_r = 0.7$ to 0.8 (Reid et al., 1977). At high reduced temperatures, liquid heat capacities are large and strong functions of temperature.

In order to calculate the liquid heat capacity at 293.15 K, the relatively simple atomic group contribution approach of Chueh and Swanson (1973) for liquid heat capacity at 293.15 K has been used.

$$C_p^0 = \sum_{i=1}^n N_i \Delta C_{p_i} + 18.83m$$

Equation 3. 24

with N_i the number of different atomic groups in the compound, ΔC_{p_i} the numeric value of the contribution of element i described in table 3.7. m represents the number of carbon groups requiring an additional contribution, which are those that are joined by a

single bond to a carbon group, which in turn is connected to a third carbon group by a double or triple bond. If a carbon group meets this criterion in more than one way, m should be increased by one for each of the ways. Exceptions: $-\text{CH}_3$ groups or carbon groups in a ring never require an additional contribution; and the first addition contribution for a $-\text{CH}_2-$ group meets the criterion in a second way, the second additional contribution reverts to the 18.83 J/mol.K value.

	ΔC_p (J/mol.K)
Non ring increments	
$-\text{CH}_3$	36.82
$-\text{CH}_2$	30.38
Oxygen increments	
$-\text{COO}-$	60.67
$-\text{COOH}$	79.91

Table 3. 8 Atomic group contribution to estimate liquid heat capacity at 293.15 K

For oleic acid methyl ester, the $-\text{CH}_2-$ group is once joined by a single bond to a carbon group, which in turn is connected to a third carbon group by a double bond, therefore $m = 1$. Following the same approach, for linoleic acid methyl ester and eruric acid methyl ester, $m = 2$ and $m = 3$ for linolenic acid methyl ester.

Bondi (1966) has reviewed many forms and modified one suggested by Rowlinson (1969) to give the specific heat as a function of temperature:

$$\frac{C_{pl} - C_p^0}{R} = 2.56 + 0.436(1 - T_r)^{-1} + \omega \left[2.91 + 4.28(1 - T_r)^{1/3} T_r^{-1} + 0.296(1 - T_r)^{-1} \right]$$

Equation 3. 25

For liquid mixtures as is Rix biodiesel, the values of the FAME can be mole-fraction averaged. This procedure neglects any heat of mixing effect. Therefore:

$$C_{p_{\text{Rixbiodiesel}}} = \sum X_i C_{pl}$$

Equation 3. 26

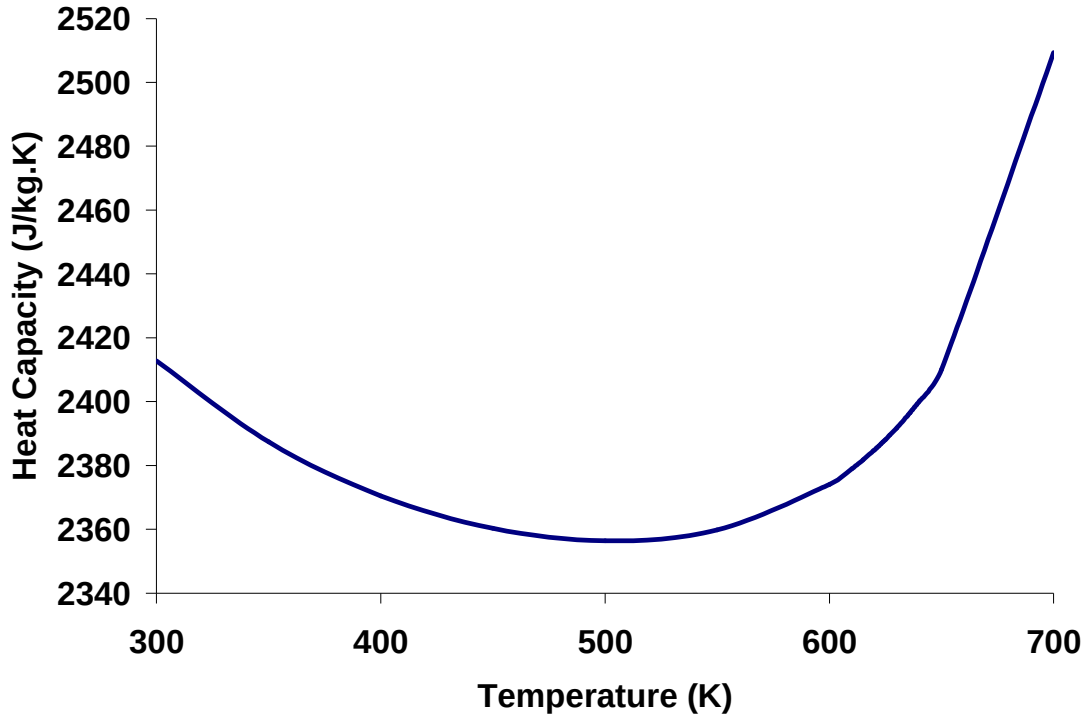


Figure 3. 4 Specific heat capacity for rix biodiesel

X_i represents the mole fraction of the different species which make part of the fuel and is calculated according to equation 3.26 based on the FAME mass fraction defined in table 3.2:

$$X_i = \frac{\frac{Y_i}{MW_i}}{\sum_i \frac{Y_i}{MW_i}} \quad \text{Equation 3. 27}$$

3.1.7 Thermal conductivity

For liquids at reduced temperature between 0.25 and 0.8 at a pressure below 3.4 MPa, an equation based on the methods of Pachaiyappan et al. (1966) may be used to determine the thermal conductivity:

$$k_l = C\rho_{mol}MW^n \left[\frac{3 + 20(1 - T_r)^{2/3}}{3 + 20\left(1 - \frac{293.15}{T_c}\right)^{2/3}} \right] \quad \text{Equation 3. 28}$$

With $C = 1.811 \times 10^{-4}$ and $n = 1.001$

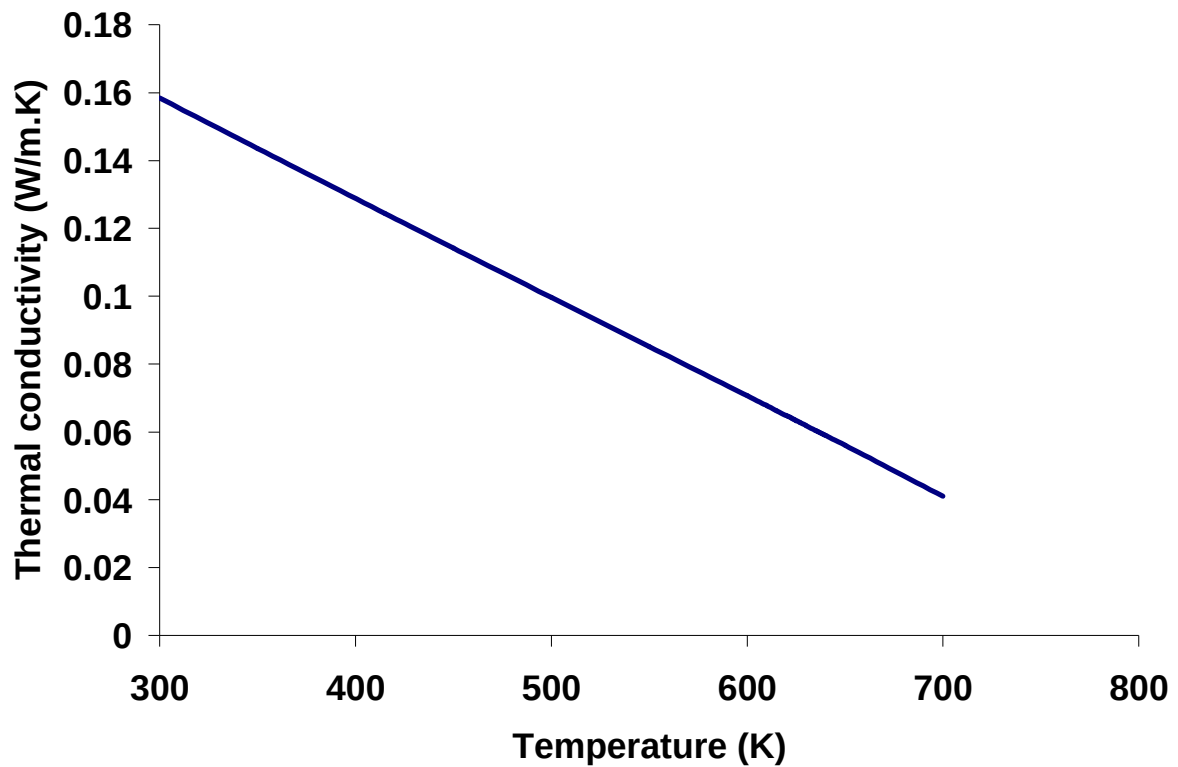


Figure 3. 5 Rix biodiesel thermal conductivity as a function of temperature

3.1.8 Binary diffusivity

For the prediction of the gas diffusivity of binary air-rix biodiesel, the method of Fuller et al. (1966) is recommended:

$$\delta_{12} = \frac{0.01013T^{1.75} \left(\frac{1}{MW_{air}} + \frac{1}{MW_{biodiesel}} \right)^{0.5}}{P \left[(Vol_{air})^{1/3} + (Vol_{biodiesel})^{1/3} \right]^2}$$

Equation 3. 29

Atomic and structural diffusion-volume increments		Number of atoms
C	16.5	19
H	1.98	32
O	5.481	2

Table 3. 9 Atomic diffusion volumes

Based on table 3.8, $Vol_{biodiesel} = 387.822$, while $Vol_{air} = 20.1$

Therefore at 1 atm and 415 K, $\delta = 7.42 \times 10^{-6} \text{ m}^2/\text{s}$

The binary diffusivity is displayed as a function of temperature figure 3.5.

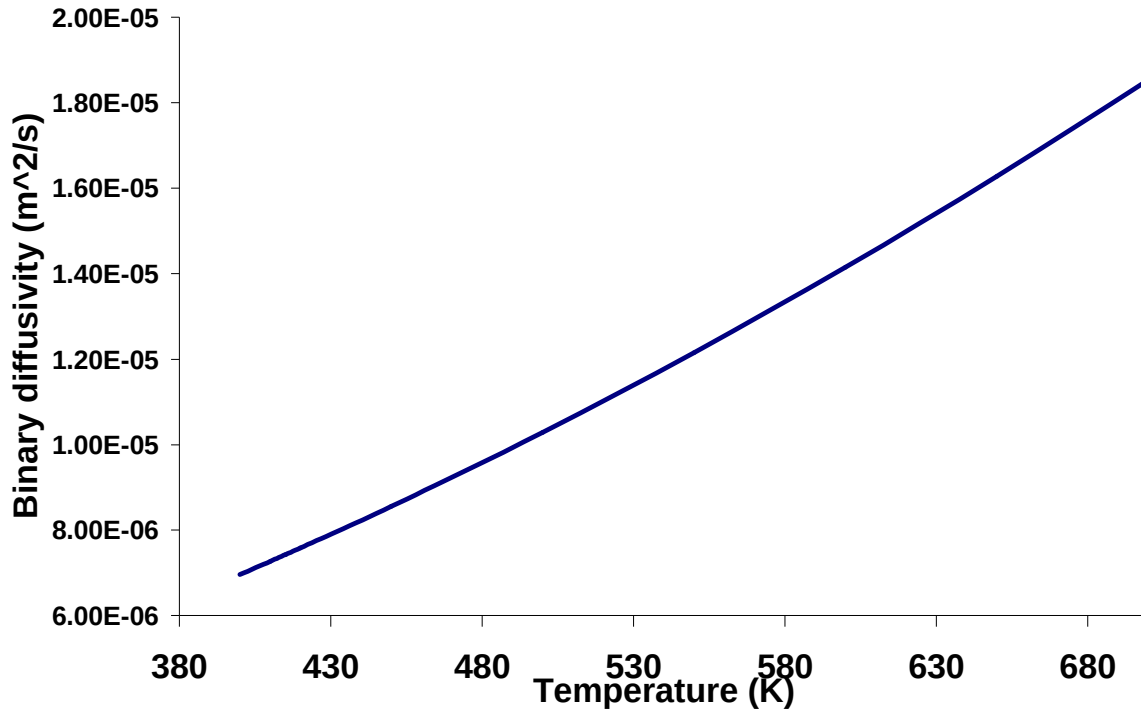


Figure 3. 6 Rix biodiesel binary diffusivity as a function of temperature

3.2 Ethanol properties

Ethanol properties already exist in the FLUENT database. Therefore, the fuel properties which are set to be constant in the simulation will be reported table 3.9, such as fuel thermal conductivity, latent heat of vaporization and density all defined at 298 K Then vapour pressure, specific heat capacity, and binary diffusivity will be plotted as a function of temperature.

	Chemical composition	Critical temperature T_c (K)	Critical pressure P_c (bar)	Critical volume V_c (mL/mole)	Thermal conductivity (W/m.K)	Latent heat of vaporization (J/kg)	Density (kg/m ³)
Ethanol	C ₂ H ₅ OH	514	63	168	0.182	855237	790

Table 3. 10 Ethanol properties set to be constant in FLUENT at 298 K

3.2.1 Vapour pressure

As for biodiesel, the vapour pressure for ethanol is calculated based on the Antoine equation.

$$P_{vi} = A_{eth} - \frac{B_{eth}}{T + C_{eth}} \quad \text{Equation 3. 30}$$

Temperature (K)	A _{eth}	B _{eth}	C _{eth}
364.8 - 513.91	4.92531	1432.526	-61.819
292.77 - 366.63	5.24677	1598.673	-46.424

Table 3. 11 Antoine constant for ethanol

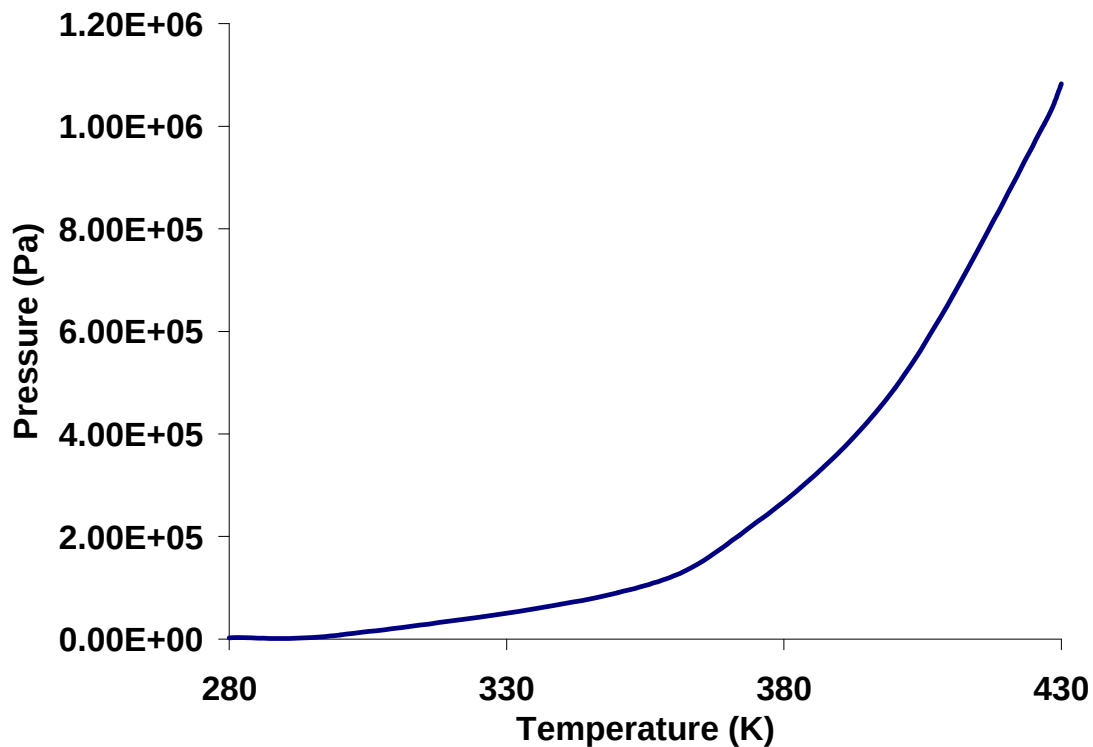


Figure 3. 7 Vapour pressure for ethanol

Pressure	1 atm	2 atm	3 atm	5 atm	10 atm
Boiling point (K)	351	371	384	399	427

Table 3. 12 Ethanol boiling point at different pressures

3.2.2 Specific heat capacity

Fluent used a piecewise polynomial function to describe the specific heat capacity as a function of temperature:

$$C_p(T) = A_1 + A_2 T + A_3 * T^2 + A_4 * T^4 \quad \text{Equation 3. 31}$$

With $A_1 = 2235.728$, $A_2 = -3.038854$, $A_3 = -0.00066$ and $A_4 = 4.42804e-5$

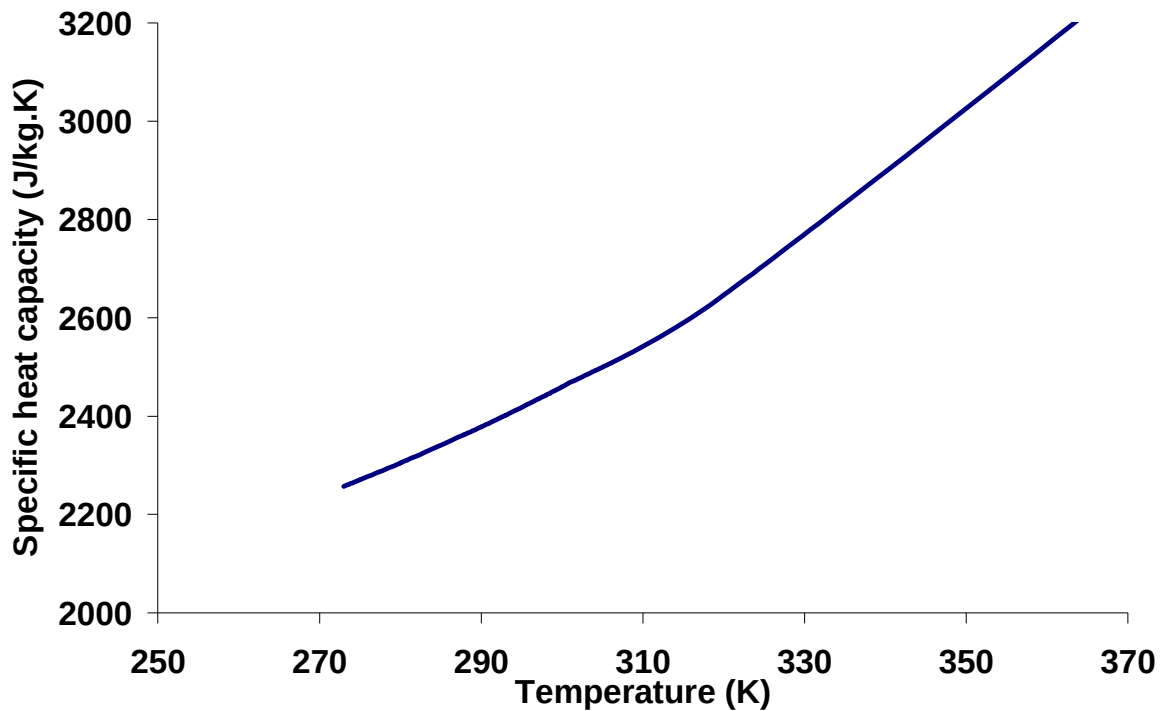


Figure 3. 8 Ethanol specific heat capacity (J/kg.K)

3.2.3 Binary Diffusivity

The theory describing diffusion in binary gas mixtures at low to moderate pressures encountered in this study has been well developed. The diffusion coefficient for binary ethanol air mixture is solved with the following equation presented in Reid (1977):

$$\delta_{AB} = 1.858 \times 10^{-3} T^{\frac{3}{2}} \frac{[(MW_{ethanol} + M_{air})/MW_{ethanol} M_{air}]^{\frac{1}{2}}}{P \sigma_{\delta_{ethanol-air}}^2 \Omega_D} \quad \text{Equation 3. 32}$$

$$\epsilon_{C_2H_5OH} / k = 362.6 \quad \text{Equation 3. 33}$$

$$\epsilon_{air} / k = 78.6 \quad \text{Equation 3. 34}$$

Therefore

$$\varepsilon_{C_2H_5OH} / k = (362.6 * 78.6)^{0.5} = 168 \text{ K}$$

$$\sigma_{ethanol} = 4.53 \text{ \AA} \text{ and } \sigma_{air} = 3.711 \text{ \AA}$$

$$\text{which results in } \sigma_{ethanol-air} = \frac{4.53 + 3.711}{2} = 4.1205 \text{ \AA}$$

Ω_D is tabulated as a function of kT/ε and described in Reid (1977) in the following manner:

$$\Omega_D = \frac{A_\delta}{T^{*B}} + \frac{C_\delta}{\exp D_\delta T^*} + \frac{E_\delta}{\exp F T^*} + \frac{G_\delta}{\exp H T^*} \quad \text{Equation 3. 35}$$

$$\text{where } T^* = kT / \varepsilon_{ethanol-air} \text{ with } A_\delta = 1.06036 \quad A_\delta = 1.06036 \quad B_\delta = 0.15610$$

$$C_\delta = 0.19300 \quad D_\delta = 0.47635 \quad E_\delta = 1.03587$$

$$F_\delta = 1.52996 \quad G_\delta = 1.76474 \quad H_\delta = 3.89411$$

Based on equation 3.29 and 3.32, the following curve is obtained:

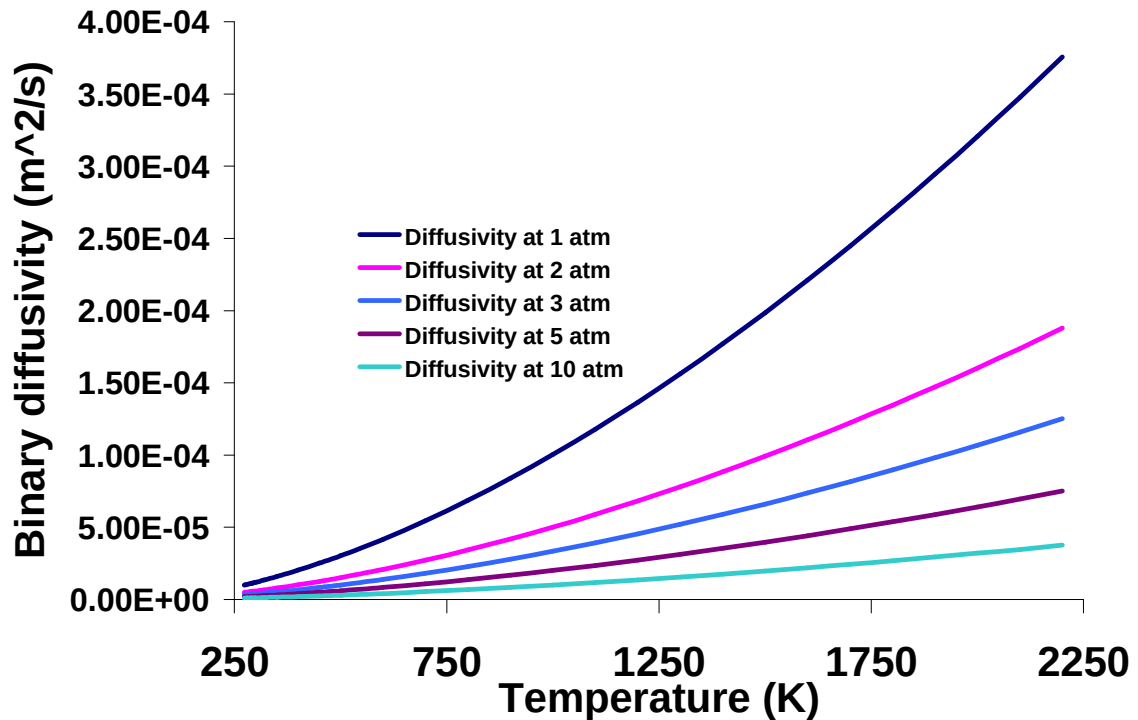


Figure 3. 9 Ethanol air binary diffusivity at different pressures

Figure 3.9 clearly shows that higher pressure can notably have a strong effect on the diffusion coefficient.

3.3 Influence of fuel properties on droplet diameter

The various physical phenomena involved in pressure swirl atomization are highly complex, and many empirical correlations have been developed to formulate mean droplet size as a function of fuel properties. Among these correlations, the following one has the advantage of being dimensionally correct (Lefebvre,1989):

$$SMD = 2.25 \sigma^{0.25} \mu_l^{0.25} m_l^{0.25} \Delta P_l^{-0.5} \rho_A^{-0.5} \quad \text{Equation 3. 36}$$

From equation 3.36, the droplet SMD highly depends on the viscosity and surface tension of the liquid fuel. These informations have been included in Appendix A for rapeseed oil. The fuel and air properties vary with temperature, therefore the Sauter mean diameter has been plotted against temperature. However, the correlation presented by Lefebvre (1989) does not describe any range of validity for temperature, therefore the temperature was limited to a variation of between 273 and 333 K (0 °C and 60 °C). The fuel and air temperature was assumed to be the same. The SMD plotted figure 3.10 against temperature was calculated based on the operating conditions described table 4.1 under 1 atmosphere for ethanol and biodiesel. It is commonly considered that the high viscosity of the injected liquid causes an increase of the Sauter mean diameter as showed figure 3.10.

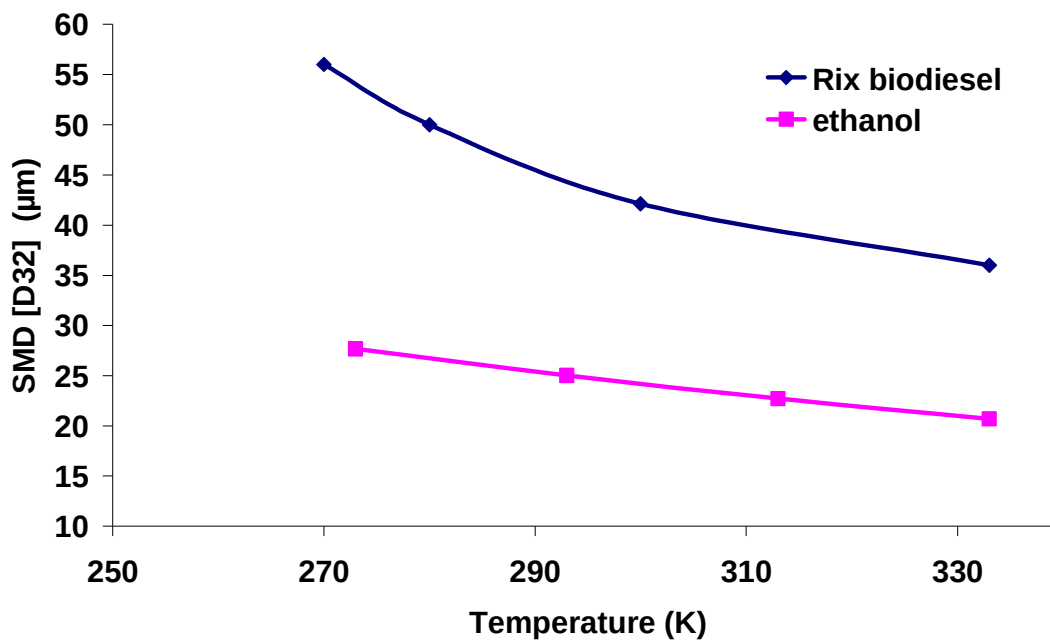


Figure 3.10 Sauter mean diameter as a function of fuel properties

Indeed, the viscosity has a direct effect upon the final atomisation process by which the drops are formed, and this final process directly affects the Sauter mean diameter. An increase in fuel viscosity will also increase spray penetration, since with more viscous and heavier fuels the jet will not be so well atomised, at a given injection pressure, and the spray will be more compact, resulting in less air resistance. With the high viscosity of vegetable oils and biodiesels compared to ethanol, the droplets tend to be bigger therefore generating atomisation problems as seen figure 3.10.

Consequently, an increase in the viscosity of the liquid has an adverse effect on the fineness of atomisation, hence any change by which the viscosity is decreased will improve the atomisation of the spray. Such an effect can be achieved, for instance, by an increase in the temperature of the liquid, operation which has been carried out in the present study for the Rix biodiesel and rapeseed oil experiments.

3.4 Concluding remarks

The fluid properties such as density, thermal conductivity, specific heat, latent heat of vaporization, vapour pressure and boiling point, have been determined over a wide range of temperatures. Viscosity and surface tension were not described since no secondary breakup occurs in the study and therefore these characteristics are not needed for the model. Rix biodiesel possess a high boiling point compared to ethanol and this study has showed that the fuel chemical structure and critical properties significantly influences the fuel properties. This section has shown that the fuels differ significantly in their physical and chemical characteristics significantly modifying the evaporation and combustion process and therefore the properties need to be accurately determined.

CHAPTER 4 – EXPERIMENTAL STUDY

4.1 Introduction

The experimental work has been carried out by Jasuja, Klaesson, Pierce and Moss. Although this work has not been carried out by the author of this study, it constitutes a vital part to validate the numerical results obtained with the CFD. This section presents data which are used to develop a qualitative and quantitative description of the structure of a spray flame. The flame has been scaled down to laboratory size and measurements have been taken which are then made available as an input for computer modelling. The objective of this section is to obtain a detailed understanding of the structure of the spray and its physics as well as being able to assess how the spray interacts with the air exiting from the swirler and how it affects the combustion process.

Indeed, it is of interest that the spray flames undergo more detailed scrutiny since there are few reports in which the accuracy of calculated results is examined by comparing to measured data for spray flames, despite the common use of spray combustion in industrial applications. The main reason for this is that the measurements of the detailed distribution of velocity, temperature and gas composition are very difficult in practical combustors, especially in dense spray regions, due to the hostile conditions and the limited optical access for carrying out the measurements.

However, experimental data are required to get a better understanding of the different physical processes involved, such as evaporation, mixing, and momentum exchange. The data will also provide information for the numerical model, especially in terms of model development and validation and information needed on the boundary conditions as well as droplet initial conditions, which are used as an input in the CFD model. The obtained data set will then be applied to simulate the behaviour of the pressure rig in different operating conditions.

Pressure swirl atomizers spray flames are shown in this section to have a complex structure. The swirling motion introduced in order to maintain the flame stability, control the flame length and increase the fuel residence time, as well as the multiphase

nature of the phenomena, added to spray evaporation, creates such a complicated situation, that even nowadays researchers struggle to fully understand all the physical implications related to these applications.

Measurements have been made at atmospheric pressures and progressively raised to 3 bar. The pressure inside the rig is regulated through an external translating plug / orifice arrangement at the top of the rig.

Previous experimental studies of turbulent ethanol and biodiesel spray flames have been briefly reviewed and the different experimental have been described. The measurement techniques chosen have been discussed and uncertainty analyses are described in section 4.3 and 4.4. Finally the experimental results are commented in the latter part of this chapter.

4.2 Experimental studies of turbulent ethanol and biodiesel spray flames

Numerous experiments have been carried out to determine swirling spray flames properties such as SMD, droplet number density and volume flux, droplet axial velocity, using Phase/Doppler technique (PDPA) and Laser Doppler Velocimeter (LDV) to measure the axial gas velocities (Mao et al., 1988; Presser et al., 1988; Edwards and Rudoff, 1991; Ghaffarpour and Chehroudi, 1993; Presser et al., 1993; McDonnell and Samuelsen, 1992). The different studies on spray measurements have been very helpful in getting some understanding of the spray structure and droplet behaviour in a spray and were also instrumental in the development of numerical models.

Most of the studies on burning sprays have been carried out using kerosene or heptane as a fuel (Mao et al. 1988; Presser et al. 1988; Edwards and Rudoff, 1991; Ghaffarpour and Chehroudi, 1993; Presser et al. 1993; McDonnell and Samuelsen, 1992), but the purpose of this study is to use ethanol and biodiesel as fuels. Quite a few studies have been reported on the characterisation of methanol or ethanol spray flames.

McDonnell and Samuelsen (1992) conducted measurements of methanol spray vaporization behaviour operating at three different conditions such as in absence of atomizing air, non swirling atomizing air and swirling atomizing air and they observed that the vaporization rate was respectively increasing according to the air flow configuration injection mode.

Wang et al. (1992) conducted experiments to determine the spray characteristics of methanol and ethanol with high-pressure swirl injector both experimental and numerically. They observed that spray patterns of methanol and ethanol are similar except that the spray penetration of methanol was a little shorter, the cone angle was a little larger, and the atomization process a little faster, since the vapour pressure of methanol is about twice that of ethanol, implying that methanol is more volatile than ethanol however the overall SMD curves of methanol and ethanol are very close to each other.

Bossard and Peck (1996), in a very interesting investigation, carried out experiments with ethanol sprays generated by air blast atomizers and showed that more complete combustion occurs in sprays possessing narrower droplet size distribution. Reduction in the burning efficiency for wide drop size distribution is attributed to their greater population of large droplets.

Various researchers (Friedman and Renksizbulut, 1999; Widmann et al., 2000; Giridharan et al., 2001; Widmann and Presser, 2002a) described a benchmark spray combustion database for the purpose of validating multiphase combustion models and submodels, using methanol where a validation of the numerical simulations with comparison of the droplet size, velocity, number density and volume flux against experimental data is presented, using phase Doppler Interferometry (PDI), temperature with the help of thermocouple and gas velocity through Particle Image Velocimetry (PIV).

A large number of experiments were carried out with vegetable oils as a replacement of conventional fuels by researchers from various parts of the world. It was often reported that the fuel depended on the location of the investigation. Most of the studies using vegetable oils were mainly investigating on NO_x, CO, HC and particulate emissions,

engine performance as compared to diesel engines using rapeseed oil (Montague, 1996; Hemmerlein et al., 1991; Murayama, 1984), rapeseed oil methyl ester (Hohl, 1995; Desantes et al., 1999; Senatore, 2000; Salvatore et al. 1993), sunflower oil (Barsic and Humke, 1981; Radu and Mircea, 1997; Abbass et al. 1990), coconut oil (Masjuki et al. 2001), coconut oil methyl ester (Shaheed and Swain, 1998), peanut oil (Barsic and Humke, 1981), palm oil (Barsic and Humke, 1981; Silvico et al. 2002), karanja oil (Ramadhas et al. 2004), waste oil (Yoshimoto et al. ; Yu et al. 2002) and biodiesel (Yoshimoto et al. 1999; Choi et al. 1997; Babu and Devaradjane, 2003; Sharp et al. 2000; Tat and Van Gerpen, 2003). Graboski et al. (1998) presented a detailed review of biodiesel properties, emissions and performance but although this literature review is not exhaustive, no detailed mapping of spray flame using vegetable oil or biodiesels, such as gas temperature, droplet size and velocity has been reported. Strykowski (2004) examined the viability of using biomass-derived oil in gas turbines, such as biodiesel and soybean oil. The fuel atomization, depending on the fuel properties such as viscosity, density and surface tension, was investigated and a preliminary study was conducted to evaluate whether the partially atomized oil could be burned. However, as mentioned, this investigation was only at its preliminary stages.

4.3 Experimental techniques

A brief review of the recent measurements techniques is presented in this section. Several key variables were identified which would be necessary to compare experimental data with the numerical predictions and obtain a detailed mapping of the flame structure:

- flame temperature which will determine the energy released by the flame
- droplet diameter, velocity and size distribution, which will help to determine the initial conditions of the spray
- and gas velocity which will provide insight into the aerodynamics of the gas related to the spray

Literature on temperature measurement techniques is quite broad such as Gilbert and Lobdell (1953) for the resistance thermometer and for thermocouples. Seebeck (1821) first demonstrated that two different metals forming a close circle, in the absence of moisture, showed magnetic properties when subjected to a difference of temperature at

the point of contact. He made sure that the magnetic properties varied for different metals and were greater for greater differences of temperature. Becquerel (1827) subsequently used Seebeck's discovery as a means of measuring high temperature and deduced that the intensity of current developed was proportional to the rise in temperature using thermocouples. However, laser based diagnostic techniques for the temperature measurements have become increasingly popular. Those which are, in principle, capable of the measurement of temperature and have received most attention are Raman scattering, Coherent Anti-Stokes Raman Spectroscopy (CARS), laser induced fluorescence Spectroscopy (LIFS) and degenerate four wave mixing (DWFM). These are reviewed by Ecbreth et al (1979), Greenhalgh (1983) and Dibble et al. (1987).

PIV is another popular technique which has been particularly used to determine the velocity field of swirling flows, the aerodynamic strain rate or to report the velocity field in luminous flames. PIV is a non intrusive technique which does not disturb the aerodynamics of the flow and the flame structure. The gas phase velocity can be deduced by measuring the seed particles displacement between two images taken at a known time interval. Seeding techniques is an extremely useful tool, showing flow streamlines and vastly improving experimental knowledge of flame structures.

For a more complete understanding of this technique, the reader can refer to Grant (1994), a book on PIV written by Raffel et al. (1998) and to a bibliography of PIV by Adrian (1996). Articles on PIV (Kompenhans and Tropea, 1997; Adrian, 2000, 2002, 2005) contain very useful collection of recent work. Although the feasibility of applying the PIV method was demonstrated by 1977 (Fourney, 1977; Dudderar and Simpkins, 1977; Grousson and Mallick, 1977), Meynart (1979, 1980, 1982a, 1982b, 1983a, 1983b, 1983c) was the leading pioneer of this method, which he defined at the time as laser speckle velocimetry (LSV) showing practical measurements could be made in laminar and turbulent flows of liquids and gases and Adrian (1984) proposed the term PIV to distinguish this mode of operation from the laser speckle mode.

The Phase Doppler Particle Analyzer (PDPA) is one of the most popular techniques for spray characterisation in combustng sprays. Mao et al. (1988), McDonnell et al. (1988), Edwards and Rudoff (1991), McDonnell et al. (1992), McDonell and

Samuelson (1996) provided very detailed information on the different spray characteristics, by being capable of directly measuring simultaneously the droplet size and velocity as well as calculating the particle number density and volume flux throughout the spray. All these gathered data help in deducing the spray trajectory, cone angle and droplet size distribution from the measurements carried out by the PDPA. The technique is thoroughly described by Bachalo (1980, 1984) while extensive testing of the method is carried out in Bachalo (1985). Bachalo provided such significant advancement to this method that it appeared a viable mean for spray diagnostics.

4.4 Measurement uncertainty

The measurements uncertainties in this study arise mainly from the thermocouple as well as PIV measurements and concerning the PDPA data, improper data filtering or derived data can significantly affect the accuracy of droplet size, velocity and volume flux.

4.4.1 Thermocouples

Thermocouples have been proven to be particularly reliable and hence it is believed that systematic errors resulting from voltage transformation to temperature data are negligible. The main sources of error may come for radiative loss and soot deposition. Indeed this would have the effect of isolating the probe from the surrounding environment, increasing the radiative heat loss from the flame (due to increased size and emissivity) and increase probe blockage effects (Young, 1993). Due to the small size of the thermocouple, aerodynamic disturbance resulting to its intrusion in the flame are believed to have no effect on the accuracy of the flame temperature measurements.

4.4.2 Spray characterisation

The accuracy of droplet size techniques has been assessed over the last 20 years in relation to the different source of errors encountered in spray measurements. Problems related to measurements techniques which are not adapted for droplets whose size is less than 10 μm because of the limitation of dynamic range of the instrument, have been mentioned and are well reported in the literature (Leport et al. 1999). Also, Hardalupas et al. (1994) found that the main source of error was the droplet rejection rate by around 25 %, due to the presence of several droplets in the probe sample area in

dense sprays, which resulted in systematic underestimation of the number density and volume flux for the reacting flow. Widmann and Presser (2002b) mentioned that the uncertainty in size and velocity distribution are generally higher than the uncertainty in measurements of individual droplets for numerous reasons, such as missed droplets, and errors in the quantification of the probe area as a function of droplet size. Leport et al. (1999) also mentioned that additional issues appear in combustor sprays, such as the presence of the flame altering the optical path of the laser beams and scattered light.

The main problems are expected to occur with the number density and volume flux measurements. In fact, droplet size and velocity are directly measured by the instruments whereas the other parameters are calculated by the equipment because they depend on more than one feature, such as volume probe area, itself dependent on the probe diameter, which varies with the droplet size and this can lead to added measurements uncertainties (Hardalupas et al. 1994). Indeed, the volume flux and number density depend on conflicting features, with the volume flux measurements being largely influenced by large particles, leading to its overestimation and number density by the detection of smaller ones (Zhu et al. 1993a), making simultaneous measurements of both parameters difficult, due to the limitation of the dynamic size range of the instrument, and further raising doubts over the reliability of the measurements. And it is known that larger droplets scatter more lights than smaller ones, making the volume flux very much affected by the larger particles, while the probe diameter is usually underestimated. Both these factors lead to an overestimation of the volume flux. On the other hand, in non-burning sprays, McDonnell and Samuelson (1989) found that the area integrated mass flux was only within 30% of the injected liquid flow, due to non-axisymmetry and steep gradients of volume flux in the radial direction. Bulzan (1995) performed the same integration and found out that only 26% of the injected flow was measurable close to the exit of the injector, where the spray is dense and is not burning.

As a whole, accurate droplet number density and volume flux measurements are difficult to make (Widmann and Presser, 2002b) and are subject to lot of uncertainty. Fridman and Renksizbulut (1999) mentioned that in light of the above, it would seem that volume flux and number density measurements should be used in qualitative fashion rather than quantitatively.

Another critical issue is that the fuel temperature will influence the fuel density, affecting the refractive index. This variation of refractive index with fuel temperature will in turn alter the measured drop size when using PDPA. Indeed, Shneider and Hirleman (1994) demonstrated that the presence of radial refractive index gradients may result in significant bias errors in sizing as well as for volume flux estimation (Leport et al. 1999) especially in burning sprays, since the droplet temperature cannot be estimated. However, if a thermo-optic coefficient for the changes in refractive index with temperature can be measured, the droplet temperature needs to be known in order to select the correct refractive index, otherwise it will result in droplet size overprediction by as much as 15 %.

4.4.3 PIV measurement

One of the main uncertainties linked with the PIV measurements resides in the failure in the vicinity of the injector to distinguish between the small droplets and the particle seed. Therefore, velocity measurements taken close to the spray nozzle should be read with extreme caution, otherwise this can be subject to misinterpretation.

Moreover, particle image velocimetry methods will in general not be able to measure components along the z-axis (towards to/away from the camera). These components may also introduce an interference in the data for the x/y-components.

Also, the size of the recordable flow field is limited by the size of the tracer particles. If the recorded area is too large, this will result in the loss of sub pixel resolution. The typical maximum size of the recordable plane is in the region of 10cm to 50cm square, depending on the technology and complexity of the analysis algorithms used.

4.5 Experimental Operating Conditions

The experiments were carried out using ethanol and biodiesel.

	Ethanol	Biodiesel			Rapeseed oil
$P_{\text{rig atm}}$	1	1	2	3	1
$M_{\text{fuel}} \text{ (g/s)}$	0.36	0.75	0.75	0.75	0.75
$M_{\text{air,sw}} \text{ (g/s)}$	1.6	3.0	6.0	9.0	3.0
$M_{\text{air,coflow}}$	12.0	12.0	12.0	12.0	12.0
$T_{\text{air,sw}} \text{ (}^{\circ}\text{C)}$	20.6	150.6	187.4	189.6	165.0
$T_{\text{air,co}} \text{ (}^{\circ}\text{C)}$	15.7	13.4	14.4	15.4	14.4
$T_{\text{fuel}} \text{ (}^{\circ}\text{C)}$	20.5	141.4	155.8	156.3	157.1
Injection pressure (p.s.i)	116.8	147.6	231.0	281.5	313.6

Table 4. 1 Experimental operating conditions

The fuels considered in this study were ethanol and biodiesel. The experimental conditions are described in table 4.1. Although increasing the secondary air resulted in no discernible difference in terms of the flame structure, increasing the secondary air from 12 g/s to 16 g/s resulted in a corresponding increase in re-circulated combustion products entering between the heat shield and pressure casing. This caused condensation problems on the optical windows (Pierce et al., 2007). Therefore the experiments were all carried out at the lower secondary air flow rate of 12 g/s.

The boiling point of biodiesel is significantly higher than for ethanol – respectively 623 K and 351 K under 1 atm – therefore biodiesel is much less volatile than ethanol. For this reason, these fuels need to be preheated in order to reduce their viscosity and atomize into droplets within the size range of ethanol droplets, so that significant evaporation can occur in the pressure rig and avoid to a maximum wall wetting which would tend to reduce combustion efficiency.

4.6 Unconfined ethanol experimental data

Drop mean properties (size, number density, volume flux, velocity) and gas properties (temperature, axial velocity) are presented to describe the global features of the spray. A traverse was made of the flame centreline and radial traverses at six axial locations of 10, 20, 30, 40, 50 and 60 mm downstream of the nozzle as illustrated figure 4.1 where

all the necessary data required to determine the spray and gas characteristics were taken.

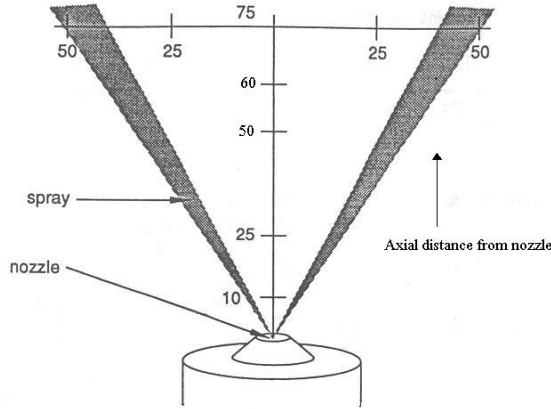


Figure 4.1 Spray measurement locations

4.6.1 Droplet size measurements

Figure 4.2 shows the droplet Sauter Mean Diameter, D_{32} , for different downstream distances. The Sauter Mean Diameter (SMD) is the diameter of a droplet whose volume to surface area ratio is that of the entire spray and is frequently used to characterize a polydisperse spray via a single representative droplet. The Sauter Mean Diameter is defined as (Mugele and Evans, 1951):

$$D_{32} = \frac{\sum_i n_i d_i^3}{\sum_i n_i d_i^2} \quad \text{Equation 4. 1}$$

Where n_i and d_i are the number of count in and the droplet diameter corresponding to, the i^{th} class, respectively.

Based on the experimental data shown figure 4.2, the droplets enter the flame front as a hollow cone spray since there are no droplets present inside the cone. At a distance of up to 20 mm downstream of the spray nozzle, it is interesting to note that the largest droplets are located on the inner side of the spray, whose presence is revealed by the local peaks, while the smallest droplets tend to be located on the outer edges of the

spray. In fact, the small drops have a relatively high velocity near their point of formation and they initially have straight trajectories.

But as the spray moves further away from the nozzle exit, the average Sauter Mean diameter (D32) of the droplets at the inner side of the spray begins to decrease, while on the other hand the droplets size at the outer edge increase significantly. As a result, from a height of 20 mm, the biggest droplets are at the outer edges of the spray since they possess sufficient inertia to penetrate deep into the spray region while essentially maintaining straight trajectories and the finest drops, which tend to relax more rapidly than the larger drops and have little inertia, follow the flow structure and will be shifted to the inner edge of the spray and will be confined to fuel rich regions. This is attributed to the characteristic design of hollow cones.

Moreover, the flame sits on the spray centreline and therefore the droplets on the inner edges, surrounded by hot gases, tend to evaporate much quicker than the droplets on the outer edges, which manage to escape the main flame zone and consequently are less subject to evaporation. On the inner edge, the small droplets present from 30 mm are initially large droplets which have partially undertaken evaporation as they go through the flame, while on the outer edge, preferential vaporization of small droplets, which are more affected by the heat exchange than the larger ones as the weight function is a function of the cube of the diameter, leads to a shift of the droplet size distribution to the larger droplets resulting in an increase in mean diameter of droplets.

The PDPA data show that the profiles of droplet diameter reveal that the main body of the spray is composed of droplet ranging from 5 μm to 120 μm but the number of droplets beyond 50 μm is marginal. However, accurately defining the size range of droplets still represents a challenge for the attempts to give an accurate representation of the droplet size distribution, since it will significantly affect the flame structure, as it will be demonstrated in the computational study.

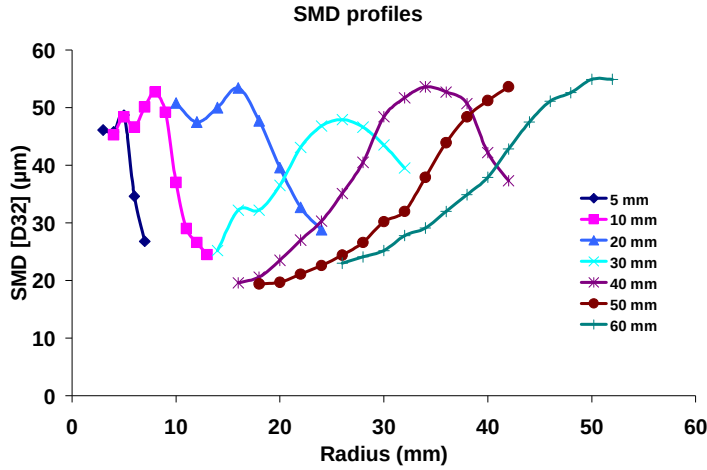


Figure 4. 2 SMD PDPA measurements as a function of distance from the nozzle exit

4.6.2 Droplet mean axial velocity distribution

The mean axial velocities of the droplets is presented figure 4.3. The axial velocities of the droplets progressively decays from a maximum value of 22 m/s in the most dense region at 5 mm downstream of the injector and become more uniform radially to a low value of around 4 m/s at 60 mm from the nozzle exit where the droplet velocities continue to adjust to the rapidly changing gas phase until they are in velocity equilibrium with the gas phase as seen figures 4.5 and 4.6. The absence of negative axial velocity for the droplets implies that even the finest droplets, which possess less inertia than the larger ones, are not sufficiently small to be carried away by the gas field into the recirculation zone.

The outer edges of the spray display low axial velocities and high velocities on the inner side of the spray, up to a distance of 20 mm downstream of the injector due to the fact that the largest droplets close to the fuel atomizer are located nearer to the centreline as illustrated on the SMD PDPA measurements.

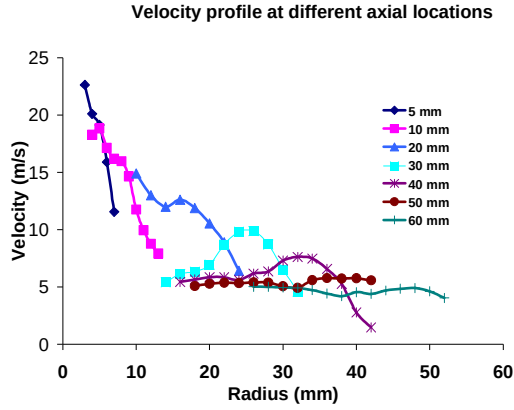


Figure 4. 3 Axial velocity profile at different axial locations

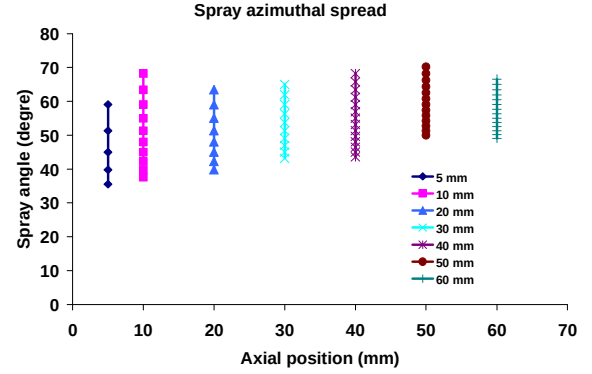


Figure 4. 4 Spray azimuthal spread

The wide droplet radial distribution implies that the azimuthal spread of the cone angle is significant, and the PDPA data seem to imply that the spray angles ranges approximately from around 40° to 70° as illustrated figure 4.4.

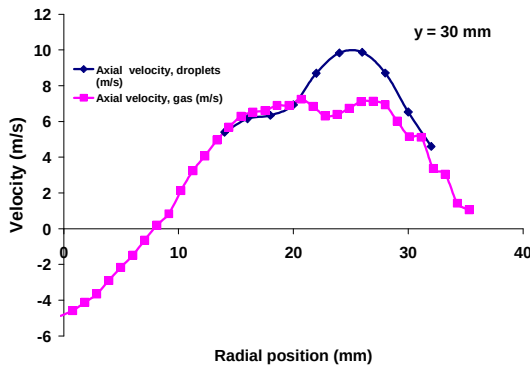


Figure 4. 5 Axial velocity droplet and gas at 30 mm

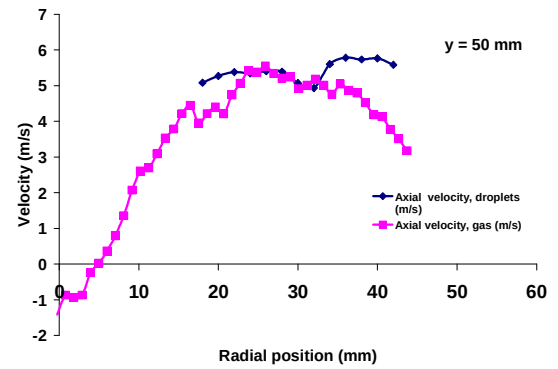


Figure 4. 6 Axial velocity droplet and gas at 50 mm

4.6.3 Breakup phenomena

Figure 4.7 illustrates the visualization of the spray features realised with the help of laser imaging data using higher imaging magnification camera optics. Although described by the manufacturer as a solid spray, laser sheet imaging rather suggests the hollow cone nature of the spray and the spray region even in the vicinity of the atomizer, appears to be dilute, setting aside the perspective of significant droplet collision and coalescence but dense enough to make proper observation and measurements in the vicinity of the fuel nozzle difficult.

The figure shows that at 5 mm downstream of the injector, the droplets still have a ligament-like droplet structure and still breaking up so it is difficult to conclude on the droplet size measurements at that particular location. In fact, the near-field of the injector presents a particularly challenging problem for CFD. Droplet primary break-up becomes effective further downstream, likely from a distance of 10 mm. Therefore, although the closest possible measurements were made at 5 mm downstream of the nozzle the measurements were assumed to be reliable only from 10 mm downstream of the spray nozzle.

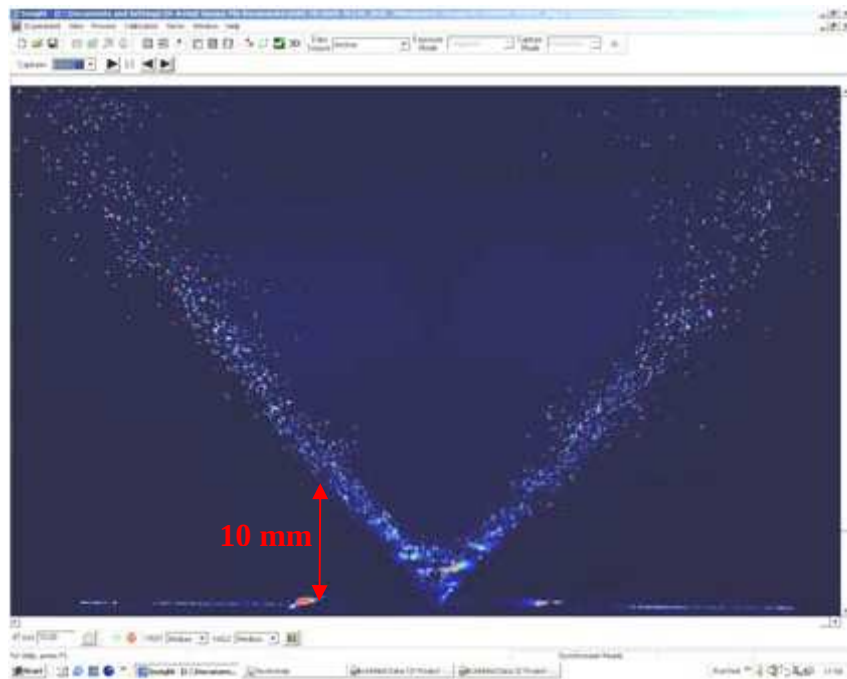


Figure 4. 7 Planar sheet image of the spray

Since the Weber number is well below a critical value of 12 as seen figure 4.8, secondary breakup is not believed to be occurring in the experiments. Weber number calculations with biodiesel also showed that the value obtained is too low to consider secondary breakup. At higher pressures the velocities remain the same since the mass flow rate is scaled with pressure therefore the Weber number will not exceed the critical value unless the initial injection velocity is dramatically increased (at least 4 or 5 times the injection velocity encountered at 1 atm which is not the case in these experiments).

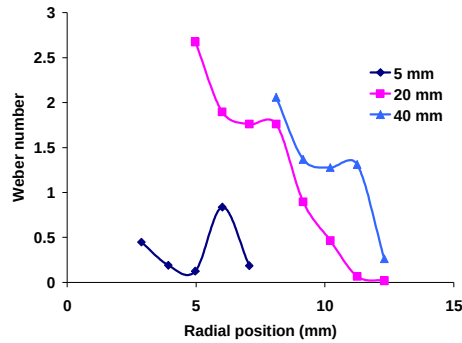


Figure 4. 8 Weber number calculation

4.6.4 Gas velocity

Direct comparison between the preliminary swirling cold flow measurements (without fuel) and those for the combusting ethanol spray is not possible since the level of swirler air flow had to be substantially reduced from initial estimates in order to stabilize the flame (Pierce et al., 2007).

4.6.5 Temperature profiles

Thermocouples have been chosen to measure the temperature since they are robust, relatively easy to use, take a relatively small volume and are particularly reliable. The temperature accuracy is estimated at ± 50 K. A thermocouple is illustrated in Appendix B. The measured temperature field is described figure 4.9 and illustrates the flame structure around the spray and allows a direct comparison with the numerical model.

The flame, once ignited, is anchored near the spray nozzle and extends to a distance of around 10 cm. At 5 mm downstream of the fuel nozzle, the gas temperature reached 1810 K and a sharp reduction in temperature at a radial distance of about 4 mm are caused either by the cooling effect of the spray or by the droplet impingement on the thermocouple, and a second peak is apparent further out radially since the spray influence is no longer felt at this location. Consequently, the spray flame appears as a dense column of droplets burning with a flame surrounding the spray region. It appears that the presence of the thermocouple can affect the flow field immediately downstream of the nozzle, and a non intrusive technique, would have been suitable, to see if the measurement technique would have influenced the flame structure, especially in the

vicinity of the fuel atomizer where the spray is generally dense. If the cool region is due to the cooling effect of the spray, this makes a spray flame sensibly different from a gas diffusion flame, as the spray will have a significant impact on the structure of the flame.

At 10 mm downstream of the fuel nozzle, gas phase temperature is substantially elevated and has increased to a maximum temperature of close to 1900 K. The steep reduction in temperature due to droplet impingement are still present and are found at a radius of about 10 mm, corresponding to the spray trajectory. At 20 mm downstream, the maximum corrected temperature is about 1860 K but the cooling effect of the spray or eventual thermocouple interference is no longer present. Further downstream the temperature gradually falls down to a temperature of 1427 K at Z=60mm while the width of the higher temperature region becomes larger. All the profiles are bell shaped with the maximum temperature always located on the centreline. The temperature peak corresponds to the region where the most intense combustion is taking place.

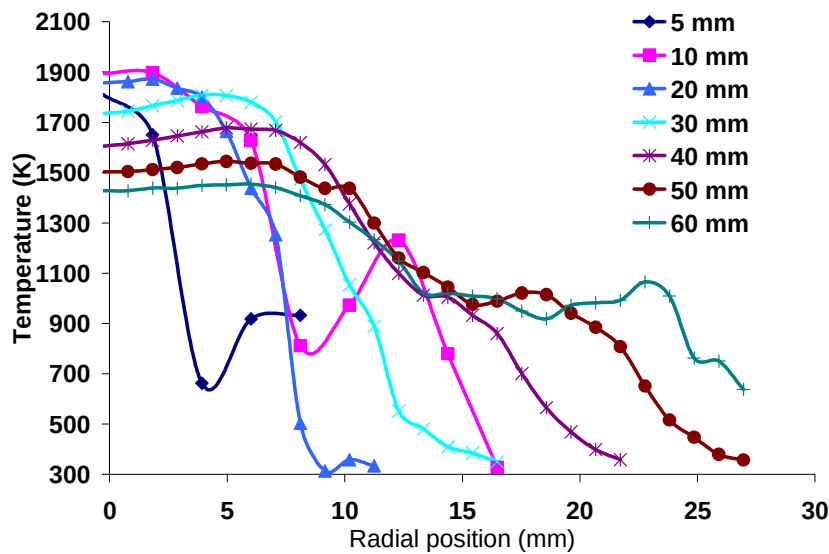


Figure 4. 9 Unconfined ethanol temperature profile (distances measured from the nozzle exit).

4.7 Confined Ethanol experiments

Drop size and axial velocity as well as the gas axial velocity and temperature are presented. The number density and volume flux are not described since they are not believed to be reliable enough.

4.7.1 Droplet size measurements

The droplet size in the confined rig remains largely unchanged with downstream distance and displays similar values to those obtained in the open experiments but it appears that there is more radial spread of the spray in the open than in the confined experiments. Moreover, the droplet initially are of the same size, but thereafter the measurements in the confined rig show that the droplets have a lower size as they move further downstream. The large radial spread encountered in the open experiment (cf. figure 4.10 and 4.11) has a larger cooling effect on the ambient air, since spray evaporation acts as a heat sink on the gaseous phase. As a result, the cool region surrounding the spray is larger in the open experiment and consequently, the droplets do not undergo as strong evaporation as in the confined rig, leading to higher droplet size especially at 20 and 30 mm as illustrated figure 4.12 and 4.13.

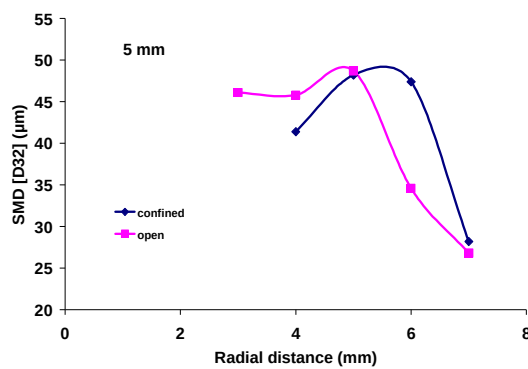


Figure 4.10 Droplet SMD at 5 mm from the nozzle exit

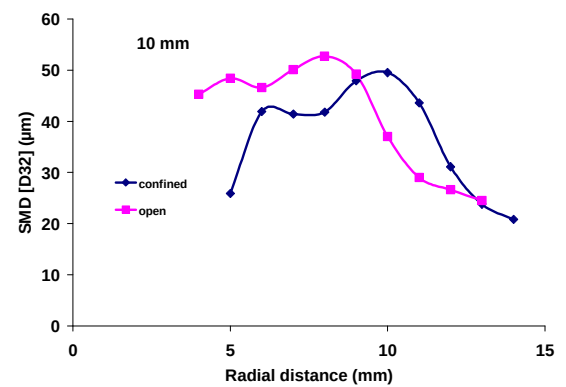


Figure 4.11 Droplet SMD at 10 mm

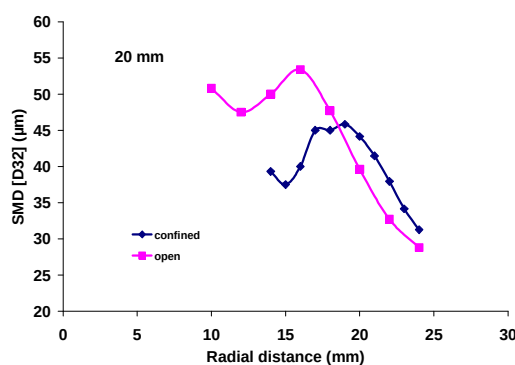


Figure 4.12 Droplet SMD at 20 mm

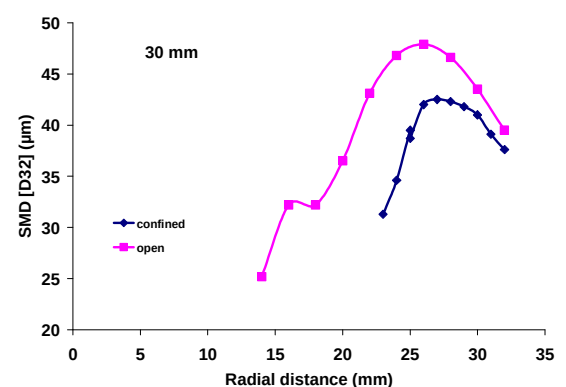


Figure 4.13 Droplet SMD at 30 mm

4.7.2 Droplet velocity

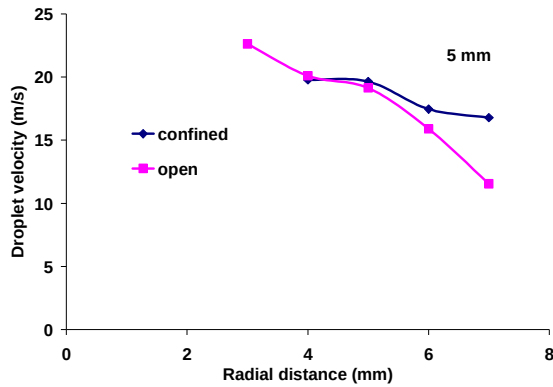


Figure 4. 14 Droplet axial velocity comparison at 5 mm

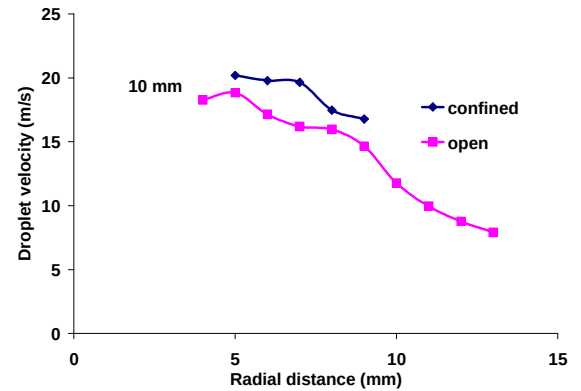


Figure 4. 15 Droplet axial velocity comparison at 10 mm

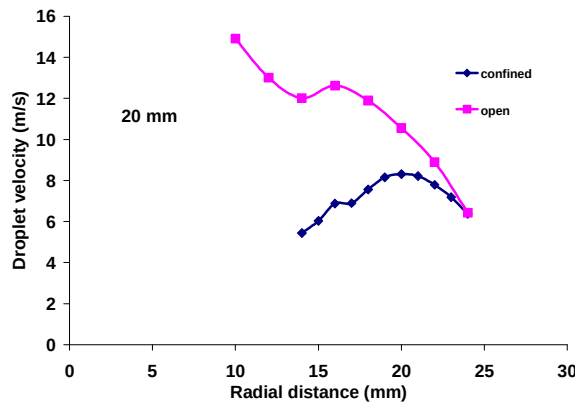


Figure 4. 16 Droplet axial velocity comparison at 20 mm

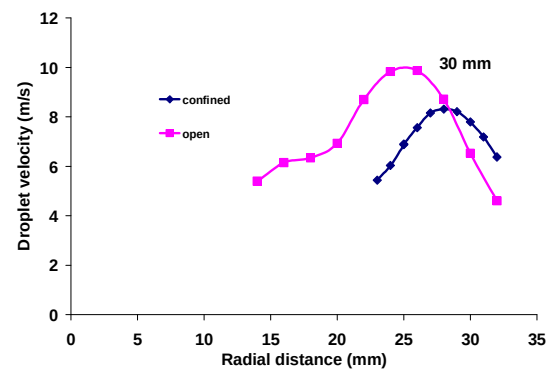


Figure 4. 17 Droplet axial velocity comparison at 30 mm

The experimental conditions being the same as for the open flame, the droplet velocities initially show the same features with a gradual decay of the droplet axial velocity as they penetrate further into the flow field (cf. figure 4.14 and 4.15) but as the droplets move downstream they show a lower velocity than in the open experiments as illustrated figure 4.16 and 4.17. It is explained by the fact that the droplets in the confined rig have a lower Sauter mean diameter, and as a result lose their momentum more rapidly than the larger droplets encountered in the open experiment.

4.7.3 Temperature profiles

The temperature profiles between the open and the confined rig look broadly similar, except that at 10 mm (cf. figure 4.18), the flame is quenched closer to the spray centreline due to the fact that the droplets expand more in that particular radial direction in the open flame experiments. Further downstream, up to a distance of 30 mm downstream (cf. figure 4.19 and 4.20), the larger spread of the cone angle in the open

experiments leads to lower flame width due to the cooling effect of the spray. However, from 40 mm, the flame temperature profiles appear to be similar in the open and confined rig as illustrated figure 4.21 and 4.22.

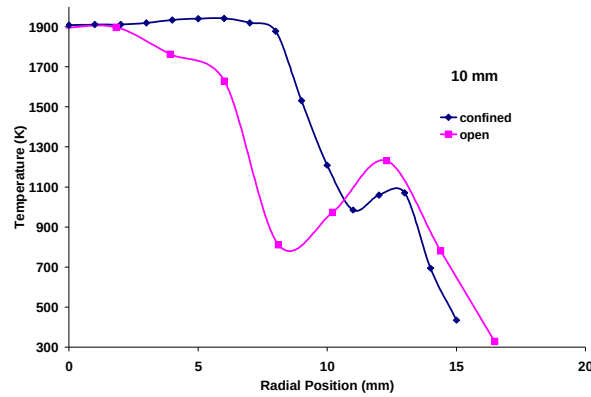


Figure 4. 18 Temperature profiles at 10 mm

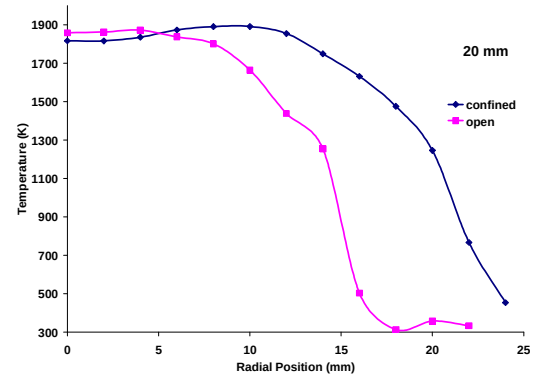


Figure 4. 19 Temperature profiles at 20 mm

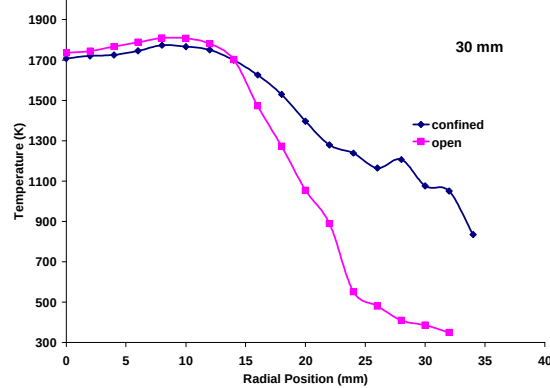


Figure 4. 20 Temperature profiles at 30 mm

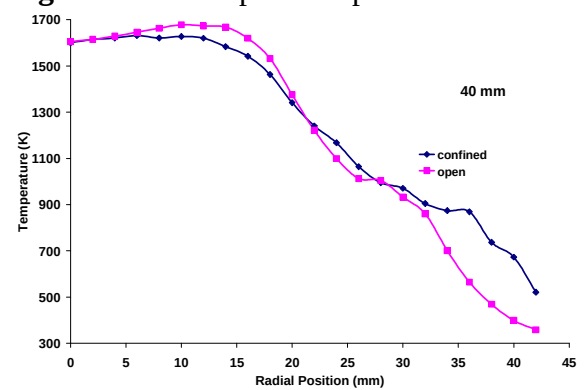


Figure 4. 21 Temperature profiles at 40 mm

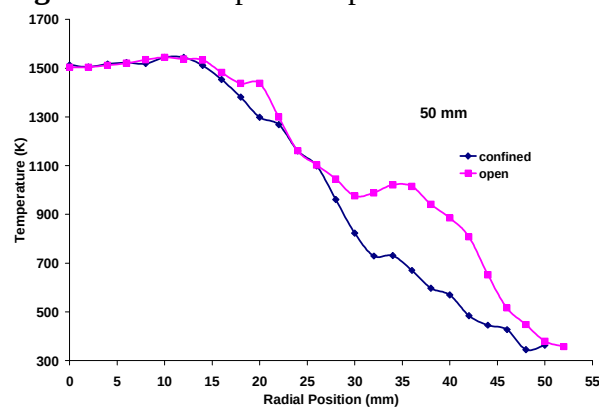


Figure 4. 22 Temperature profiles at 50 mm

4.8 Biodiesel experiments

4.8.1 Droplet size

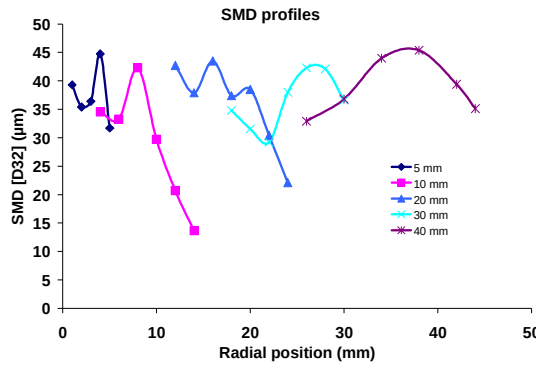


Figure 4.23 SMD PDPA measurements at 1 atm

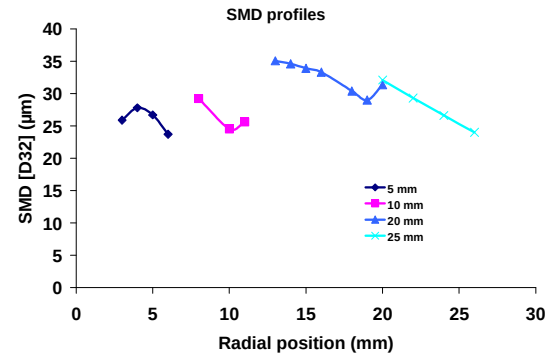


Figure 4.24 SMD PDPA measurements at 2 atm

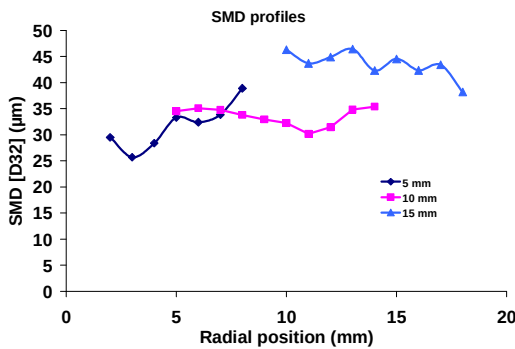


Figure 4.25 SMD PDPA measurements at 3 atm

As for the ethanol experiments, the droplets enter the flame front as a hollow cone spray. The droplet SMD appears to be in the same range, between 30 and 45 μm , regardless of the pressure as illustrated figure 4.23 to 4.25. Clearly it is observed that the penetration of the spray decreases when the ambient pressure is increased. Indeed, the PDPA measurements show that, although the initial droplet Sauter mean diameter is initially similar at all pressures, from 40 mm at 1 atm, the furthest measurement at 2 atm is taken at a distance of 25 mm, and decreases down to 15 mm at 3 atm. This is the result of an increased drag force and ambient gas density. At 3 atmospheres, it appears that the SMD has increased at 15 mm to a value of 45 μm , against a value of around 35 μm at a height of 10 mm. Due to an increase of droplet collision frequency with increasing ambient pressure, as a result of the reduced spray penetration and an increased number density of the droplets. In fact, Kim and Sung (2003) demonstrated that collisions are more frequent as a result of an increase in pressure.

Figure 4.26 to 4.29 represent the size histograms for biodiesel under 1 bar. They illustrate that the spread of drop size is fairly narrow and there is no convincing evidence of much larger droplets with the number of droplets beyond 70 μm being marginal. The drop size distribution $D_{0.9}$ at 40 mm height is perhaps due to errors in the PDPA measurements since it coincides with a small volume flux. However, it could be possible that the calibration of the instrument is such that much larger droplets are not accounted for in the spray drop size distribution. As there can be a significant amount of measurement uncertainty regarding the spray drop size characterisation, the reliability of the simulation comes into question, as the spray flame is highly dependent on the drop size distribution, and this will be discussed in section.

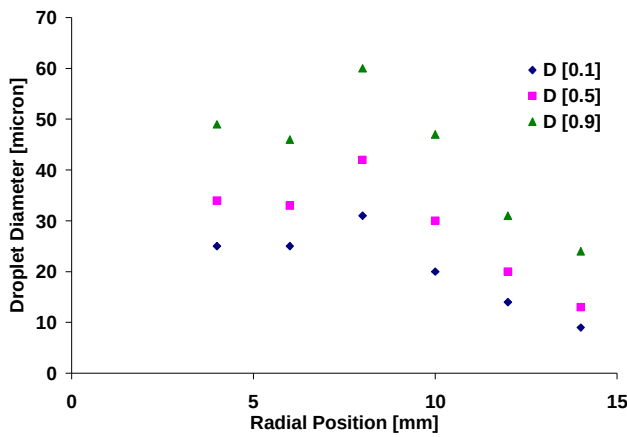


Figure 4. 26 Drop size distribution: Biodiesel; 1 atmosphere; 10 mm height

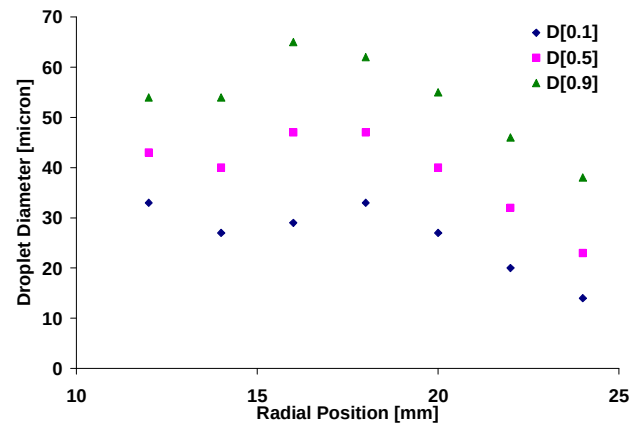


Figure 4. 27 Drop size distribution: Biodiesel; 1 atmosphere; 20 mm height

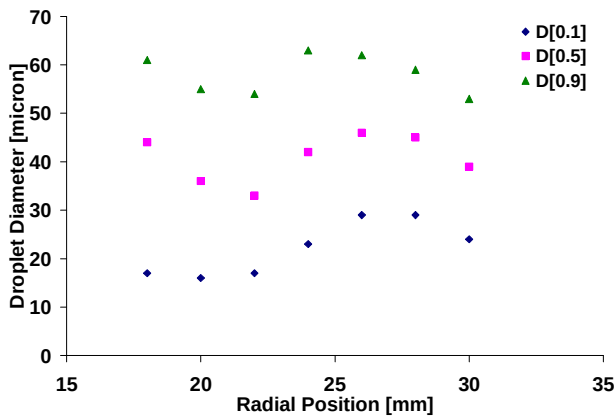


Figure 4. 28 Drop size distribution: Biodiesel; 1 atmosphere; 30 mm height

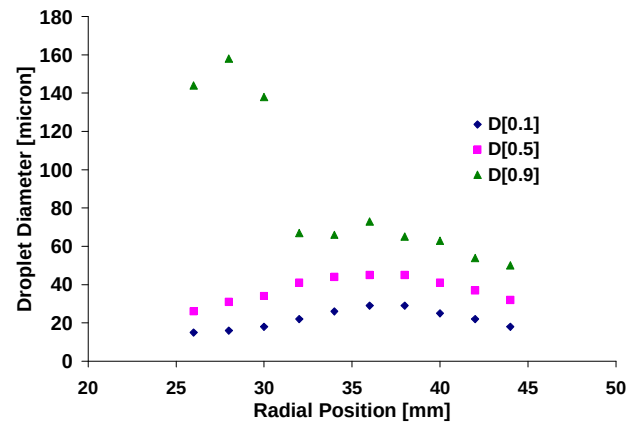


Figure 4. 29 Drop size distribution: Biodiesel; 1 atmosphere; 40 mm height

4.8.2 Droplet mean axial velocity distribution

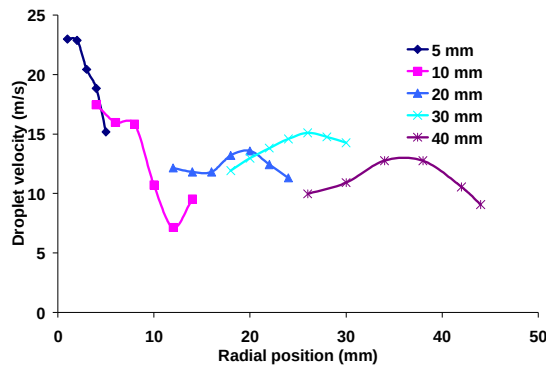


Figure 4.30 Axial velocity profile at different axial locations at 1 atm

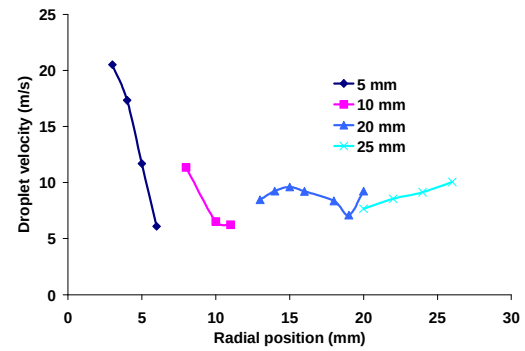


Figure 4.31 Axial velocity profile at different axial locations at 2 atm

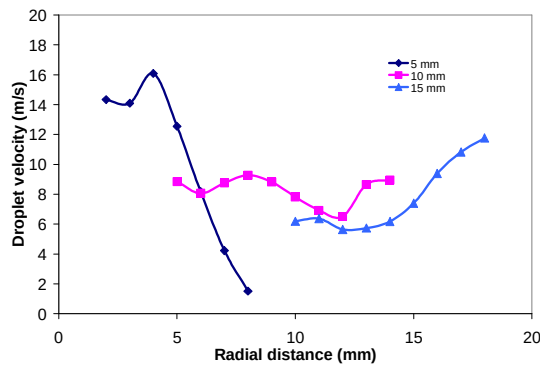


Figure 4.32 Axial velocity profile at different axial locations at 3 atm

The observations are the same as for the droplet SMD, with the visible effect of the ambient pressure on the spray velocity, since an increase in pressure will lead to a stronger deceleration of the droplet velocity as illustrated from figure 4.31 and 4.32 compared to figure 4.30.

4.8.3 Gas velocity

The axial gas velocity profile of reacting biodiesel sprays is presented figure 4.33. The velocity profiles at 2 and 3 atm are presented in Appendix B since they are similar to 1 atm, as the velocities are scaled with pressure. In the vicinity of the spray nozzle, the flow field displays a positive axial velocity on the spray centreline. This behaviour results from the spray momentum and heat release from the flame which causes an acceleration of the gas through their effect on gas density. Hence close to the burner exit, where the liquid loading is at its highest, spray momentum has a significant impact on the gas flow field. Indeed, in this region there is a strong two-way coupling between the gas and the spray phase, since the positive axial velocity is a result of the added

momentum created by the spray. Therefore, the spray has a dominant effect on the gas phase in the vicinity of the fuel atomizer.

However, the PDPA measurements did not show any droplets on the spray centreline, rather showing features of a hollow cone spray. In fact it is believed that, although the PDPA does not appear to pick up the droplets, small droplets are present on the spray centreline. The absence of PDPA data on the centreline is probably due to the limitation of dynamic range of the PDPA measurements, calibrated so that the lowest drop size resolution is set at 5 μm . Consequently, it can be concluded that the droplets responsible for the positive axial velocity in the vicinity of the atomizer have a SMD of less than 5 μm , up to 10 mm downstream.

Further downstream, the axial velocity shows a decrease with axial distance on the spray centreline, as the momentum of the small droplets which are not captured by the PDPA in the central region of the spray close to the nozzle gradually subside. In fact the heat release is progressively less pronounced in that region and the spray is no longer the dominant factor on the flow field. Consequently, a strong recirculation zone due to the swirling air flow is visible from a height of 20 mm, with a maximum negative value of close to 7 m/s at 30 mm and peak positive axial velocities of 27 m/s from the air exiting at 5 mm downstream of the swirler.

The axial velocities display the same trend and values regardless of the pressure since they have been scaled accordingly with an increase in pressure. For instance, from 1 to 2 atm, the mass flow rate has been doubled and tripled from 1 to 3 atm, hence the velocities are conserved.

Figure 4.34 to 4.37 presents a comparison of the axial velocity profiles for air alone and the reacting spray at 1 atm, with the same air flow conditions of 3 g/s for the primary air flow and 12 g/s for the secondary air flow. These data illustrate the potential of the PIV measurements in discriminating fuel effects rather than for detailed analysis at this stage. The burning air field displays a stronger positive axial velocity than for the cold air alone due to the presence of the burning spray. The expanding gas add significant momentum to the gas phase and the momentum of the spray has broaden the recirculation zone by pushing further out radially the air jets coming out of the swirler.

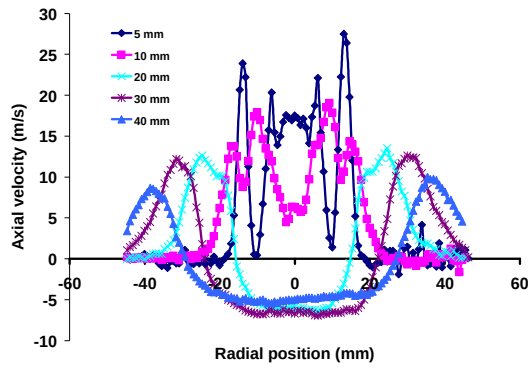


Figure 4.33 Axial velocity profile at 1 atm

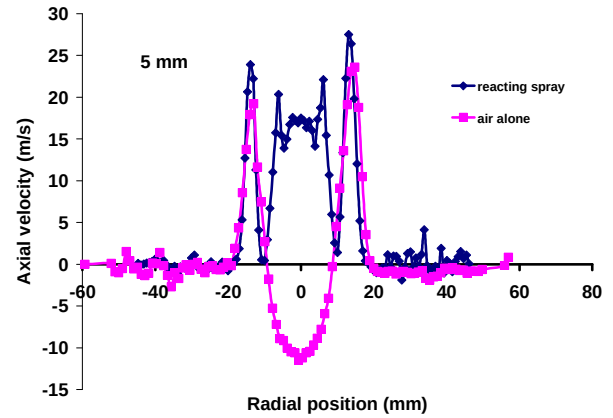


Figure 4.34 Axial gas velocity profile at 5 mm

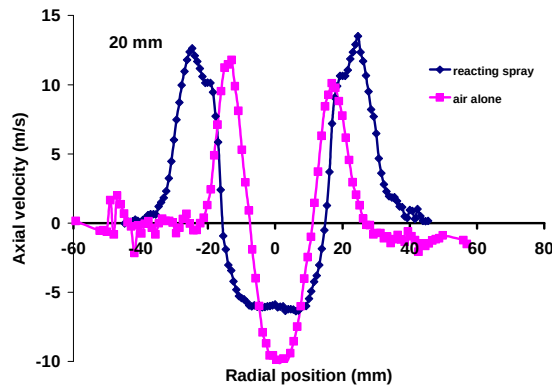


Figure 4.35 Axial gas velocity profile at 20 mm

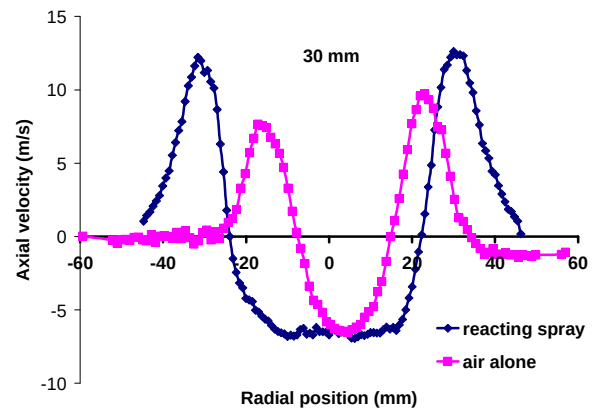


Figure 4.36 Axial gas velocity profile at 30 mm

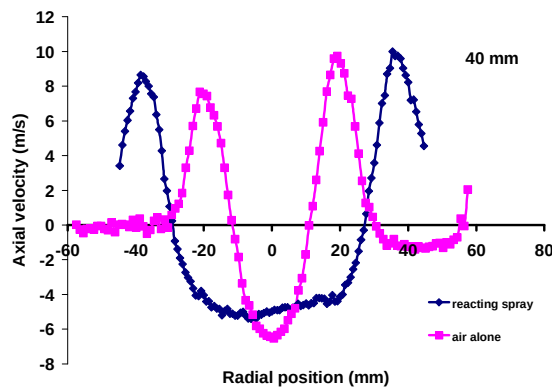


Figure 4.37 Axial gas velocity profile at 40 mm

Figure 4.38 shows the velocity magnitude for a burning biodiesel spray, at 1 atm. Velocity vectors at 2 and 3 atm are presented in Appendix B. The impact created by the 45° angle from the spray is clearly seen with the green arrows strongly influencing the flow field. The swirlers air jets, located further out radially on either side of the spray and highlighted with the red arrows in the vicinity of the horizontal plane, collide with the spray and are pushed by its momentum along its trajectory. Without the spray, the

air jet would have had a more upward trajectory and the recirculation zone would be much narrower. The effect of the spray on the air jets at 1 atm is clearly seen figure 4.39.

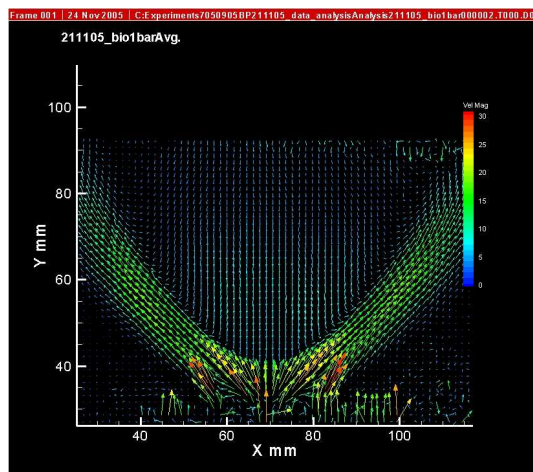


Figure 4. 38 PIV image of the velocity magnitude at 1 atm (velocity vectors)

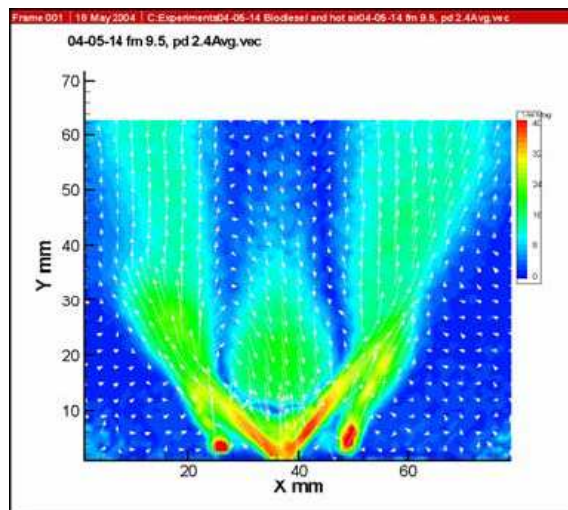


Figure 4. 39 PIV image of the velocity magnitude at 1 atm (contours)

4.8.4 Temperature profiles

Difficulties have been encountered to measure the temperature 5 mm downstream of the spray nozzle, therefore, thermocouple measurements will be taken into account only from a distance of 10 mm. The temperature profile looks similar to the confined ethanol simulation, since a peak flame temperature of 1850 K is located at $Z = 10$ mm before progressively decreasing down to a temperature of 1400 K as seen figure 4.40. The dip in temperature at 10 mm is also predicted due to the cooling effect of the spray or the droplet impinging on the thermocouple. As the gas temperature decreases when moving further downstream, the higher temperature region tends to widen. Contrary to the ethanol experiments, the peak temperature at each axial location is positioned further out radially from the centreline. No temperature measurement is available at 2 and 3 atm.

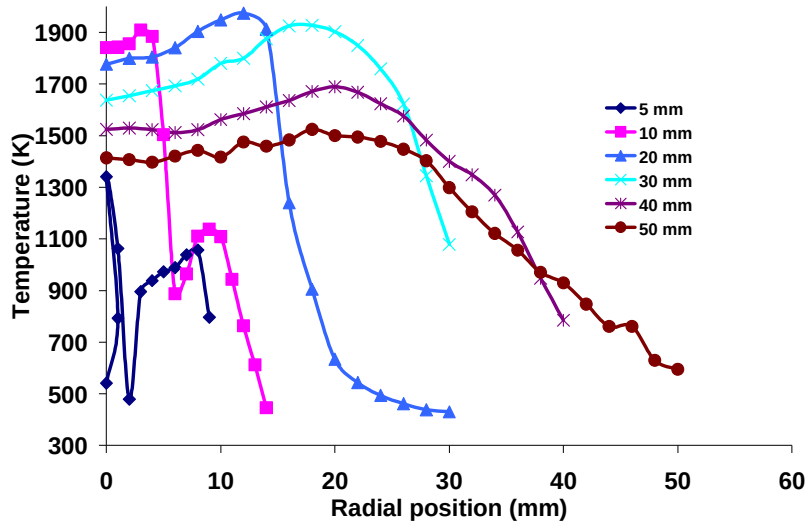


Figure 4.40 Confined biodiesel temperature profile at 1 atm

4.9 Summary

This chapter has attempted to provide experimental data obtained under controlled operating conditions which give a quantitative as well as qualitative description of the spray structure, which could possibly lead to a better understanding of the spray physics and its interaction with the swirling air. These experimental data are obtained for the purpose of providing an input for the initial conditions for the droplet size and velocity conditions as well as a set of boundary conditions, and ultimately the database obtained is used for validation purpose and assessing the performance of the CFD simulations.

In the present study, the spray structure is transformed from solid in an isothermal chamber to hollow cone in a swirl-stabilized combustor. Measurements of droplet size and velocity as well as gas velocity and temperature have been reported on ethanol and biodiesel spray flames using respectively PDPA, PIV and thermocouple techniques. The strongly coupled processes involved in a reacting spray make it compulsory to possess several measurement techniques in order to obtain meaningful enough data to fully capture the spray structure. The results show the strong effects of the spray on the gas flow field, due to the momentum imparted by the droplets. The broad features of the confined rig look quite similar to the experiments in an open configuration in terms of temperature profile, droplet size and axial velocity, except that there is more radial spread for the open configuration, which affects the flame structure. The biodiesel data have been analysed and the effect of increase in pressure on the spray have been commented.

CHAPTER 5 – COMPUTATIONAL STUDY

Modelling turbulent spray flames is a complex task that needs to be solved with sufficient accuracy in order to allow validation of the model and permits enough flexibility to conduct numerical experimentations to determine the effect of different parameters on the structure of the spray flame.

This section provides an overview of the different submodels chosen in the present study, which account for the mesh, numerical methods, models describing the effect of turbulence, multiphase interactions, evaporation, combustion and breakup. Spray wall interaction is not considered to be significant in the present study and hence will not be treated here.

5.1 Mesh

Any desired level of numerical accuracy can be obtained in principle by the use of a sufficiently fine grid. However, care must be taken as to avoid a too fine grid, which for the same results will increase significantly the computational time. The method employed to solve the equations is a computer based numerical model, where the domain is divided into a number of finite volumes called cells, at which all the variables are calculated.

The FLUENT software operates on a wide variety of hardware platforms and operating systems in an efficient and economical manner. Using the Cranfield HPC facilities, domains with a number of cells approaching one million can be completed within one week, using parallel processing. In fact, to increase simulation turn-around time, the computational domain is evenly distributed using parallel processing which is a viable substitution for classic serial processing due to the high number of cells, too demanding for a single computer. The parallel implementation of the solver is based on MPI, allowing it to be used across networks of clustered workstations and also on symmetric multiprocessor machines such as the SGI.

The machine used was a SunFire v880 server. It has 8 processors and 16Gb shared memory and is running on Solaris 9, equipped with 72 processors, with 4 processors per board and a fast interconnect between them. All of the machines have Sun's MPI libraries installed and FLUENT use the MPI version of the code. Sun Grid Engine is used for the queue management of the machines.

The full three-dimensional flow of air through the swirler and the downstream domain up to a distance of 20 cm away from the swirler has been represented. The grid used was a high quality, semi-structured multiblock cylindrical grid system generated using GAMBIT, the mesh generating software normally associated with FLUENT. As the flow is strongly swirling, a 3-dimensional model is required for this geometry; however exploiting a cyclic symmetry it is only necessary to simulate a 36° portion of the vane-cascade as seen figure 5.1. A full geometry would require too much computing power and modelling 1/10th of the full geometry brings significant relief in the computational effort. The grid system contained 814 380 cells and was nearly orthogonal to the flow everywhere. Use of this mesh resolves the flow very efficiently, and in particular, results in high resolution and accuracy near the fuel nozzle, where the pressure and velocity gradients are the highest, fuel mass fraction gradients are the most important and evaporation rates need to be captured accurately. Also, the overall system performance depends heavily on the design of air swirlers and their characteristics. Therefore, the flow through the swirl slots must be accurately represented. The CFD simulations reported were made using Fluent 6.2.

The same simulations with different levels of grid resolutions were completed for the same geometry and boundary conditions. In addition to the previously mentioned grids, a coarser grid was also completed to investigate the resolution of the results and assess overall performance as reflected in the ratio of quality of results/time of the solution. The results have been demonstrated to be grid independent with the computational grid which contained 5400 horizontal cells x 150 vertical cells = 814 380 cells when the computational domain representing the swirler is included and the same mesh has been used for the confined rig simulations. The spacing between the cells in the vicinity of the spray nozzle has been reduced, in order to accurately represent the high pressure, momentum and mass fraction gradients encountered in this area and as the flow move downstream the cells size has been progressively

increased. The height of the domain was limited to 20 cm from the spray nozzle, since the experiments showed that the flame height in all the experiments did not go beyond a height of 10 cm. A typical cell size in the vicinity of the injector was around 0.2mm, which corresponds to the fuel orifice diameter.

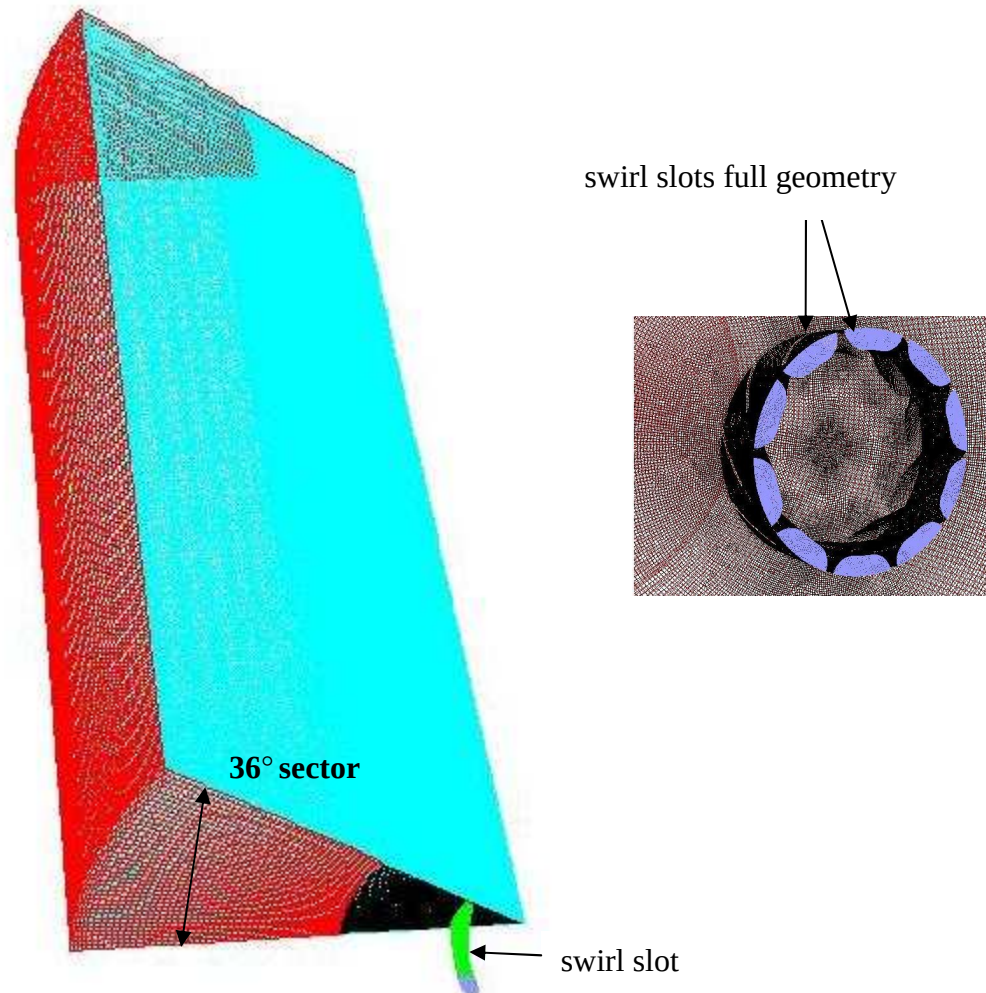


Figure 5. 1 Meshing of the geometry

5.2 Turbulence model

Unfortunately there is no single turbulence model which can be adopted for all types of flows. In fact, there are turbulence models which are superior to others according to the type of application. Reitz and Rutland (1995) have demonstrated that the turbulence model can have a significant effect on the peak temperature prediction for

example, and as a consequence, great care must be taken in the choice of the turbulence model.

The present modelling approach is based on the RSM turbulence model which is well adapted to compute strongly swirling flows. The RSM turbulence model has been proven to be giving accurate results in the prediction of flow with strong swirl, as it is the case in this study as proved in the section 6.3.2.

Since the RSM accounts for the effects of swirl, rotation, and rapid changes in strain rate in a more rigorous manner than $k-\epsilon$ models, it is of greater potential to give accurate predictions for complex flows. In spite of the 30 % additional computational time generated by the use of the Reynolds Stress Model, it might not always yield results that are clearly superior to the simpler models in all classes of flows. However, use of the RSM must be considered when the flow features of interest are the results of anisotropy in the Reynolds stresses, such as highly swirling flows encountered in this study. Equations describing the RSM model are written in Appendix C.

5.3 Evaporation model

Due to the complexity of the evaporation process, CFD tools are of prime importance for the design of low emission combustors involving liquid fuels. Therefore the choice of a particular evaporation model over another is crucial, since it can significantly influence the evaporation rate and determine the fuel mass fraction in a fuel/air mixture and as a consequence the combustor performance. Consequently, a proper evaporation model with the most accurate gas film model which can apply for a wide range of operating conditions should be used. Moreover, CFD codes must strive to achieve a proper balance between results accuracy and computational efficiency and stability rather than the accuracy of the models alone. Consequently, a major compromise for the treatment of the liquid within the droplet is needed. The default FLUENT model is quite a simple model based on the infinite conductivity model and will be described in this section. User defined alternative models do not appear to possess any major demonstrated advantage over the default model. Drawbacks and advantages of those alternative options will be presented in the Discussion section.

In the present simulations the liquid conductivity is assumed to be infinite such that the droplet internal temperature is uniform. Heat transfer operates at the droplet surface and the heat is transferred by convection and conduction from the liquid phase towards the gas phase. The droplet surface is assumed to be regressing as droplet evaporation occurs and the onset of vaporization is initiated whenever the droplet temperature exceeds the vaporization temperature.

In common with most CFD codes, the models in FLUENT assume that the temperature gradients inside the droplets can be ignored, essentially due to the fact that droplet evaporation has to be modelled alongside turbulence, combustion and other related phenomena. This simplifying assumption also represents a major constraint to the use of user defined alternative droplet heating models. However, it is expected to be a good approximation in the case of stationary or very fast moving droplets, when the isotherms almost coincide with the streamlines (Abramzon and Sirignano, 1989b). Even in intermediate situations, errors introduced by this assumptions are assumed to be acceptable (Sazhin, 2006b). Moreover, Sazhin (2006a) investigated the effect of temperature gradients on droplet evaporation using the infinite and effective conductivity models and he concluded that in the absence of break-up, the temperature gradients do not have a significant effect on droplet evaporation, but if secondary breakup occurs, this will lead to a significant decrease in the droplet evaporation time. However, as demonstrated in Section 5.1.3 of the Experimental Study, no secondary breakup occurs in the current study due to the low Weber number, therefore description of the droplet temperature gradients is not needed in the present study.

5.4.3 Heat transfer to the droplet

For groups of models that do not offer representations of temperature gradients inside the droplets, the following relationship is commonly used to calculate the droplet temperature from the following energy balance equation:

$$m_p C_p \frac{dT_p}{dt} = \text{flux}_{\text{conv}} + \text{flux}_{\text{vap}} \quad \text{Equation 5. 1}$$

The droplet evaporation is defined by a heat balance between the convective and the latent heat transfer between the continuous and the droplet phase. This equation implies that the heat transferred from the gas to the droplet is spent on raising the droplet temperature and supplying the heat for vaporization with the convective heat flux widely used for practical applications in CFD defined as:

$$flux_{conv} = hA_p (T_{\infty} - T_p) \quad \text{Equation 5. 2}$$

And the vaporization heat flux:

$$flux_{vap} = h_{fg} \frac{dm}{dt} \quad \text{Equation 5. 3}$$

The Ranz-Marshall (1952) correlation is used to account for convection and to calculate the heat transfer coefficient h :

$$Nu = 2 + 0.6 Re^{1/2} Pr^{1/3} = \frac{hd_p}{k_{\infty}} \quad \text{Equation 5. 4}$$

According to Aggarwal et al. (1984), although this type of correlation is very simple, there is very little theoretical justification for it (Aggarwal et al. 1984). Indeed, this correlation is based on experiments conducted under quasisteady conditions, atmospheric pressure, relatively low air temperature and the transient droplet heating stage as well as internal circulation are not taken into account. The Ranz-Marshall correlation overpredicts the vaporization rate and can yield to inaccurate results, especially for low Reynolds number, as noticed by Abramzon and Sirignano (1989a). However, this correlation is commonly used for the d^2 -law, conduction limit and infinite conductivity models and as mentioned in the literature review, even though this correlation has some flaws, Sirignano (1999a) used it to characterise the droplet lifetime in a convective environment.

The extension of the empirical 1/3 averaging rule for the Prandtl and the Reynolds number in the Ranz and Marshall correlation is necessary when large temperature differences exists across the gas film surrounding the droplets, conditions which have not been tested in the original experiments by Ranz and Marshall (1952). The

Reynolds number based on averaged conditions can be five times the Reynolds number based on ambient properties (Sirignano, 1999).

Renksizbulut-Yuen (1983) and Abramzon and Sirignano (1989a) developed some other correlations but the CFD code Fluent incorporates the correlation of Ranz and Marshall (1952) by default in their equation for the calculation of the heat transfer coefficient. Indeed, despite the fact that the Renksizbulut and Yuen's correlation seems to be offering some advantages, it has been tested only at atmospheric pressure and testing was limited to water, methanol and heptane droplets, therefore this correlation cannot be generalised to be adopted in a CFD code. These correlations are again based on experimental results under atmospheric pressure and relatively low air temperature. The correlation developed by Abramzon and Sirignano (1989a) is described in the Discussion section.

5.4.4 Mass transfer to the droplet

The droplet mass is calculated in the following manner:

$$m_p(t + \Delta t) = m_p(t) - N_{vap} A_p MW \Delta t \quad \text{Equation 5. 5}$$

The molar flux of droplet vapour N_{vap} into the gas phase is related to the gradient of diffusion between the gas phase and the droplet surface:

$$N_{vap} = k_c (C_{i,s} - C_{i,\infty}) \quad \text{Equation 5. 6}$$

The concentration of vapour at the droplet surface is calculated based on the ideal gas law:

$$C_{i,s} = \frac{P_{sat}(T_p)}{RT_p} \quad \text{Equation 5. 7}$$

In order to calculate the concentration of vapour at the droplet surface in an accurate manner, it is important to know the relationship between the vapour pressure and the

temperature. These relationships are defined in the Fuel Properties chapter, section 3.1.2 for Rix biodiesel and 3.2.1 for ethanol.

The concentration of vapour in the bulk gas used in equation 6.5 is calculated based on the mole fraction of the species x_i :

$$C_{i,\infty} = x_i \frac{P_{op}}{RT_{\infty}} \quad \text{Equation 5. 8}$$

Fluent uses the Ranz-Marshall (1952) correlation which allows to calculate the mass transfer coefficient.

$$Nu = 2 + 0.6 Re^{1/2} Sc^{1/3} = k_c d / \delta \quad \text{Equation 5. 9}$$

5.4.5 Evaporation at elevated pressures

Section 2.3.4 in the Literature Review showed that once the critical temperature is reached, the ambient gas is soluble into the liquid phase and as a consequence solubility effects should be taken into account under high pressures. Moreover, the ideal gas assumption is no longer valid beyond the critical pressure. However, since the operating pressure in the simulations for both Rix biodiesel and ethanol will not exceed 10 atm and the fuel temperature will not go beyond 767 K and 428 K respectively for biodiesel and ethanol, these operating conditions are well below the critical pressure and temperature of both fuels, determined respectively at 12 and 64 atmospheres and 788 and 514 K as demonstrated in Fuel Properties section 3.1.3 and 3.2. Consequently, assumptions based on the ideal gas law and gas insolubility in the liquid phase still prevail under the operating conditions encountered in this study.

5.5 Combustion model turbulent non-premixed flames

The non premixed model is used since the fuel and the air are introduced in two separate locations. The combustion model used in this study is the laminar flamelet model introduced by Liew et al. (1981). The flamelet model with presumed PDF shape approach was adopted for its ease of use and also bearing in mind the number

of simulations to be undertaken turnaround time is an important issue for this study. The local structure of these flamelets may show significant deviations from a typical open laminar flame due to local turbulence flame stretch effects and this is where the advantage of the laminar flamelet model lies since the laminar flamelet concept has its origin in the idea that a turbulent flame can be viewed locally as an ensemble of thin, laminar flame structures, called flamelets. Bilger (1976) showed that diffusion flame structure may be expressed as functions of a single conserved scalar under the constraints of infinite reaction rate, equal species diffusivity, unity Lewis number and zero heat loss. In the laminar flamelet model, when flame stretch is incorporated, the governing equations are expressed not only as a function of the mean mixture fraction Z but also of the scalar dissipation, χ_{st} . This may be further extended to include the effects of radiation heat loss. The laminar flamelet model by taking into account the stretch effect on the flame presents itself as a natural extension of the chemical equilibrium model. The laminar flamelet model treats the coupling between chemistry and turbulence in an elegant and simple manner. The advantage of the laminar flamelet approach is that realistic chemical kinetic effects can be incorporated into turbulent flames. Advantages and inconvenients of the FLUENT laminar flamelet model advantages and drawbacks are further commented in the Discussion section.

The mixture fraction Z can be defined as:

$$Z = \frac{Y_i - Y_{i,o}}{Y_{i,f} - Y_{i,o}} \quad \text{Equation 5. 10}$$

and is normalized to lie between zero and one. The mixture fraction Z is defined in such a manner that its value is zero in the air stream and unity in the fuel stream. Applying the flamelet assumption, it has been shown that the governing equations for species and temperature may be written as a function of mixture fraction instead of the spatial coordinates (Liew et al. 1984a; Liew et al. 1981).

The scalar dissipation rate has been introduced into the flamelet equations to define the effect of strain on the flame and is defined in the following manner:

$$\chi = 2\delta \left(\frac{\partial Z}{\partial x_k} \right)^2 \quad \text{Equation 5. 11}$$

The scalar dissipation rate is at the centrepiece of the flamelet assumption, since it is a parameter which defined the amount of stretch on the laminar flamelet. In FLUENT, the scalar dissipation rate is derived from the strain rate a using the equation developed by Peters (1984a):

$$\begin{aligned} \chi_{st} &= (a/\pi) \exp \left[-2 \left[\text{erfc}^{-1}(2Z_{st}) \right]^2 \right] \\ &\approx 4aZ_{st}^2 \left[\text{erfc}^{-1}(2Z_{st}) \right]^2 \end{aligned} \quad \text{Equation 5. 12}$$

and the strain rate is calculated according to the formula proposed by Bray and Peters (1994):

$$a = \frac{\mathcal{E}}{k_{turb}} \quad \text{Equation 5. 13}$$

The species governing equation is written in the following manner:

$$\rho \frac{\partial Y_i}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 Y_i}{\partial Z^2} \quad \text{Equation 5. 14}$$

And the following equation defines the temperature:

$$\rho \frac{\partial T}{\partial t} = \frac{1}{2} \rho \chi \frac{\partial^2 T}{\partial Z^2} - \frac{1}{C_p} \sum_i H_i S_i + \frac{1}{2C_p} \rho \chi \left[\frac{\partial C_p}{\partial Z} + \sum_i C_{p,i} \frac{\partial Y_i}{\partial Z} \right] \frac{\partial T}{\partial Z} \quad \text{Equation 5. 15}$$

As mentioned earlier in this section, a turbulent flamelet is an ensemble of laminar flamelets. Therefore, it is possible to take into account the effect of stretch in the turbulent ensemble. Since for adiabatic systems, species mass fraction and temperature in the laminar flamelets are closely linked to the mean mixture fraction and the scalar dissipation rate, mean values of the thermochemical state variables, such as gas density, species mass fraction and temperature in the turbulent flame can

be determined from the PDF of the mixture fraction and the scalar dissipation rate in the following manner:

$$\bar{\phi} = \iint \phi(Z, \chi_{st}) p(Z, \chi) dZ d\chi_{st} \quad \text{Equation 5. 16}$$

The probability density function of a conserved scalar determines the state of mixedness of the fluid (Bilger, 1989). The values obtained in equation 5.15 are preprocessed and stored in look up tables, saving computational time. The look-up table will be used in Fluent to determine mean species mass fractions, density, and temperature from the values of mixture fraction $(\bar{f})$, mixture fraction variance $(\overline{f'^2})$ and possibly enthalpy $(\bar{H})$ and scalar dissipation $(\bar{\chi})$ as they are computed during the FLUENT calculation of the reacting flow. In the flamelet concept, only the PDF of the conserved scalar, as such the mixture fraction Z , is necessary. Indeed, in FLUENT, Z and χ_{st} are assumed to be statistically independent and as a result the joint PDF can be written $p(Z)p(\chi_{st})$. Transport equations for Z' and $\overline{Z'^2}$ are solved in FLUENT in order to determine $p(Z)$ and a β PDF function is assumed for $p(Z)$. Two popular forms of the assumed PDF are the normalized beta function (Liew, 1983) and the clipped Gaussian (Lockwood and Naguib, 1975). The beta function is more attractive since it is naturally bounded between 0 and 1 and is simply defined by its mean mixture fraction and mixture fraction variance. Since Bilger (1988) found that both forms of the PDF gave good agreement with the experimental results, it seems more appropriate to use the beta function. Girimaji (1991) has also demonstrated that the β -PDF is appropriate in capturing the nature of the relevant mixing processes in non-premixed combustion.

The β -PDF is defined as a function of the mean mixture fraction and mixture fraction variance and written in the following manner:

$$p(Z) = \frac{Z^{\alpha-1} (1-Z)^{\beta-1}}{\int Z^{\alpha-1} (1-Z)^{\beta-1} dZ} \quad \text{Equation 5. 17}$$

where the exponents α and β are:

$$\alpha = \bar{Z} \left[\frac{\bar{Z}(1-\bar{Z})}{Z'^2} - 1 \right] \quad \text{Equation 5. 18}$$

$$\beta = (1-\bar{Z}) \left[\frac{\bar{Z}(1-\bar{Z})}{Z'^2} - 1 \right] \quad \text{Equation 5. 19}$$

Fluctuations in χ_{st} are ignored and the PDF of the scalar dissipation rate is a delta function such that $p(\chi_{st}) = \delta(\chi - \bar{\chi})$. According to Liew et al. (1984a), χ_{st} is defined as a function of the turbulent field and the mixture fraction variance:

$$\chi_{st} = \frac{C_x \varepsilon \overline{f'^2}}{k} \quad \text{Equation 5. 20}$$

Where C_x has a default value of 2.0 and expresses the time scale ratio for dissipation of scalar and velocity fluctuations. This value is cemented in FLUENT and therefore will remain unchanged throughout this investigation.

The flamelets generated with CHEMKIN are adiabatic, since radiative heat transfer and soot modelling was not included in the simulations, and the introduction of enthalpy loss is not coupled to the composition. However, the mean temperature and density PDF tables have an additional dimension of mean enthalpy. To avoid complications due to the prohibitive cost of modelling flamelets with a range of enthalpies, FLUENT have made some simplifications. Heat loss/gain is assumed to be negligible for species mass fraction, except for the case $\chi_{st}=0$ where the species mass fraction is computed as a function of the mixture fraction, mixture fraction variance and enthalpy and the temperatures are calculated from equation 5.21 for a range of mean enthalpy gain/loss $\bar{H}$.

$$H = \sum_i Y_i H_i \quad \text{Equation 5. 21}$$

5.6 *Flamelet generation using CHEMKIN*

The flamelet libraries can be generated in two different manners, either by carrying out experimental measurements or through the use of a computer code. However, it is generally impractical to make sufficient detailed measurements to satisfactorily define the flamelet though this may be appropriate in relation to validation. Consequently, the flamelet libraries have been generated with CHEMKIN, where the species mass fraction and temperature are to be defined as a function of the mixture fraction and the strain rate.

In order to represent the full range of strain encountered in the turbulent flow, a certain number of flamelet are generated which account for the varying strain, and these flamelets are labelled flamelet libraries. In the early development of the flamelet methodology, flamelet libraries were constructed using experimental data or an opposed laminar diffusion flame calculation (Peters, 1984b; Liew et al. 1984b). As explained in section 2.6 in the Literature Review, a common laminar flame used to represent a flamelet in a turbulent flow is the counterflow diffusion flame as illustrated figure 2.14. This geometry consists of opposed, axisymmetric fuel and oxidiser jets and has been demonstrated to be suitable for the fundamental study of diffusion flames since it offers great flexibility in varying the experimental boundary conditions with a well defined flow field using a simple configuration. Indeed, using this kind of configuration, the flames are flat, allowing for a detailed study of the flame structure and its chemistry. As the distance between the jets is decreased and/or the velocity of the jets increased, the flame is strained and increasingly departs from chemical equilibrium until it is eventually extinguished. CHEMKIN uses an Opposed-flow Diffusion Flames model, or OPPDIF, which uses the conservation equations and assumption that govern the behaviour of opposed flow flames, reducing the three-dimensional nature of the flow to a one-dimensional (axial) dependence of the governing equations. For the Opposed-flow flame model, a steady-state solution is computered for either axisymmetric or planar diffusion flames between two opposing nozzles.

The OPPDIF model predicts the species mole and mass fraction and the flame temperature as a function of mixture fraction. More data such as velocity profiles are

generated with OPPDIF but these information are sufficient to generate the flamelet libraries. The OPPDIF flame model used in CHEMKIN is derived from a model that was originally developed by Kee et al. (1988) for premixed opposed flow flames. In order to run a CHEMKIN simulation, data are required in the form of chemistry sets such as:

- a file containing a description of the reactions occurring in the gas phase
- a file containing thermodynamic data for the different chemical species which take part in the reaction mechanism
- a file containing the gas phase transport data

Thermodynamic data are needed for all chemical species included in a reaction mechanism. The thermodynamic data are needed to calculate reaction rates for reverse reactions and heats of reaction, used to solve the energy equation. In CHEMKIN, thermodynamic data are generally provided in the form of a therm.dat file, which can be found from various sources (Kee et al. 1987b; Chase and Lide, 1985; NIST, 2005; Burcat, ; NASA, 2005). If the desired thermochemical data are not available in the literature, such data can be calculated through various means. For example, Benson proposed group additivity methods which are a systematic way of extrapolating known species to chemically related species that have not been studied experimentally. Eventually the user can refer to known species to estimate thermodynamic parameters, but this will lead to large uncertainties (Reaction Design, 2005).

The reaction mechanism lists the chemical reaction and rate parameters for the molecule of interest. Detailed reaction mechanisms are widely used to describe the fragment of a reacting molecule into products, through a large number of elementary steps. Quite often, reaction mechanisms are built from a previously developed mechanism. Reaction mechanisms are generally found in the literature but there are a number of standard sources of chemical kinetics data for individual reactions such as the well known NIST chemical database (2000) or a chemical kinetics data written by Kondratiev (1972). Each reaction has to be validated against experimental results but reaction mechanisms are known to be valid only for a set range of operating conditions.

In certain cases, where the transport is assumed to be infinitely fast within the section of the gas considered, such as for perfectly stirred reactors, the effect of transport properties can be neglected whereas in many other cases, transport data are of critical importance such as for diffusion flames and hence play a key role in the burning of fuel droplets (Liñán and Williams, 1993). When transport data are involved, increased computational time is to be expected due to the increased difficulty of resolving spatial transport (Westbrook and Dryer, 1984). In addition to the increased computational cost, additional physical data are required. In fact, the term “diffusive transport processes” refers to molecular diffusion, thermal conductivity, viscosity and thermal diffusion. Transport processes are crucial to the description of flame ignition since they are the mechanism by which heat and reactive species are transported ahead to the unburned gas (Oran and Boris, 1981).

CHEMKIN provides a transport database of over 200 species provided in the form `tran.dat`, but the list of species is not exhaustive and some other species transport data are needed for this study. Some data can be found in standard references such as Hirschfelder et al. (1964) and Svehla (1962b). Some of the numbers in the database have been determined by computing “best fits” to experimental measurements of macroscopic transport properties (e.g. viscosity) while in other cases the Lennard-Jones parameters were estimated and all ethanol transport data are listed in Appendix F.

5.6.3 Ethanol flamelets

Methanol has been the most extensively studied of all alcohols but fewer studies of ethanol are available (Norton and Dryer, 1992; Norton, 1990; Norton, 1990). This investigation concerns turbulent ethanol/air diffusion flames. Marinov (1999b) has developed a detailed kinetic model for ethanol oxidation with new rate constant expressions for ethanol decomposition and validated it against a set of experimental data sets obtained under a variety of operating conditions. The modelling study presented by Marinov (1999b) examined ignition delay from shock tubes, laminar flame speeds data from a combustion bomb and a counterflow twin flame, and species profiles from ethanol oxidation in jet-stirred and turbulent flow reactions and good

agreement was found in modelling of those data sets obtained from the five different experimental systems. The data sets considered span the temperature range of 1000-1700 K, a pressure range of 1.0-4.5 atm and an equivalence ratio range of 0.5-2.0.

The present modelling computations were performed using OPPDIF (Lutz et al. 1997) in CHEMKIN 4.0.2, that is capable of modelling combustion between two opposed jets and widely used in the analysis of a steady 1 D counterflow flame. The detailed chemical kinetic model was assembled using reaction sub mechanisms developed previously for hydrogen (Marinov et al. 1995), methane (Marinov et al. 1996), ethylene (Marinov and Malte, 1995), ethane (Marinov et al. 1996), and propane (Marinov et al. 1997) oxidation mechanisms. The compiled ethanol oxidation mechanism consists of 56 species and 351 reversible reactions.

Transport properties were obtained from the Sandia CHEMKIN transport database (Kee et al. 1986). Transport properties for species not found in the database were estimated using the method of Norton and Dryer (1992) or following the method outlined by Svehla (1962a) and listed in Appendix F.

The thermodynamic properties for the species used in this study were primarily obtained from the CHEMKIN thermodynamic database developed by Kee et al. (1987a) and Burcat and McBride (1993). Thermodynamic properties for those species not found in the database were estimated by group additivity (Ritter and Bozzelli, 1991). These estimated specific heats, standard state enthalpies, and standard state entropies data were fitted for the 300-1500 K range and extrapolated to 5000 K using the Harmonic Oscillator Equation and Exponential Function methods of THERM (Ritter and Bozzelli, 1991). The THERM program generates the fourteen polynomial coefficients as used in the NASA Chemical Equilibrium program.

The configuration used for this study is the diffusion flame stabilized between counterflowing streams of prevaporized ethanol and air. Numerical calculations were performed for different values of strain rate to determine the structure and determine the extinction strain rate of ethanol-air diffusion flames using the detailed reaction mechanism presented by Marinov (1999a). The calculations were performed at a value of the thermodynamic pressure equal to 1, 2, 3, 5 and 10 atmospheres and

emphasis was placed on the diffusion flames response to strain rate variations. Temperature and concentration profiles of the main species were plotted as a function of the mixture fraction. Extinction limits were also predicted. The present study is motivated by a need to use this detailed chemical kinetic mechanism that can be used to generate a flamelet library, which will be then exported into prepdf, where the PDF function of the flamelet will be generated and incorporated into the computational fluid dynamics code.

Gutheil (2001) carried out a numerical study of structure of laminar ethanol-air spray flames in a counterflow configuration and the results show that ethanol-air flames are more stable than methanol-air spray flames, up to extinction. The extinction strain rate is 1375 s^{-1} with a maximum flame temperature of 1983 K compared with 1225 s^{-1} and 1962 K for methanol. Gutheil (2001) mentioned that the principal differences in properties between the fuels is the higher boiling point for ethanol (351.4 K) compared with methanol (337.7 K), the latent heat of vaporization (13 % lower for ethanol), the heat of combustion (15 % higher for ethanol) and the stoichiometry that requires almost 40% more liquid mass to be vaporized for methanol compared with ethanol for stoichiometric mixture since the stoichiometric $\text{AFR}_{\text{methanol}} = 6.46$ and stoichiometric $\text{AFR}_{\text{ethanol}} = 9$. A survey of differences in fuel properties is given by Gutheil (2001). The higher liquid mass of methanol causes the reduced flame temperature of methanol flames compared with ethanol flames. However, this study relates to spray flames and not prevaporized fuel like the ones considered in the current study.

5.6.3.1 Flamelet data

In the present configuration, a fuel stream made up of prevaporized ethanol at boiling point is injected from one end and an oxidizer stream made up of undiluted air (mole fraction $X_{\text{N}_2} = 0.79$ and $X_{\text{O}_2} = 0.21$) is injected from the other end. These jets flow into the mixing layer. The value of the strain rate, on the oxidizer side of the stagnation plane is presumed to be given by Seshadri and Williams (1978):

$$a = \frac{2V_2}{L} \left(1 + \frac{|V_1| \sqrt{\rho_1}}{|V_2| \sqrt{\rho_2}} \right)$$

Equation 5. 22

The temperature of the ambient oxidizing gas stream is $T_\infty = 300\text{K}$. The mass flux, temperature and species mass fraction at the fuel jet are given as are the temperature and species mass fraction on the air side. The fuel temperature corresponds to the boiling point of ethanol at different pressures and is shown in the following table based on the values obtained in the Fuel Properties chapter, in section 3.2.1 using the Antoine equation. All these information, fuel and oxidiser temperature, composition, as well as the fuel and oxidizer velocities have been used as input into CHEMKIN. The output of the code gives the species mole fraction as a function of distance, which are converted into mixture fraction.

	1 bar	2 bar	3 bar	5 bar	10 bar
Boiling point (K)	351	371	384	399	427

Table 5.1 Boiling point of ethanol at different pressures

It is convenient to express the flame position in terms of the mixture fraction Z , a conserved scalar quantity which is defined as $Z = (Y_i - Y_{i,o}) / (Y_i - Y_{i,f})$ (Peters, 1991), where Y_i represents the mass fraction of the element i at any location in the flow field. The subscript o denotes the value at the oxidizer stream inlet and the subscript f denotes the value at the fuel stream inlet. From this definition, $Z = 0$ in the oxidiser stream and $Z = 1$ in the fuel stream.

The comparison for different strain rates are conducted in both a shifted flame coordinate and the mixture fraction coordinate. Figure 5.2 shows the predicted temperature as a function of mixture fraction in an opposed-flow diffusion flame with a strain rate varying from 50 to 492 s^{-1} . The flamelet library consists of laminar diffusion flames for the following values of strain rate: $a = 50 \text{ s}^{-1}$, 103 s^{-1} , 192 s^{-1} , 242 s^{-1} , 342 s^{-1} and 492 s^{-1} . The local instantaneous value of the scalar dissipation in the turbulent flow selects each one flamelet from the ensemble of all possible flamelets. The local values of temperature and species mass fraction are found by linear interpolation between the strain rate values. The results of the numerical simulation

show that as the strain rate is increased, the flame moves toward extinction. To determine the extinction strain rate of the ethanol-air diffusion flames, calculations were performed at a number of values of the strain rate with increasing values of the oxidiser and fuel velocity, until no numerical solution was obtained for the set of equations. No solution was obtained for values of a greater than 492 s^{-1} and as a consequence it is estimated that extinction occurs at 500 s^{-1} for this system at 1 atm. Unfortunately there is no experimental data or numerical results available for ethanol in the literature to compare with the results obtained. However, Seshadri et al. (1989) performed numerical calculations to determine the extinction strain rate of diffusion flames stabilised between counterflowing streams of methanol and air and they obtained an extinction strain rate of 521 s^{-1} . But there is considerable uncertainty in the result since an extinction strain rate of 168 s^{-1} was obtained when a slightly modified methanol mechanism is used. Puri and Seshadri (1986) obtained values at extinction for propane C_3H_8 , which has a close molecular weight compared to ethanol ($\text{MW}_{\text{C}_2\text{H}_5\text{OH}} = 46 \text{ g/mol}$ and $\text{MW}_{\text{C}_3\text{H}_8} = 44 \text{ g/mol}$) of 305 s^{-1} . Based on the values obtained for different fuels and in the absence of any experimental data for ethanol diffusion flames, the extinction strain rate obtained for ethanol looks quite plausible.

For each of the ethanol flames, the temperature tends to decrease as the strain rate is increased. The peak temperature falls off nearly linearly from 1940 K to 1793K respectively at 50 s^{-1} and 492 s^{-1} before the flame is suddenly extinguished. However, it would have been expected that the temperature falls off to a lower value before being extinguished. It may be linked to CHEMKIN numerical failure to predict high temperature gradients close to extinction. The peak value of the temperature profiles progressively decreases with increasing value of strain rate until reaching the critical value of extinction strain rate. Critical conditions of extinction are therefore predicted to be at around 500 s^{-1} .

Low strain rates correspond to conditions where the flame is close to equilibrium. The stoichiometric mixture fraction is estimated at around 0.11. Beyond this value, the mixture is estimated to be fuel rich, and fuel lean below.

Figure 5.3 compares the temperature profiles for the different strain rates as a function of the distance from the oxidizer nozzle. As illustrated figure 5.3, the flame is shifting towards the oxidiser side as the strain rate is increased. From 103 s^{-1} to 146 s^{-1} , the flame is strongly shifting by 27 mm towards the oxidiser side and then there is a regular 13 mm shift as the strain rate is increased by 50 s^{-1} from 192 s^{-1} . The figure clearly shows that the temperature profile becomes thinner with increasing strain rate and they overlap with each other and the flame shifts towards the oxidizer side.

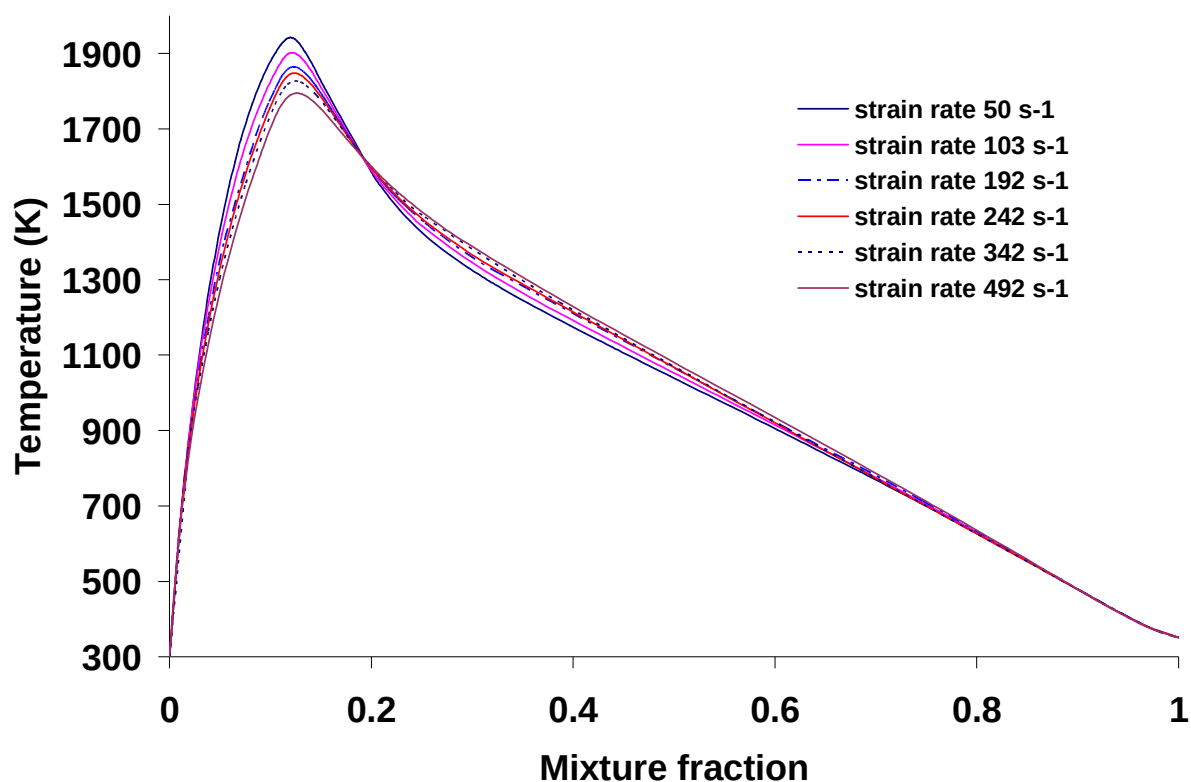


Figure 5. 2 Ethanol temperature as a function of mixture fraction at different strain rates

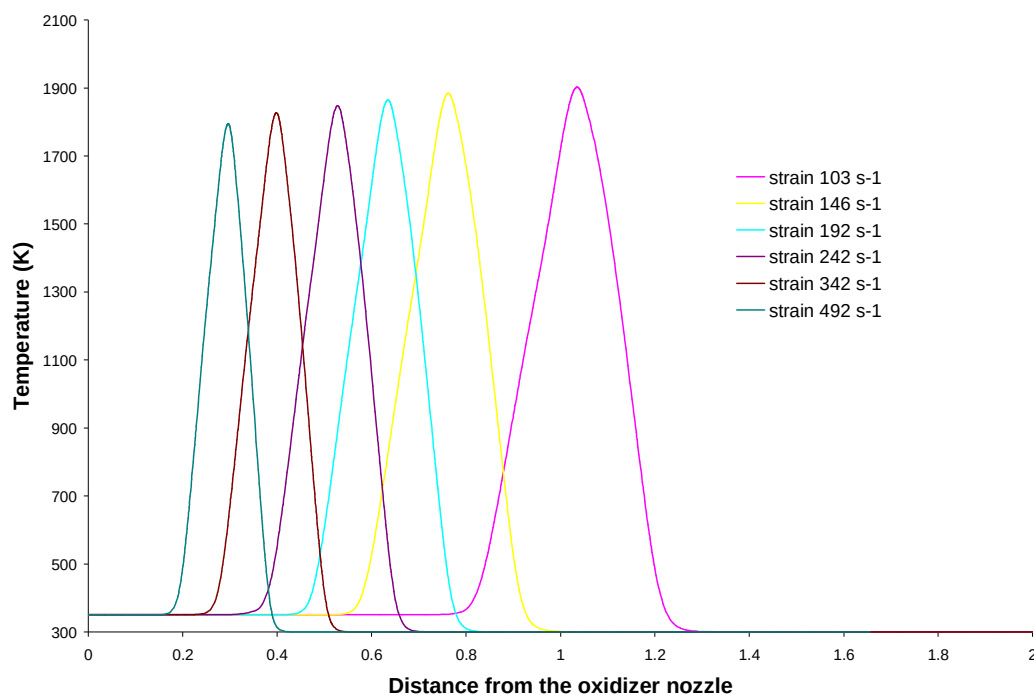


Figure 5. 3 Ethanol flame position as a function of strain rate

Figure 5.4 and 5.5 show plots of major species mole fraction versus mixture fraction. Figure 5.4 shows that the nitrogen concentration decreases monotonically towards the fuel side. Figure 5.5 shows that CO_2 and H_2O , which are the final combustion products, as well as CO , which has considerable concentration among the intermediate products, have their maximum concentration in the fuel side of the flame zone. The concentration of carbon dioxide decreases rapidly on both fuel and air side of the flame. CO tends to peak slightly further to the fuel side than CO_2 . Carbon monoxide exist on the fuel side as well as on the air side and its concentration decreases rapidly on both sides. CO_2 and CO concentration decrease toward both fuel and air sides of the flame, but these species exist over a wide region of the fuel and air sides. Hydrogen concentration is maximum on the fuel side. Hence CO , H_2O and H_2 peak mass fraction occur on the rich side of stoichiometry.

Figure 5.6 to 5.8 show that the concentration of CO_2 , H_2 and OH decrease with increasing value of the strain rate but there is an increase in CO mass fraction seen figure 5.9. In fact, as the strain rate is increased the flame is further from equilibrium.

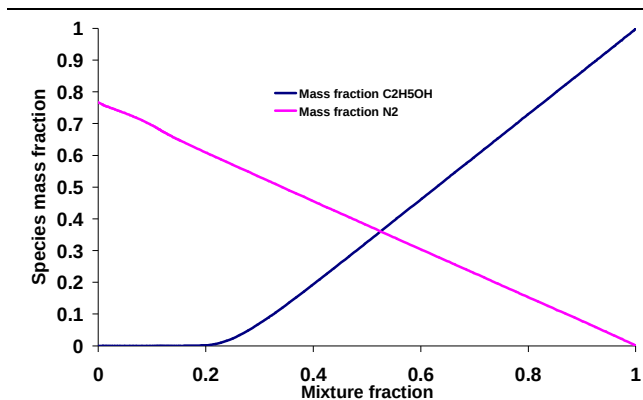


Figure 5.4 Computed values for profiles of $\text{C}_2\text{H}_5\text{OH}$ and N_2

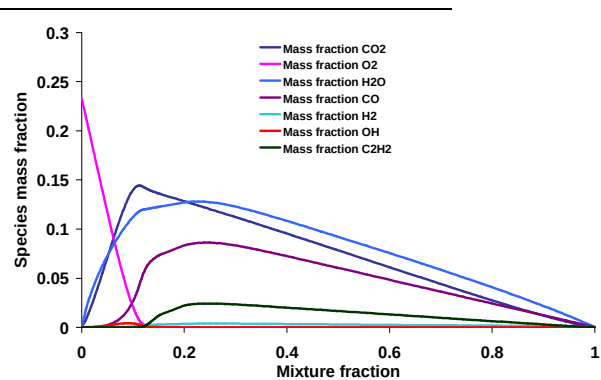


Figure 5.5 Computed values for profiles of CO_2 , O_2 , H_2O , CO , H_2 , OH , C_2H_2

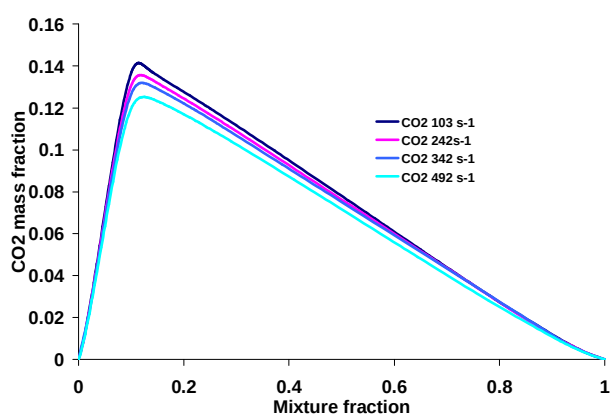


Figure 5.6 CO_2 mass fraction as a function of strain rate

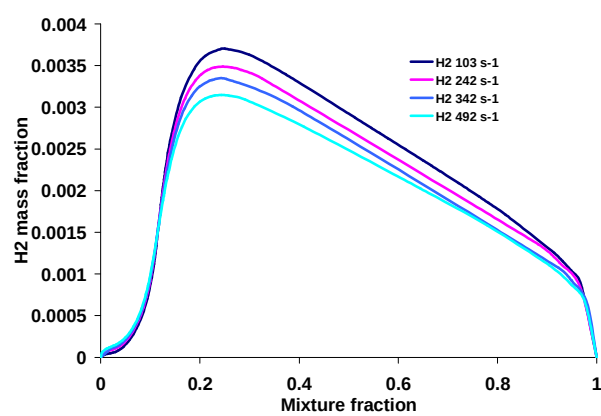


Figure 5.7 H_2 mass fraction as a function of strain rate

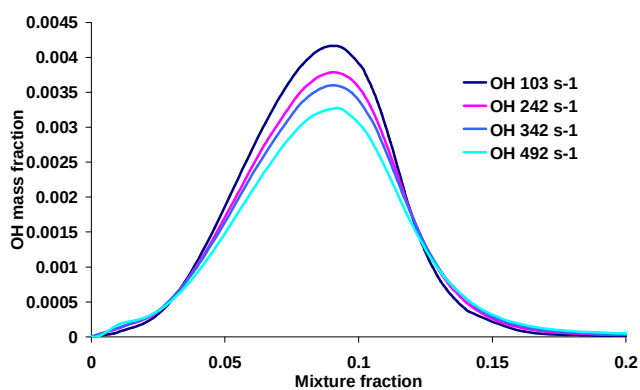


Figure 5.8 OH mass fraction as a function of strain rate

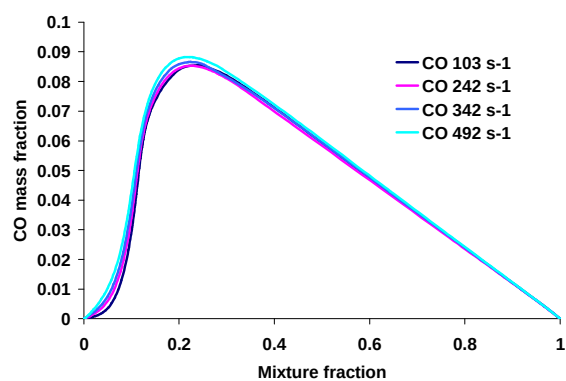


Figure 5.9 CO mass fraction as a function of strain rate

5.6.3.2 At higher pressures

One method to improve overall thermal efficiency in gas turbine is to increase operating pressures, hence many practical combustion processes takes place under such pressures and the current investigation must account for this effect on the flame behaviour.

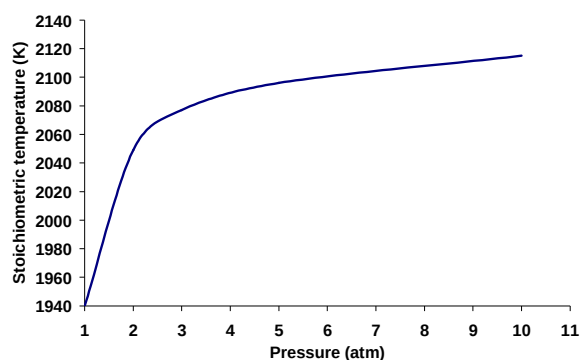


Figure 5.10 Effect of pressure on stoichiometric temperature

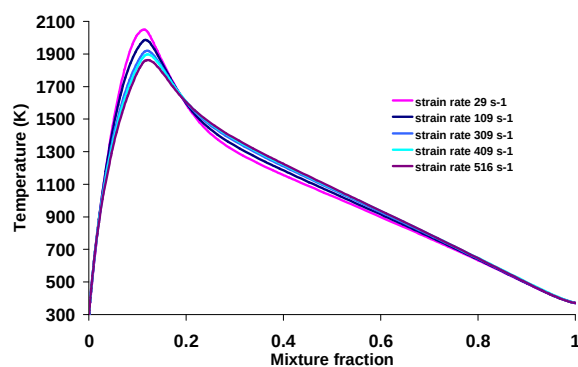


Figure 5.11 Temperature versus mixture fraction at 2 atm

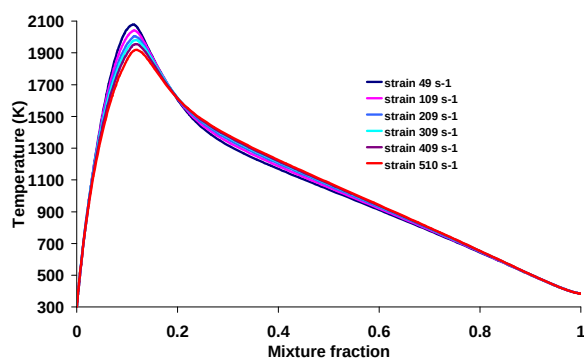


Figure 5.12 Temperature versus mixture fraction at 3 atm

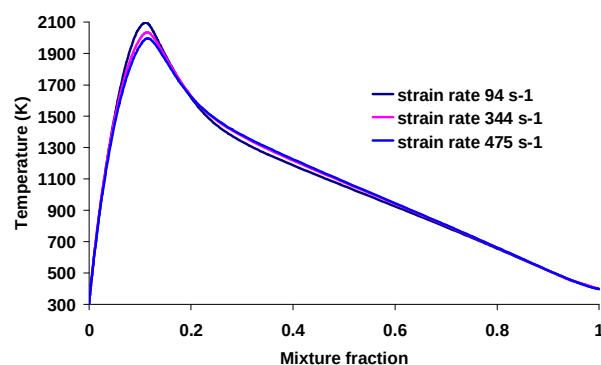


Figure 5.13 Temperature versus mixture fraction at 5 atm

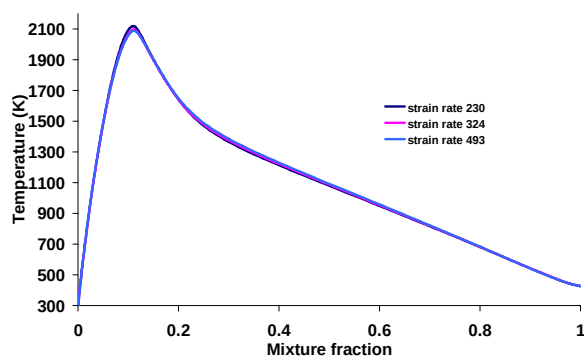


Figure 5.14 Temperature versus mixture fraction at 10 atm

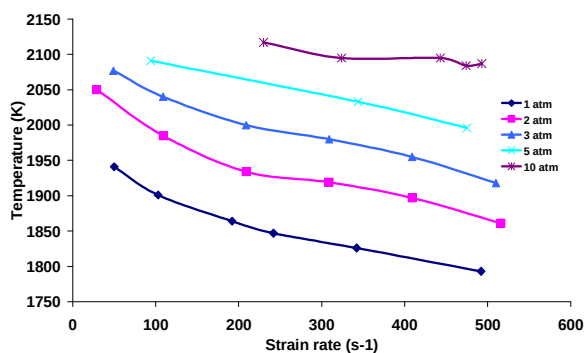


Figure 5.15 Temperature versus extinction strain rate at 1,2,3, 5 and 10 atm

Increase in pressure results in a continuous increase in the stoichiometric temperature from a value of 1940 K at 1 atm to 2115 K at 10 atm as illustrated figure 5.10. Temperature profiles versus mixture fraction at 2,3, 5 and 10 atm are presented from figure 5.11 to figure 5.14. Effects of pressure and strain rate on flame structure, extinction are presented in this section. Extinction characteristics at high pressure are different from that at low pressures. In the literature, the extinction strain rate increases linearly with pressure for methane and hydrogen (Sohn et al. 2002; Sohn and Chung, 2000). With hydrogen flames Sohn et al. (Sohn and Chung, 2000; Sohn and Chung, 1998) showed that the extinction strain rate increases at low pressure (below 1.5 atm) , decreases at moderate pressures and increase again at high pressures (above 10 atm). However, the current results demonstrate that the extinction limits have not increased as the oxidiser temperature is raised, as illustrated in figure 5.15, for the range 1 to 10 atm but have rather remained in the same range as seen table 5.1.

Pressure	1 atm	2 atm	3 atm	5 atm	10 atm
Extinction strain rate (s^{-1})	492	516	510	475	493

Table 5. 1 Extinction strain rate as a function of pressure

The structure of counterflow diffusion flames burning ethanol has been characterised using CHEMKIN, and the calculated profiles of temperature and species mixture fraction were determined with the help of detailed chemical kinetics and transport. This configuration provides a convenient and well-characterised combustion environment because of its one dimensionality. All the flamelet data destined to be exported into FLUENT are written in Appendix H.

5.6.4 Methylbutanoate flamelet

As mentioned in the literature review in Section 2.7, the methylbutanoate reaction mechanism developed by Fisher et al. (2000) has been chosen as a surrogate for biodiesel fuel.

Thermodynamic properties and detailed chemical kinetic models have been developed for the combustion of methyl butanoate, a model compound for biodiesel fuels. Bond additivity methods and rules for estimating kinetic parameters were adopted from hydrocarbon combustion and extended.

Methyl butanoate was chosen as a surrogate molecule for the larger methyl esters, in order to obtain a reaction of manageable size. However, some of the shortcomings of the methylbutanoate reaction mechanism are that the operating conditions under which the simulations are run range from 520 to 740 K and 13 to 54 kPa. In fact, the resulting mechanisms have been tested against the limited combustion data available in the literature, which was obtained at low temperature and subatmospheric conditions.

5.6.4.1 Flamelet data

The temperature of the ambient oxidizing gas stream is $T_{\infty} = 420\text{K}$. The fuel temperature corresponds to the boiling point of methylbutanoate at different pressures and is shown in table 5.2.

	1 bar	2 bar	3 bar	5 bar	10 bar
Boiling point (K)	375.9	401	417	440	475

Table 5. 2 Boiling point of methylbutanoate at different pressures

The comparison for different strain rates are conducted in both a shifted, flame coordinate and the mixture fraction coordinate. The following figure shows the predicted temperature as a function of mixture fraction in an opposed-flow diffusion flame with a strain rate varying from 15 to 550 s^{-1} . The flamelet library consists of laminar diffusion flames for the following values of strain rate: $a = 15 \text{ s}^{-1}$, 100 s^{-1} , 200 s^{-1} , 330 s^{-1} , 450 s^{-1} and 550 s^{-1} . No solution was obtained for values of a greater than 550 s^{-1} and as a consequence it is estimated that extinction occurs immediately beyond this value at 1 atmosphere. For each of these flames, the temperature tends to decrease as the strain rate is increased. The peak temperature falls off nearly linearly from 1940 K to 1793K respectively at 50 s^{-1} and 550 s^{-1} before the flame is suddenly

extinguished. The peak value of the temperature profiles progressively decreases with increasing value of strain rate until reaching the critical value of extinction strain rate. The variation of the flame temperature with strain rate is shown in figure 5.16. The stoichiometric mixture fraction is estimated at around 0.12. Unfortunately, no data has been found in the literature that can be a basis for comparison with the numerical results found with CHEMKIN.

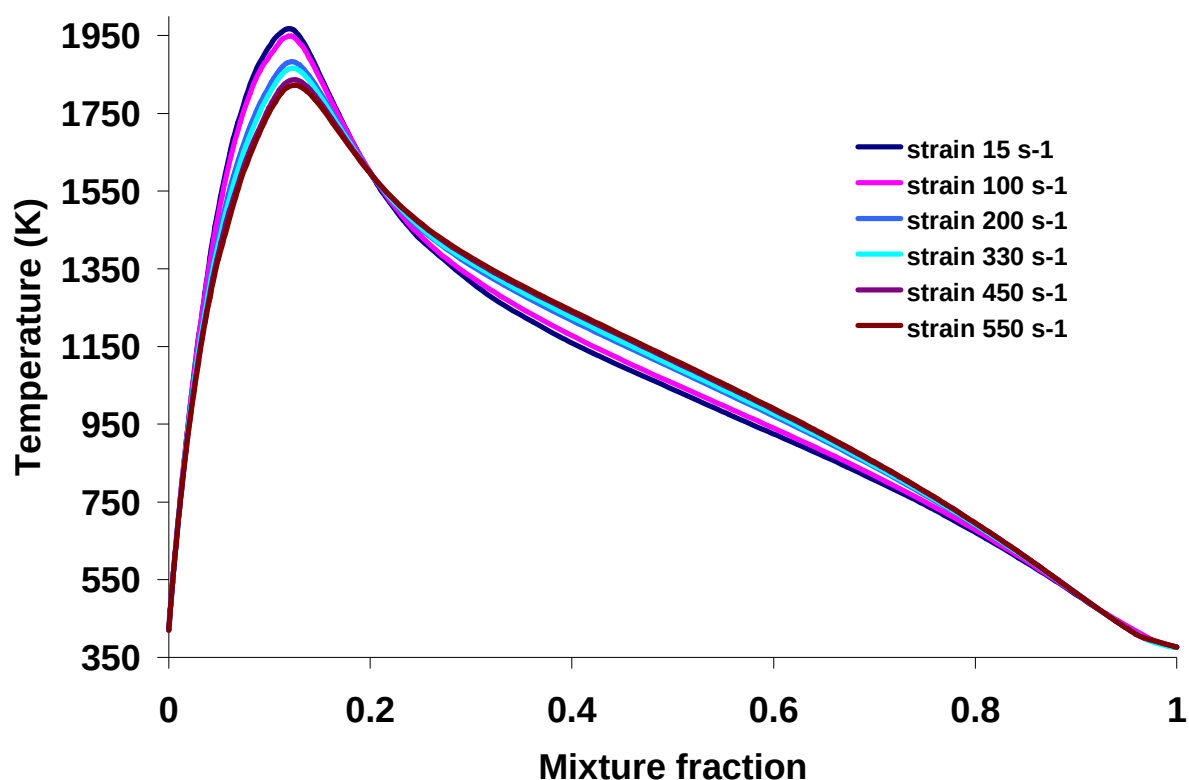


Figure 5. 16 Temperature versus mixture fraction for methylbutanoate

5.7 Spray Modelling

5.7.1 Eulerian/Lagrangian representation

In this study, the gas phase properties are computed by an Eulerian approach, while the liquid phase properties are obtained by a Lagrangian approach and the discrete phase modelling (DPM) approach is used to model the vaporization and boiling of liquid droplets.

FLUENT offers two types of two-phase flow approach, based on the Eulerian-Eulerian and the Eulerian-Lagrangian approaches. In an Eulerian-Lagrangian formulation also called Lagrangian, the particles are treated as discrete entities. A large number of physical droplets are grouped in FLUENT as computational droplet or parcels, where a certain number of droplets share the same characteristics such as size, mass, and temperature. The physical droplets are so numerous that the simulation would be too expensive to run as it involves determining whether liquid or gas is present at every point and changing the governing equations according to the phase. The time dependent, mass, momentum, energy and species conservation equation, in principle can be applied to describe the flow and spray combustion. Individual trajectories are predicted as a result of the forces on the droplet from the existing solution of the gaseous phase equations. Lagrangian techniques are applied to dilute flows and are characterised by a well defined dispersed phase (e.g. spherical) and relatively small locally dispersed phase volume fraction ($<10\text{-}12\%$). For the current study, the maximum dispersed volume fraction reached a maximum of 3.2% for biodiesel at 1 atm, based on a total air flow rate of 15 g/s (3 g/s primary air flow and 12 g/s secondary air flow) and a fuel flow rate of 0.75 g/s . As a result, droplet interactions are assumed to be negligible with the DPM approach and collisions are infrequent and heat transfer, mass transfer and drag coefficients are not directly influenced by adjacent droplets. However, the mass loading may exceed 12% and the dispersed phase flow rate might be greater than that of the continuous phase.

On the other hand, Eulerian formulations treat the particles as a continuous phase, intermixed with the fluid phase. Such an approach is usually applied to dense flows, ie. flows in which the particle motion is controlled principally by collisions between particles and where dispersed-phase volume fractions exceed 10% , which is not the case in this study. Moreover the Eulerian needs an extremely fine mesh – unlike for the Lagrangian method- at the interface between both phases when the droplet is small. Handling of the droplet evaporation using an Eulerian method is also more complex than with the Lagrangian approach. Consequently the model in this investigation describes a spray where the gas phase is formulated in Eulerian coordinates and the spray is described through Lagrangian equations with two-way coupling between phases.

5.7.2 Turbulent dispersion of particles

In FLUENT, droplet dispersion due to turbulence can be treated either through the stochastic model or with the cloud model. The particle cloud model tracks the statistical evolution of a cloud of particles about a mean trajectory. However, the cloud model is not available for parallel processing, therefore this model cannot be used in this study. Hence the stochastic approach has been chosen for this investigation. In the stochastic tracking approach, the turbulent dispersion of particles is predicted using the instantaneous fluid velocity for the droplet trajectory equation integration. The instantaneous fluid velocity is defined by:

$$u = \bar{u} + u'(t)$$

Equation 5. 23

By computing the trajectory in this manner for a sufficient number of representative particles, the random effects of turbulence on the particle dispersion may be accounted for. Generally a number of tries equal to 5 was specified so that the trajectories can be computed five times in order to get a good statistical representation of the spread of droplet due to turbulence. Each trajectory calculation includes a new stochastic representation of the turbulent contributions to the trajectory equation. Increasing the number of tries would lead to an increase in the number of droplet which would improve the statistical accuracy of the spray computation, but it would require a significant increase in the computational time, which is one of the main drawbacks highlighted using a Lagrangian method in the Literature review. Hence the maximum number of parcels and tries had to be limited. The total number of injection streams tracked for the surface injection will be equal to the number of diameters in each multiplied by the number of tries and the total number of injections. To see the sensitivity of the solution to the number of tries, a simulation was carried out with 10 tries but this resulted in more than double computational time while the numerical predictions remained largely unchanged, therefore it was decided that setting to 4 the number of tries was sufficient. Typically a number of tries comprised between 3 and 5 is judged acceptable.

In FLUENT, the Discrete Random Walk (DRW) model is used. The DRW follows Gosman and Ioannides (1983) and assumes that the droplet interacts with the gas phase over a succession of turbulent eddies.

5.7.3 Particle force balance

The force balance is written in the Lagrangian reference frame. The force balance is represented by the particle inertia and the forces acting on the particle. As a result, FLUENT predicts the trajectory of a discrete phase particle in the following manner:

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad \text{Equation 5. 24}$$

where F_x is an additional acceleration (force/unit particle mass) term, $F_D(u - u_p)$ represent the drag force per unit particle mass and

$$F_D = \frac{18\mu}{\rho d_p^2} \frac{C_D \text{Re}}{24} \quad \text{Equation 5. 25}$$

Where μ is the molecular fluid viscosity, ρ is the gas density, d_p is the particle diameter, ρ_p the particle density, u the gas velocity and u_p the particle velocity. Re is the relative Reynolds number defined as follow:

$$\text{Re} = \frac{\rho(u - u_p)d_p}{\mu} \quad \text{Equation 5. 26}$$

The Weber number defined as

$$\text{We} = \frac{\rho D |u - u_d|^2}{\sigma} \quad \text{Equation 5. 27}$$

will remain small as shown figure 4.19 therefore the droplet will remain spherical throughout the domain hence, the drag coefficient is described as:

$$C_d = \begin{cases} 0.424 & \text{Re} > 1000 \\ \frac{24}{\text{Re}} \left(1 + \frac{1}{6} \text{Re}^{2/3} \right) & \text{Re} \leq 1000 \end{cases} \quad \text{Equation 5. 28}$$

5.7.4 Coupling between the gas and the discrete phase

In order to solve the discrete phase model, the following steps have to be followed:

- solve the continuous phase prior to introduction of the discrete phase
- set up the discrete phase properties
- introduce the discrete phase by calculating the particle trajectories for each discrete phase injection
- recalculate the continuous phase flow, using the interphase exchange of momentum, heat, and mass determined during the previous particle calculation
- recalculate the discrete phase trajectories in the modified continuous phase flow field

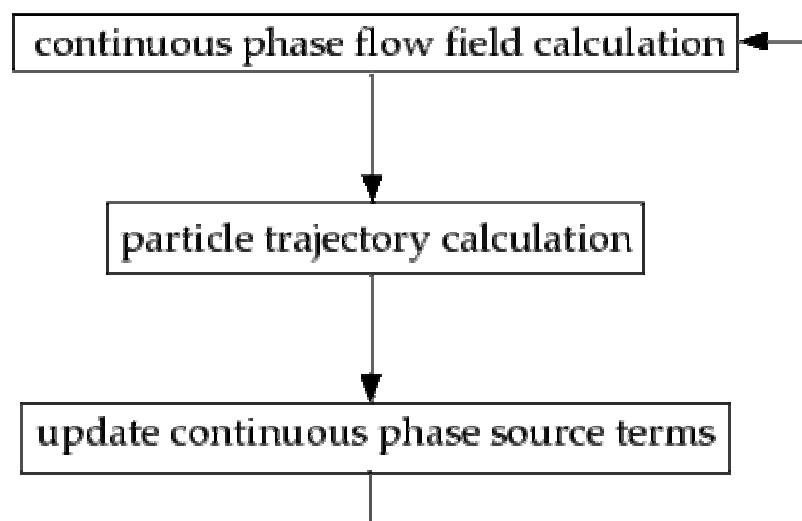


Figure 5. 17 Coupled discrete phase calculation (FLUENT, 2004)

A typical coupled calculation procedure is illustrated figure 5.17. While the particle travels throughout the domain, FLUENT keeps track of the heat, mass and momentum lost by the particles and which are in turn incorporated into the gas phase calculation. The interaction between the continuous and the dispersed phase is taken into account by coupling both phases. Indeed, the dispersed phase can exchange momentum, heat and mass with the gaseous phase and for each discrete-phase iteration, FLUENT computes the particle/droplet trajectories and updates the interphase exchange of

momentum, heat, and mass in each control volume. Hence the impact of the droplets (discrete phase) on the gas (continuous) phase is monitored as well as the impact of the gas phase on the droplets. The discrete phase is solved every 20 gas-phase iterations and again the gas phase run for 20 iterations before the new calculated particle sources are introduced in the domain, until convergence is obtained. This way the spray solution is updated, and the effect of heat transfer of the spray towards the gas phase is regularly monitored until reaching a stable solution, which at this stage is supposed to remain unchanged with each additional calculation. Reducing the number of continuous phase iteration per DPM iteration would make the solution less stable. In general, 400 external iterations were performed, hence computing for at least 8000 iterations. Convergence is reached when changes in solution variables from one iteration to the next is negligible and residuals are quite helpful in monitoring convergence. Generally, a decrease in residuals by at least three orders of magnitude indicates convergence. A relative error of 10^{-5} is used as the criterion for convergence for the continuity, velocity and turbulence terms and residuals of 10^{-6} are required for the energy equation. Rather than only relying on residuals, it is possible to get a complementary indication of convergence by checking the mass and energy balance, the energy balance being available only for cases with combustion from the particles to the gas phase, like encountered in this study. To ensure convergence, the DPM mass and enthalpy source should be algebraically equal respectively to the mass and energy imbalance in the Report-> Flux panel. The numerical model is applied to predict the flow properties of the pressure rig.

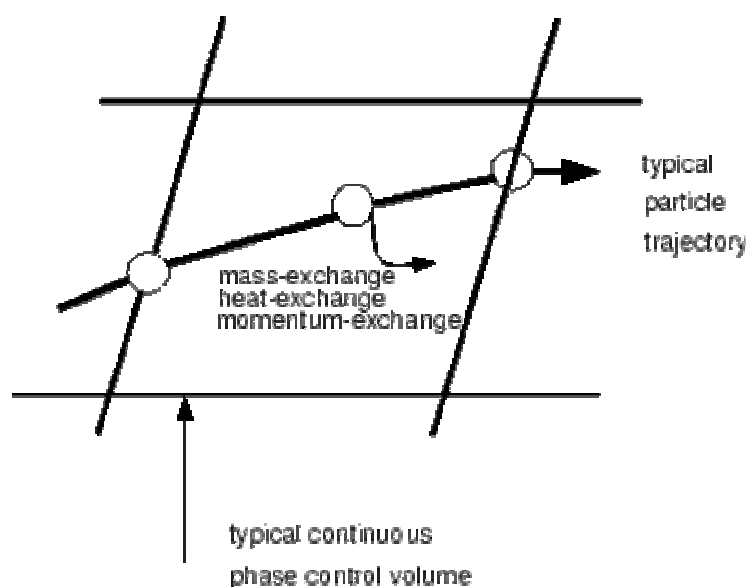


Figure 5. 18 Heat, momentum and mass transfer between the discrete phase and the continuous phase throughout the domain.(FLUENT, 2004)

The momentum transfer in FLUENT from the continuous phase to the discrete phase is calculated as the particle passes through the control volume in the following manner:

$$F = \sum \left(\frac{18\mu}{\rho d_p^2} \frac{C_D \text{Re}}{24} (u - u_p) + F_{\text{other}} \right) \dot{m} \Delta t \quad \text{Equation 5. 29}$$

The heat transfer from the continuous phase to the discrete phase is computed by analyzing the energy change of the particle as it passes through the control volume:

$$Q = \left[\frac{\overline{m_p}}{m_{p,0}} C_p \Delta T_p + \frac{\Delta m_p}{m_{p,0}} \left(-h_{fg} + \int_{T_{ref}}^{T_p} c_{p,i} dT \right) \right] \dot{m}_{p,0} \quad \text{Equation 5. 30}$$

The mass exchange from the continuous phase to the discrete phase is computed by examining the mass loss as the particle passes through the control volume:

$$M = \frac{\Delta m_p}{m_{p,0}} \dot{m}_{p,0} \quad \text{Equation 5. 31}$$

5.7.5 Under-relaxation of the interphase exchange terms

The interphase exchange of momentum, heat and mass is under relaxed during the discrete phase calculation as follows:

$$F_{\text{new}} = F_{\text{old}} + \alpha (F_{\text{calculated}} - F_{\text{old}}) \quad \text{Equation 5. 32}$$

$$Q_{\text{new}} = Q_{\text{old}} + \alpha (Q_{\text{calculated}} - Q_{\text{old}}) \quad \text{Equation 5. 33}$$

$$M_{\text{new}} = M_{\text{old}} + \alpha (M_{\text{calculated}} - M_{\text{old}}) \quad \text{Equation 5. 34}$$

Where α is the under relaxation factor for particles/droplets. This value is set by default at 0.5 but was set at 0.05 in this study to allow a smooth evolution of the solution towards a converged value and hence improve the stability of the solution.

5.7.6 Discrete phase model set up

In order to use the discrete phase model it is necessary to define the injection location, the droplet size (minimum, maximum and mean diameter) as well as the spread parameter, the droplet velocity components and the droplet temperature. These initial conditions are used to initiate the heat and mass transfer with the input of the physical properties. Some alternative options are available which give a choice between different atomizer models, corresponding to a particular injection type. The flow characteristics are predetermined in the literature based on the nozzle type and fuel flow rate. The different atomizer types are:

- plain orifice atomizer
- pressure swirl atomizer
- effervescent atomizer
- airblast atomizer
- flat fan atomizer

Although the pressure swirl atomizer type corresponds to the type of injection used in this study, the Linearized Instability Sheet Atomization (LISA) model of Shmidt et al. (1999) was not used in this study. Indeed, the approach in this work has been to use experimental measurements to set the initial drop size and characteristics in the CFD model. Consequently detailed droplet data is required as a starting point for the numerical simulation. Since the spray depends not only on the flow configuration but also on a variety of operating parameters such as fuel and air flow rates, pressure or temperatures, droplet size and velocity correlations of a specific atomizer often can not be applied in complex combustor designs. In many cases, spray measurements on large scale combustors test rigs are the only mean to provide initial spray data of sufficient quality for the numerical simulation (Schmehl et al. 2000).

The trajectory and heat/mass transfer calculations are based on the force balance on the particle and on the convective/radiative heat and mass transfer from the particle, using the local continuous phase conditions as the particle moves through the flow.

A maximum number of steps was increased from a default value of 500 to 3 000 to compute a single particle trajectory via equation 5.23. Increasing this number gives a better chance to converge the DPM equations. If the maximum number of steps is exceeded, FLUENT abandons the trajectory calculation for the current particle injection and reports the trajectory fate as "incomplete".

It is necessary to specify the type of particles that is necessary for the spray calculations. The choice exists between three types of particles: inert, droplet or combusting particle. The droplet particle type is required for this study as it is the one designed when heat transfer to and from the particle is present and when the non-premixed combustion model is used, which is the case here.

There are several ways of setting up the spray injection method using non atomizer injection type:

- surface injection
- group injection
- cone injection

For the surface injection, an injection point has been created in the domain, and defined as a surface. With this type of injection, there is no need to define the location of the injection since the surface represents the position where the fuel is atomized from. Each injection is assigned a name so that it is easily possible to distinguish them when a large number of injections is defined. In this study, the injection name was defined in such a manner that the cone angle was quoted as well as the injection number for this angle, for instance "injection-45deg-1" "injection-45deg-2" or "injection-50deg-1" and generally, 20 injections points were assigned for each spray angle. Indeed, for this study the number of droplet particle streams is set at 20 for one sector of 36° , hence the particle streams were injected each 1.8° .

Besides the injection location, the injection parameters defined at the beginning of this section have to be described, starting by the injection velocity components. In

order to compute the injection velocity, the pressure on the injected fluid in the nozzle is required. The resulting injection velocity was computed from the following equation:

$$V_{inj} = C_d \sqrt{\frac{2(P_{inj} - P_{atm})}{\rho_l}} \quad \text{Equation 5. 35}$$

It was assumed that the discharge coefficient, C_D , remained fixed at 0.7. For instance, the injection pressure for ethanol fuel under atmospheric pressure being around 117 psi (0.80 MPa), the injection velocity magnitude obtained was around 30 m/s. Assuming that the velocity magnitude remains constant and based on the spray angle, the velocity components, V_x , V_y and V_z were determined. Once V_z was determined, corresponding to the axial velocity, this value remained constant for any injection corresponding to this cone angle. V_x and V_y varied so that the particle streams were injected uniformly from 0 to 36° corresponding to 1/10th of the full geometry represented in this study.

$$V_{axial} = V_{tot} * \sin \theta \quad \text{Equation 5. 36}$$

$$V_{radial} = V_{tot} * \cos \theta \quad \text{Equation 5. 37}$$

The axial and radial velocities are determined according to the spray half-angle, in this case 45° and according to the spray dispersion angle varying in the current study generally from 40 to 65°. The droplet velocity is defined by the experimental measurements and since only the 1/10th of the real geometry is represented, only 1/10th of the experimentally measured mass flow rate was considered as the total fuel flow rate for all the injectors. Then this total fuel flow rate was divided by the number of injectors to obtain the fuel flow rate per injector. For instance, the ethanol mass flow rate in the experiments was determined to be 0.36 g/s. Hence, the fuel flow rate in the simulation for all the injectors was based on 1/10th of this value, 0.036 g/s, value which was uniformly divided by the number of injectors. Figure 5.19 shows the trajectories of the fuel droplets. These trajectories are in three-dimensional space but this figure shows a projection of the paths in a vertical midplane.

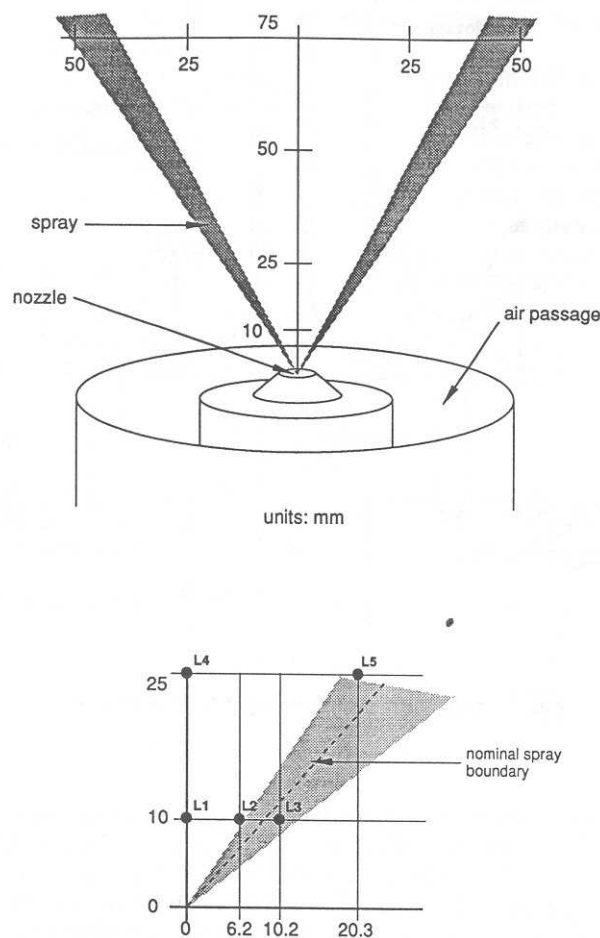


Figure 5. 19 Schematic of the spray boundary position (Presser et al. 1988)

The surface injection is quite convenient since it allows flexibility for the user to directly set the injection properties for each particle stream, thereby allowing to change the drop size and velocity distribution for each injection. However, this task is particularly cumbersome, since for instance in the current study, with 7 different angles and a value of 20 particle streams used per angle, 140 injection points had to be created defining the different velocity components and droplet size distribution.

Group injection represents a good compromise since while losing partially the accuracy required with the surface injection method, it allows to gain a considerable amount of time in the injection method definition. Indeed, for group injection, only the first and last point of a particular angle are needed. The “point” represented one particle stream. Consequently, while the first and last injection velocity components are defined for a particular injection angle, FLUENT will interpolate for the values comprised in between depending on the number of particle streams defined by the

user. However, the droplet size distribution defined for the first point is automatically assigned for the last one, therefore offering a little less flexibility for that aspect compared to the surface injection method. This deficit can be compensated by setting another group or if needed only a point injection with a changed droplet size distribution.

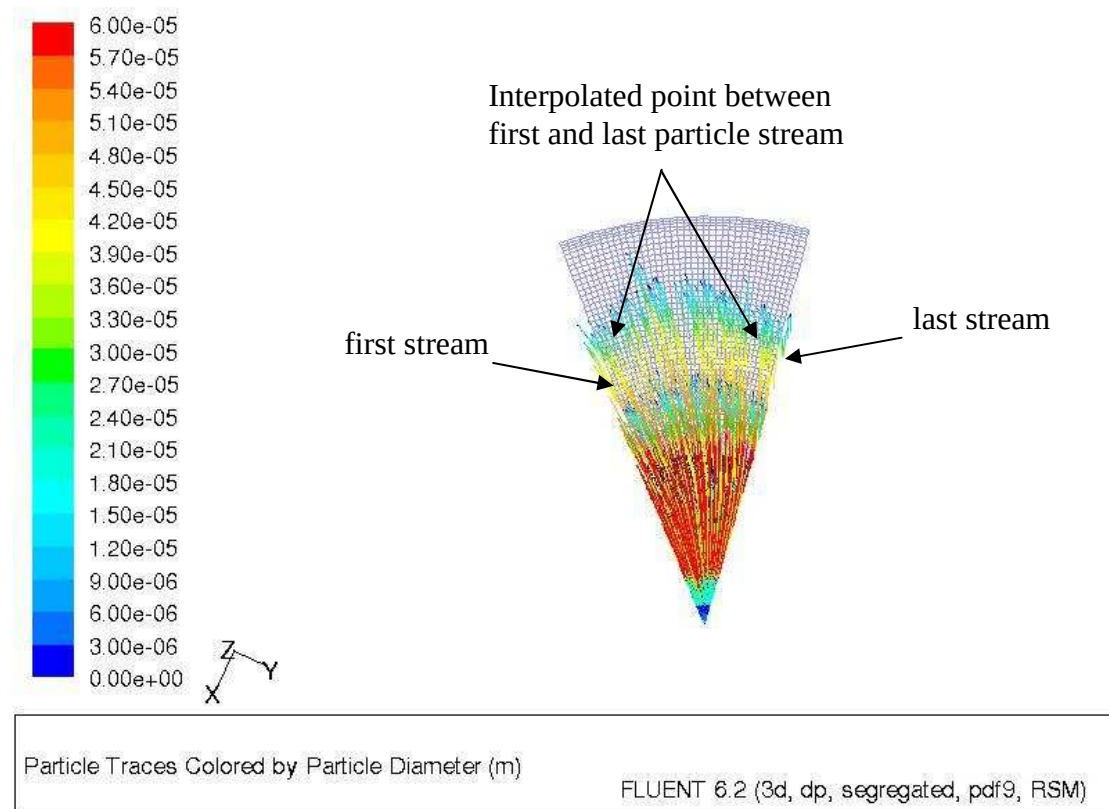


Figure 5.20 Group injection method illustration

Finally the cone angle injection method is specifically defined for spray streams since it allows for the hollow or solid cone definition. For both types of injections, the following inputs are required:

- injection point coordinates
- temperature
- cone axis components
- velocity magnitude
- cone angle
- radius: a non-zero inner radius can be specified to model injectors that do not emanate from a single point.

-
- swirl fraction (hollow cone only): set the fraction of the velocity magnitude to go into the swirling component of the flow.
 - mass flow rate
 - mean diameter
 - maximum diameter
 - minimum diameter
 - spread parameter
 - number of diameters

The last four parameters for cone specification have been added in the FLUENT capabilities from version 6.2. FLUENT 6.1 only required the definition of a mean diameter. The cone specification method does not require the user to calculate the injection velocity components, since only the velocity magnitude is required, while the swirl fraction will define the fraction of the velocity magnitude that goes into the swirling component. It is possible to define multiple spray cones emanating from the same initial location in order to specify a known size distribution of the spray or to include a known range of cone angles; therefore this method gives flexibility in changing the droplet size distribution within the same spray angle and the cone angle specification can easily be changed without having to do some cumbersome calculations to define each velocity components as required with the surface or group injection therefore a considerable amount of time can be gained from this method. Since the cone specification method seems to be offering many advantages, it has been considered the method of choice for the current study.

5.8 Droplet interactions

Collisions among droplets seem to have a very low probability to occur in a spray in which the droplets are moving in a parallel direction or along divergent path like encountered in this study. Moreover, droplet coalescence is less important in hollow cone sprays (Reitz and Diwakar, 1987) due to the low spray density (cf. section 5.6.1). Consequently as there is a single injector in this study and the droplets are fired into divergent directions, droplet collisions and coalescence is considered to have a negligible effect on the spray combustion process. The absence of droplet coalescence is to the benefit of droplet vaporization, since droplet coalescence would have resulted

in a decrease in surface area as larger droplets would be formed (Tambour et al. 1985).

Spray breakup can have a dominant effect on the spray drop size in hollow cone sprays since droplet coalescence is minimised in such configurations (Reitz and Diwakar, 1987). However, following Reitz and Diwakar (Reitz and Diwakar, 1987), the criteria for breakup is $We_D > 12$. This criteria has never been met in any of the experiments (cf. figure 4.9) due to the low relative velocities between the air and the droplet phase, hence breakup has not been included in the simulations, except at high pressures.

The particle wall interaction are taken into account and defined in section 6.5.2 of the Results and Discussion chapter.

5.9 Numerical method

The numerical method employs a second order accurate interpolation procedure for evaluating gas-phase properties at the characteristic location from fixed Eulerian grid nodes. Sirignano (1983) indicated that unless a second or higher order accurate interpolation scheme is used then the advantage of elimination of numerical diffusion with a Lagrangian formulation for liquid phase is lost to some extent .

5.10 Summary

The RSM turbulence model has been selected since it is particularly suitable for the strongly swirling flows encountered in this study. The uniform but time varying temperature assumption in the FLUENT model means that the infinite conductivity approach is currently used for this study. The model neglects the internal vortex and liquid circulation and assumes spherically symmetric conduction. Alternative evaporation models are commented in the Discussion section. The flamelet approach has been used as a combustion model since it represents a good compromise between computational time and accuracy.

For the spray definition, the spray computations are treated with a Lagrangian approach in which the droplets are treated as a discrete phase and treated in space and time, while the gas phase is treated using an Eulerian approach. Droplet collision and secondary breakup has not been included in the simulations due to the spray operating conditions and configuration.

CHAPTER 6 – RESULTS AND DISCUSSION

This chapter describes the computational simulations of spray flame experiments carried out using carbon neutral. Although aspects of spray combustion have been simulated for several decades, very few attempts to validate the numerical results have been carried out for reacting liquid fuels in swirling flows involving biomass derived fuels, reflecting both the difficulty in getting accurate measurements and modelling challenges arising from uncertainties linked to each physical submodel.

The aim of this chapter is to describe and, where appropriate, assess the principal model elements to be incorporated in numerical spray combustion simulations. Data obtained experimentally at Cranfield such as the size distribution of the droplets within the spray, the gas temperature and gas velocity profiles are used to guide the model selection and subsequently the validation of the computational results. The simulations have been performed using two different fuels, which are considered to be of growing importance in carbon neutral applications, namely ethanol and biodiesel (FAME).

From a combustion perspective, a number of important considerations when evaluating prospective liquid fuels centre on spray atomization quality (degraded by high viscosity, density, and surface tension; often controlled by the preheating of the fuel) are determined by the droplet diameter and ensuring a high droplet vaporization rate (affecting flame length and shape) and directly influences both combustion efficiency and pollutant formation. As a consequence, it is crucial to investigate the effects of drop size distribution and cone angle, overall equivalence ratio and pressure on field properties such as gas temperature.

The main objective of this work is to assess and optimise the capability of the CFD to predict accurately the results obtained experimentally with two-phase liquid spray combustion flow using vegetable oils, under atmospheric pressure and under gas turbine operating conditions. Though physical experiments are the ultimate test to study the performance of combustion systems, they are often too expensive and complicated, and even at times impossible to achieve. Indeed, complicated interactions are involved between the air and the evaporating spray, and it is difficult

to separate one parameter at one time to analyse its effect on the combustion process. For instance, in this study, the experiments have been limited to 3 bars, while on the other hand, numerical experiments open an avenue for isolating and understanding the influence of different parameters on complex combustion situation and further extend the range of operating conditions. Calculations are compared with measurements for the reacting flow field of a fuel injected spray flame which might be considered to model a typical injector element in a gas turbine combustor. The predictions were performed with the CFD code FLUENT embodying a finely resolved unstructured mesh, especially in regions of high spatial gradients.

This chapter begins with a preliminary investigation on cold swirling flow, followed by a parametric study on different flow and spray characteristics, such as the droplet size distribution, cone angle, primary air flow rate, number of particle streams and ambient pressure on the gas temperature field. Indeed, these key factors have been identified to have a substantial effect on the spray flame structure, whose influence needs to be determined separately in the unfolding investigation.

6.1 *Introduction on swirling flows*

As a preliminary stage to burning sprays simulations, it is necessary to validate the numerical results obtained for cold swirling flows. In fact, swirling flow has a significant effect on the flow field and can affect the combustion stability in spray flame configurations.

The primary zone, also called recirculation zone, is the region where the fuel is injected and ignition occurs. The word recirculation defines the flow reversal in the combustor. In addition to its role in delivering the major heat release in the chamber, the other important function of the primary zone is to anchor the flame by recirculating burned gases through the generated flow reversal. The gases are then mixed with the incoming air and fuel in order to provide sufficient time, temperature, and turbulence to achieve complete combustion by increasing the fuel residence time and promoting chemical reaction.

One of the most efficient ways of inducing a recirculation zone in the primary zone is through the use of a swirler, located around the fuel injector and employed in a wide range of industrial applications. The overall combustion system performance depends heavily on the design of air swirlers and their flow dynamics must be well understood, explaining why swirling flows generation methods and their aerodynamics characteristics have been thoroughly investigated by many researchers. Special features of strongly swirling flows include:

1. Reduction of combustion length because of higher rates of entrainment of ambient fluid, fast moving close to the nozzle and near recirculation zone boundaries.
2. Improved flame stability because of the presence of a central toroidal recirculation zone CTRZ which recirculates hot combustion products
3. Minimised maintenance and extended life of equipment, since the blockage is aerodynamic and flame impingement on solid surfaces (with heat and deposit problems) is minimised.

This section describes the computational simulations of cold swirling flow carried out such as the strength and size of the recirculation zone and axial peak velocity. Swirl number is defined, followed by a comparison between results obtained with the $k-\varepsilon$ and the RSM turbulence models, and finally the numerical results are compared with the experimental data.

6.2 Swirl flow characterisation

6.2.1 Swirl number

The degree of swirl is usually characterized by the swirl number S , which is a non dimensional number, representing axial flux of swirl momentum divided by axial flux of axial momentum. Beér and Chigier (1972) have demonstrated that the swirl number of an annular swirler with constant vane angle α can be written as:

$$S = \frac{2}{3} \left[\frac{1 - (D_{hub}/D_{sw})^3}{1 - (D_{hub}/D_{sw})^2} \right] \tan \alpha \quad \text{Equation 6. 1}$$

Swirling flow results from the application of a spiralling motion, a swirl velocity component (also known as a tangential or azimuthal velocity component) being imparted to the flow by the use of swirl vanes, in addition to the axial and radial components of velocity encountered in the non-swirling cases. Experimental studies show that swirl has large-scale effects on flow fields. Indeed, swirling flows provoke strong centrifugal effects on entry to the combustor and very low pressure in the primary zone, especially at high degree of swirl (strong swirl, $S \geq 0.6$), resulting in the formation of a central toroidal recirculation zone (CTRZ). The usual point of onset of reversed flow is taken to occur approximately with swirl number $S \geq 0.6$ (Beér and Chigier, 1972). With sufficiently high Reynolds and swirl numbers (approximately greater than 18000 and 0.6), strong radial and axial pressure gradients are set up near the nozzle exit, resulting in flow reversal and axial recirculation in the form of a large central toroidal recirculation zone, CTRZ, which is not observed at weaker degrees of swirl. Chigier and Chervinsky (1967) observed no recirculation zone for swirl numbers below 0.64. It is essential to maintain low enough pressure and velocity in order to prevent flame blow-off or blow out. For values of swirl number less than around 0.4, the swirl is described as weak.

The swirler or swirl vane consist of a set of curved vanes at an angle α to the mainstream direction, which deflect the stream into rotation (Gupta et al., 1984). The vanes are mounted on a central hub around the fuel spray nozzle. This technique is common in gas turbine combustors.

The central hub of the swirler includes a fuel spray nozzle, as illustrated figure 6.1 and a conical swirling spray of liquid kerosene droplets, seen figure 6.2, is projected to the CTRZ, resulting in high intensity burning. Stability is enhanced by the strength of the recirculation of hot and chemically active partially burnt combustion products, and additional primary zone air entering via lateral injection holes. Heat and mass are transported effectively by the high intensity turbulence that prevails in the vortex region.

For the current study, the vane angle is maintained constant at an angle of 45° , inducing a strong swirl number of around 0.91, according to equation 6.1. This swirler

array consists of 10 swirlers as illustrated figure 6.1. Typical swirl burners in industrial burners for gaseous and liquid fuels lie in the range $0.8 < S < 1.5$.



Figure 6. 1 Burner geometry – view from top

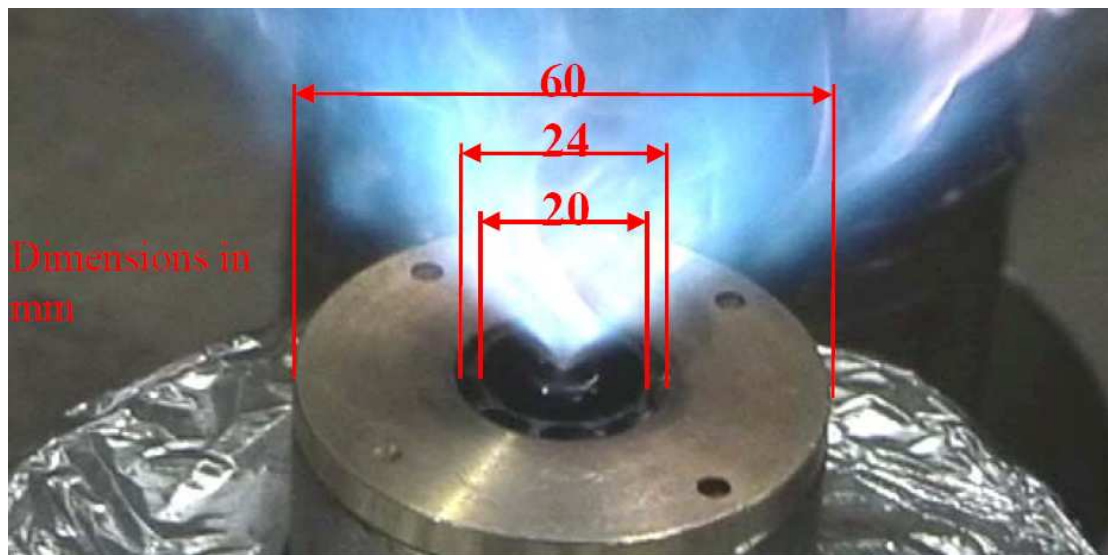


Figure 6. 2 Dimensions of swirler used in this study

6.3 Cold flow results

This section discusses the results of simulations carried out to determine the effect of change of mass flow rate on the size of the recirculation and the axial velocity profile at different heights.

Velocity profiles have been determined for swirling cold flow simulations and will be compared with the experimental data. The cold flow data presented here are only preliminary calculations. Indeed, the cold flow simulation is carried out without the

fuel spray, and it is known that the spray will have a substantial impact on the velocity flow field. Non reacting flow fields experimentations have been carried out using a curved vane type swirler. Kilik (1976) demonstrated that the efficiency of curved vanes is higher than using flat vanes, since more angular momentum can be imparted to the axial flow using the curved vanes. This means that for the same vane angle as that of a corresponding flat vane type swirler, a larger swirl number is created with curved vane typed swirler. Therefore a larger recirculation zone will be obtained using a curved vane type swirler. Measurements have been taken at different axial distances downstream of the burner from 5 mm to 6 cm and compared with the numerical results. PIV measurements were performed in the atmospheric rig to determine the flow properties of the open, isothermal, swirling flow field created in the rig.

The experimental data will help to validate modelling and justify the assumptions used for the numerical simulation employed within the CFD model and could eventually further enhance model development of these complex turbulent flows but this is beyond the scope of this study. In fact a better understanding of the swirling flow behaviour will help in defining the characteristics of the swirler. Therefore, the flow through the swirler vanes must be thoroughly understood and computational fluid dynamics offers a great advantage in helping to determine the flow characteristics.

6.3.1 Boundary conditions

The different simulations are presented table 6.1. To familiarize with the experimental techniques and to facilitate measurements, a preliminary study was carried out in an open laboratory configuration and later on the casing was installed to obtain a confined rig environment. Table 6.1 gives the value of the swirler air mass flow rate and secondary air flow rate investigated in this study as well as the Reynolds number, axial exit velocity from the swirler and the swirl number. The axial exit velocity was calculated based on the swirler area while the swirl number and the Reynolds number were calculated respectively according to equation 6.1 and 6.2. In fact, in addition to swirl strength, flow field are also characterised by their Reynolds number evaluated at nozzle exit conditions and based on the nozzle diameter:

The Reynolds number is defined as follows:

$$\text{Re} = \frac{U(D_{sw} - D_{hub})}{\nu} \quad \text{Equation 6. 2}$$

where U is the average exit axial velocity, D_{sw} and D_{hub} , respectively the swirler and the hub diameter.

	Swirler air mass flow rate (g/s)	Secondary air mass flow rate (g/s)	Axial exit velocity (m/s)	Reynolds number	Swirl number
Case A	3.5 (open)	12	27	6328	0.91
Case B	1.6 (open)	12	12.43	2892	0.91
Case C	1.6 (confined)	12	12.43	2892	0.91
Case D	3.5 (confined)	12	27	6328	0.91
Case E	3 (confined)	12	23.32	5424	0.91

Table 6. 1 Experimental boundary conditions for the cold flow in open and confined rig

The air mass flow rate in the CFD simulation was varied between 1.6 g/s and 3.5 g/s. 3.5 g/s corresponds to the air mass flow rate used for a heptane experiment while 1.6g/s was the swirling air flow rate used throughout the ethanol experiments. A uniform mass flow rate distribution was considered at the air swirler inlet. The temperature of the air was estimated at around 298 K for the ethanol experiments and 423 K for the experiments carried out with biodiesel.

The preliminary experiment carried out in an open laboratory environment were made in order to obtain a comprehensive set of data in a relatively simple flow configuration, while at the same time allowing full optical access to the flow field which would not be possible in a confined pressure rig.

The degree of swirl remain constant despite the change in the Reynolds number, and the value of swirl of 0.91 based on equation 6.1 represents a high value of swirl, constant in all the cases and as a consequence a recirculation region will be present in every flow field for this study. Since the primary concern is the immediate

downstream region the measurements were extended up to a maximum distance of $3D_{sw}$ in the axial direction.

6.3.2 Comparison of turbulence models for swirling flows

Swirling flows are generally difficult to simulate due mainly to the non-isotropic turbulence field. The $k-\varepsilon$ and the RSM model were used in this study for the prediction of the swirling flow and their performance was compared. The $k-\varepsilon$ is widely used for engineering application because of its simplicity and reduced computational time as well as facility of convergence compared to more sophisticated turbulence models. In this study, a converged solution is first obtained using the standard $k-\varepsilon$ turbulence model, which offers the advantage of fairly rapid convergence.

The axial velocity profiles predicted by the $k-\varepsilon$ and RSM are presented figure 6.3 to figure 6.5 and illustrates typical comparisons between the PIV measurements and the numerical results obtained with the $k-\varepsilon$ and the Reynolds Stress Model (RSM) which accounts for the non-isotropic stresses generated by highly swirling flows.

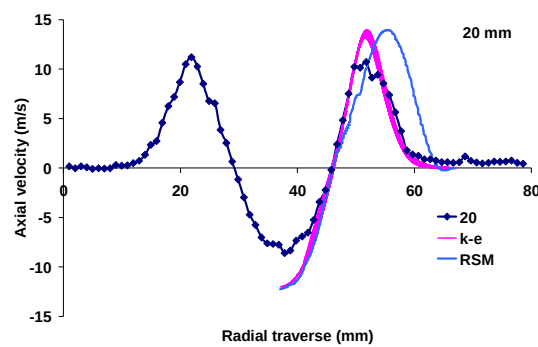


Figure 6.3 Cold air velocity profile, air mass flow rate 3.5 g/s at 20 mm

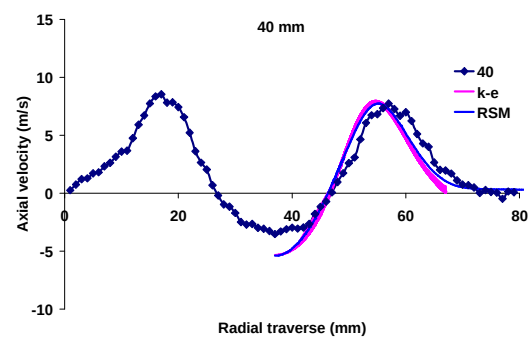


Figure 6.4 Cold air velocity profile, air mass flow rate 3.5 g/s at 40 mm

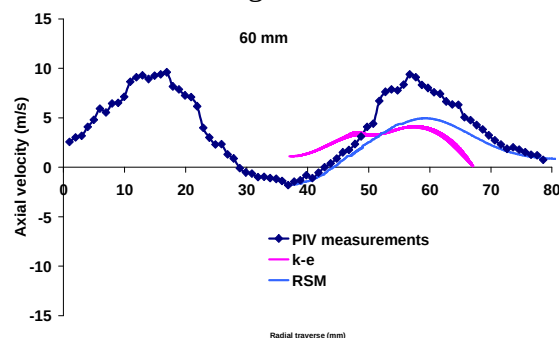


Figure 6.5 Cold air velocity profile, air mass flow rate 3.5 g/s at 60 mm

The $k-\varepsilon$ model, although computationally less expensive than the RSM model, managed to predict the flow recirculation as the RSM model up to a distance of 40 mm on the burner centreline. However, at 60mm, the flow recirculation is not predicted with the $k-\varepsilon$ model unlike what is obtained with the RSM model. The advantages of the RSM model over the $k-\varepsilon$ model are apparent in far downstream regions in strongly swirling flows, therefore the RSM model was consequently selected to simulate the effects of turbulence on the flow, although the $k-\varepsilon$ model brings relatively accurate results at a low computational cost.

6.3.3 Axial velocity distribution

Figure 6.6 illustrates the PIV measurements taken at different heights, from 1 mm up to 60 mm downstream of the swirler. The shape of the profiles changes rapidly in both the radial and axial directions. A peak axial velocity of around 27 m/s is obtained in a region close to the air swirler. The axial velocity decays very fast and at a 60 mm location, the peak axial velocity has already gone down to a value of 7 m/s. The air jets expand in the downstream direction with the peak axial velocities progressively moving further out radially.

A large and strong recirculating region is observed in the centre region of the flow, with reverse flow extending from the nozzle exit towards a region of around 60 mm further downstream. The CTRZ present the maximum reverse velocities close to the swirler exit and as the fluid flows downstream, the swirl gradually decays and the recirculation zone tends to vanish with a lower negative velocity. Figure 6.6 represents PIV measurements of velocity vectors which clearly illustrates these observations.

Comparison between the PIV measurement and FLUENT predictions of the axial velocity profiles of the cold flow exiting from the swirlers is shown from figure 6.7 to 6.9. The shape of the central recirculation is satisfactorily predicted by CFD. However, the magnitude of centreline velocity predicted by the numerical simulation at 20 mm is slightly larger than the measurements but generally the numerical results are in qualitative agreement with the measurements. The difference between computed velocity and measured velocity is under 10% except at 20 mm where the

maximum difference between measured and computed reverse velocity is between 15% and 25%.

The figures 6.7 to 6.11 show that the predicted CFD results agree satisfactorily with the measurements. The width and strength of the recirculation zone and maximum positive axial velocities are correctly captured. The CFD results show that the overall flow patterns in the open rig, especially the recirculation in the centre above the burner is correctly captured. Overall, the CFD analysis did accurately capture the flow pattern in the whole area and reproduced faithfully the features captured by the PIV measurements in the experiments.

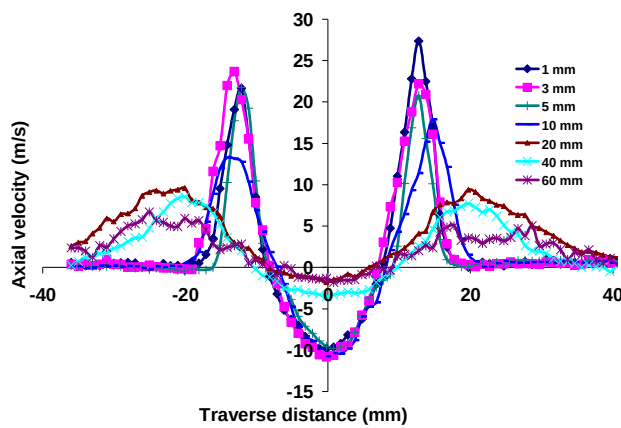


Figure 6.6 PIV measurements of axial velocity for cold flow, air mass flow rate 3.5 g/s

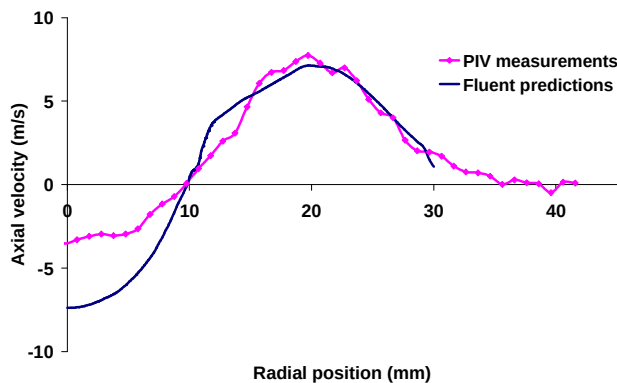


Figure 6.8 Cold air axial velocity profile in open configuration at 40 mm, air mass flow rate 3.5 g/s

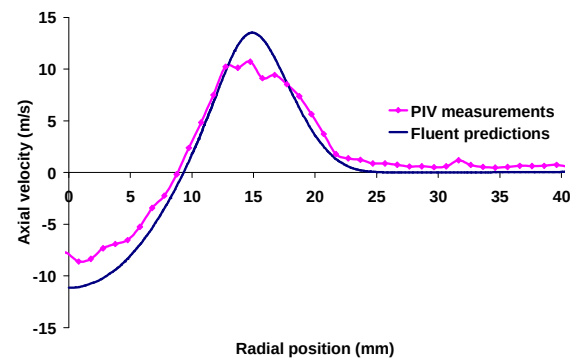


Figure 6.7 Cold air axial velocity profile in open configuration at 20 mm, air mass flow rate 3.5 g/s

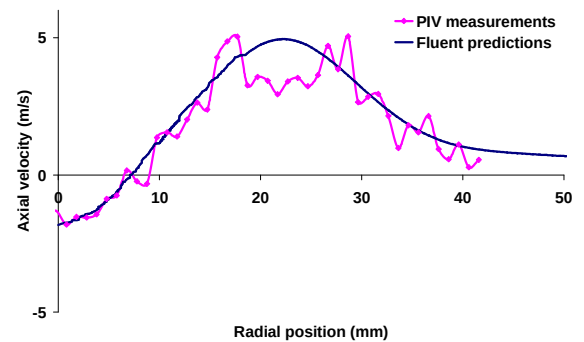


Figure 6.9 Cold air axial velocity profile in open configuration at 60 mm, air mass flow rate 3.5 g/s

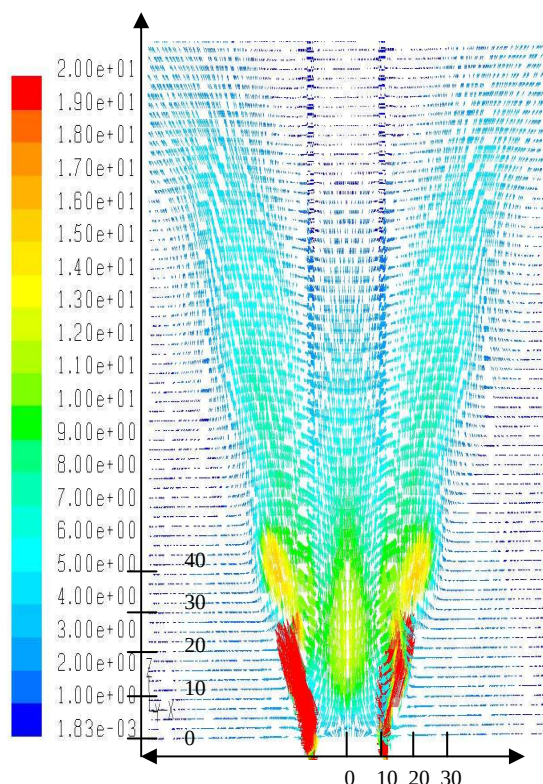


Figure 6.10 Fluent predictions for cold flow velocity magnitude (m/s) flow field for air flow rate of 3.5 g/s in open configuration

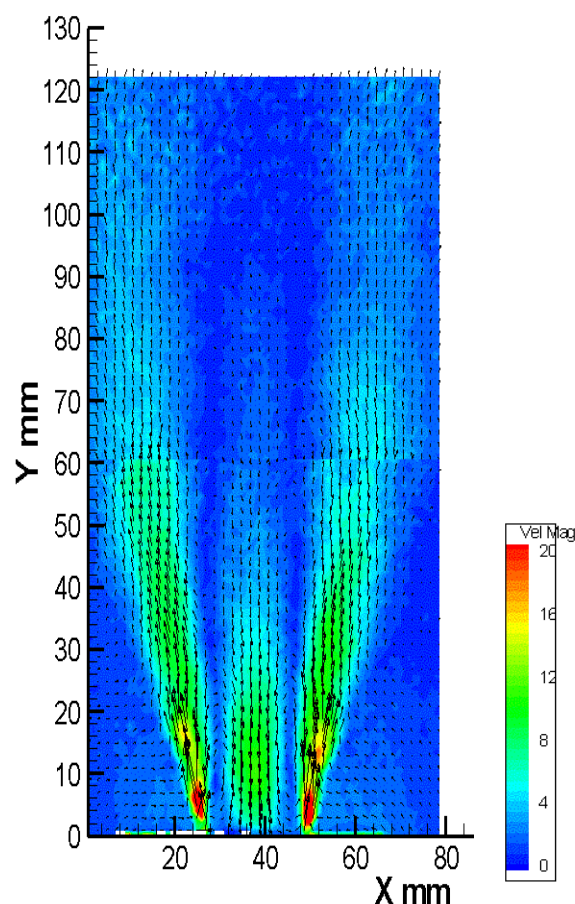


Figure 6.11 PIV velocity magnitude for air flow rate of 3.5 g/s under non-burning conditions in open configuration

6.3.4 Comparison of structure of the recirculation region

Different cold flow cases have been investigated with a swirl air mass flow rate ranging from 1.6 g/s corresponding to the ethanol case air flow rate to 3.5 g/s, assigned to the heptane experiments, while the secondary air flow has been maintained constant, with an air flow rate of 12 g/s. Biodiesel run on a air flow rate of 3 g/s, since the different fuels require to run on different flow conditions. Due to the geometry of the domain, there is no possibility of changing the swirl number, as the axial flux of swirl momentum divided by axial flux of axial momentum will remain constant.

Figures 6.12 to 6.14 show the velocity vectors distribution in a vertical plane passing through the middle of the swirl vane where the increase in air mass flow rate is clearly visible. The swirling air flow of 3 g/s seen figure 6.14 expands radially more rapidly

than when the air flow rate is set at 1.6 g/s. Moreover the peak axial velocity is significantly increased proportionally to the increase in air mass flow rate and the strength of the recirculation zone is reinforced, from a value of 5.55 m/s at 1.6 g/s to 7.30 m/s when the air mass flow rate is raised up to 3 g/s. Therefore increasing the cold swirling flow results in a significant modification of the air flow field, with increase in air exit velocity and strength of the recirculation zone. Figures 6.12 to 6.14 show the significant impact of the swirling flow on the mean axial flow field with a strong recirculation zone that extends from the swirler exit to a distance depending on the air mass flow rate coming out of the swirler. Figures 6.12 to 6.14 show that the air velocities are not perfectly symmetric because the vertical plane does pass only through one swirler.

In the current setup, as the pressure rig is large compared to the swirler exit diameter, since the ratio of the chamber diameter over the swirler diameter is around 6, the air jet behaves similarly to an unconfined air jet, the large distance between the swirler and the walls justifying this, so it can be safely believed that the air flow is relatively unaffected by the presence of walls in the case of cold swirling flow. As a consequence, the shape of the central recirculation predicted by the simulations is the same for the open than in the confined rig as illustrated figure 6.12 and 6.13. However, the presence of the walls will affect the flow field in presence of combustion, as described in the Experimental Study.

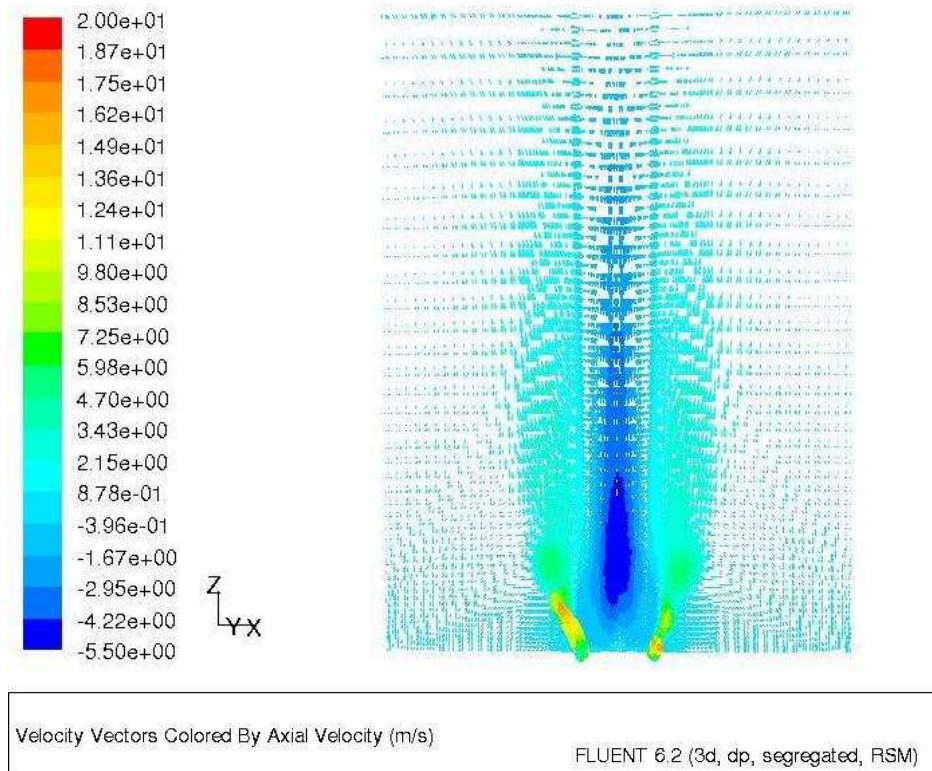


Figure 6.12 Fluent predictions for cold flow axial velocity flow field for air flow rate of 1.6 g/s in open configuration

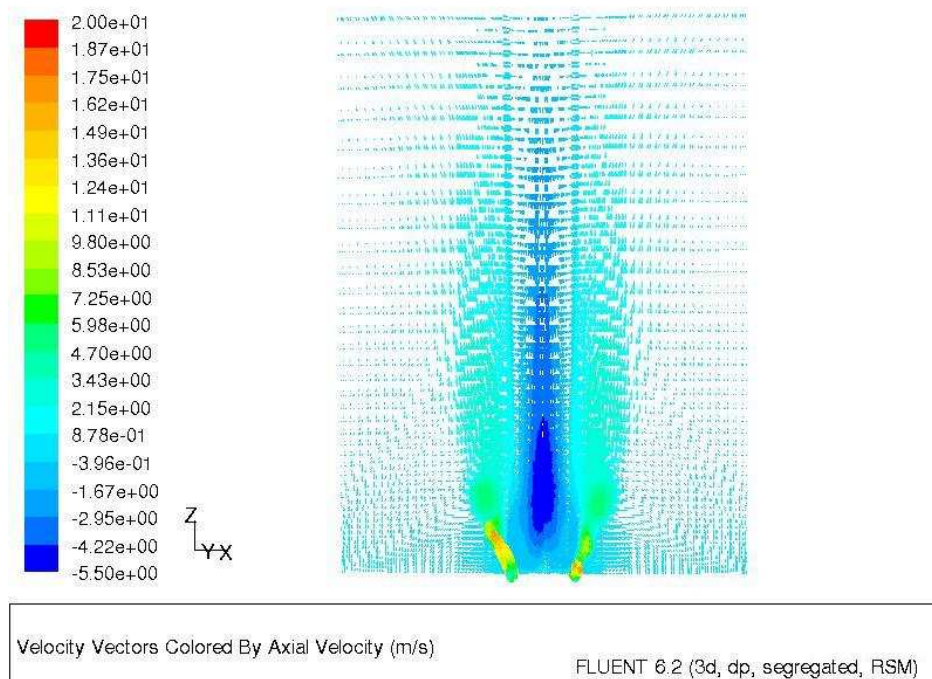


Figure 6.13 Fluent predictions for cold flow axial velocity flow field for air flow rate of 1.6 g/s in open configuration

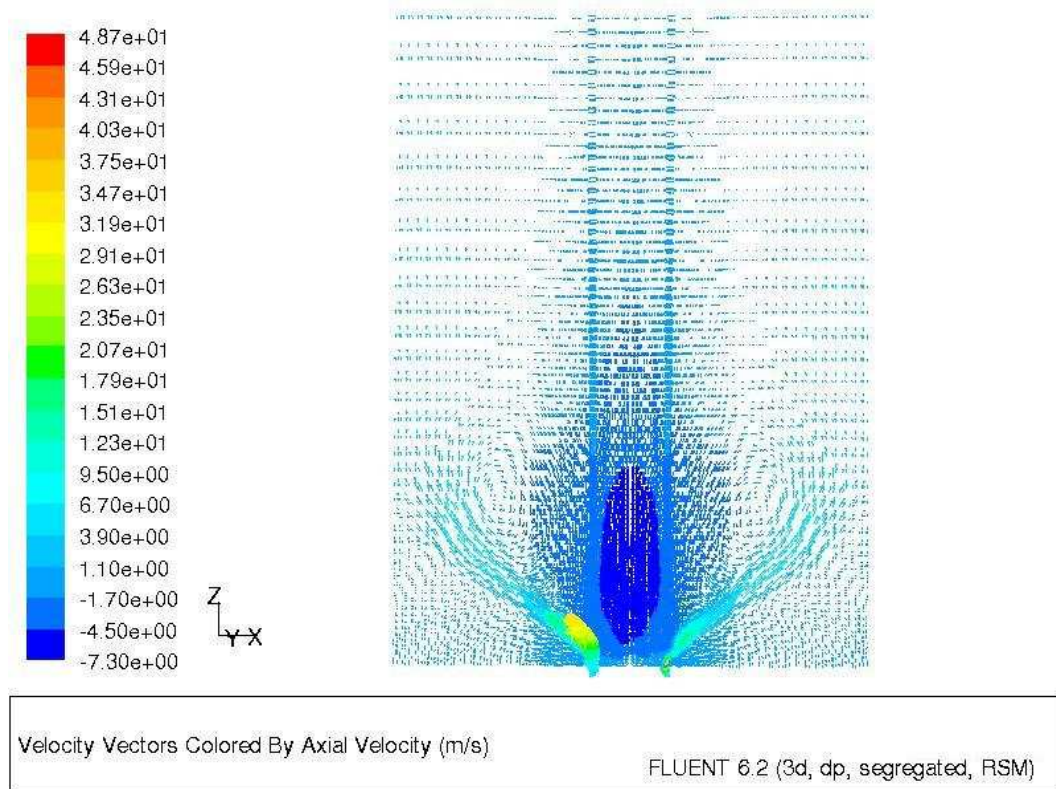


Figure 6. 14 Fluent predictions for cold flow axial velocity flow field for air flow rate of 3 g/s in confined rig

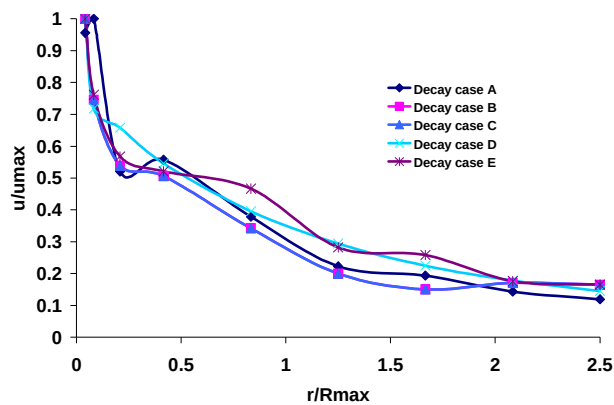


Figure 6. 15 Decay of the maximum value of the axial components of velocity along the length of the jets

As the flow moves away from the swirler, the central recirculation zone gradually expands with the expansion of the air jet. All the velocity components gradually decay in the downstream direction following the same trend regardless of the mass flow rate, as illustrated figure 6.15. Decay of the peak values in the axial velocity profiles remains approximately the same even though the air mass flow rate is increased, because of the constant swirl number.

A typical recirculation region is represented in figure 6.16, where the region OAB encloses the recirculation region. The point B is called the stagnation point. Beyond this location the flow becomes supercritical as described by Escudier and Keller (1985). Indeed, after this point, the flow axial velocities become positive because the reverse flow disappears as the effect of the swirler gradually vanish. Escudier and Keller (1985) defined that if the flow is supercritical, the flow waves are swept downstream from the originating disturbance, whereas for subcritical flows these waves propagate against the flow, carrying with them information about the nature of the downstream geometry and conditions. The phenomenon representing the flow reversal as a transition is referred as vortex breakdown (Benjamin, 1962). The position of the stagnation point defines the length of the recirculation zone and the flow outside the region OAB constitutes the main flow. The recirculation region in the case A and E are shown respectively figure 6.17 and figure 6.18.

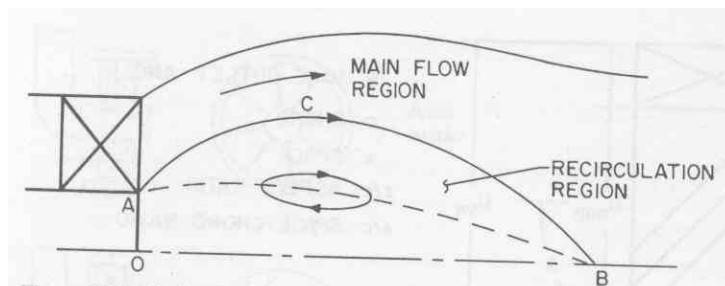


Figure 6. 16 Recirculation region in a swirling flow field (Lefebvre, 1998a)

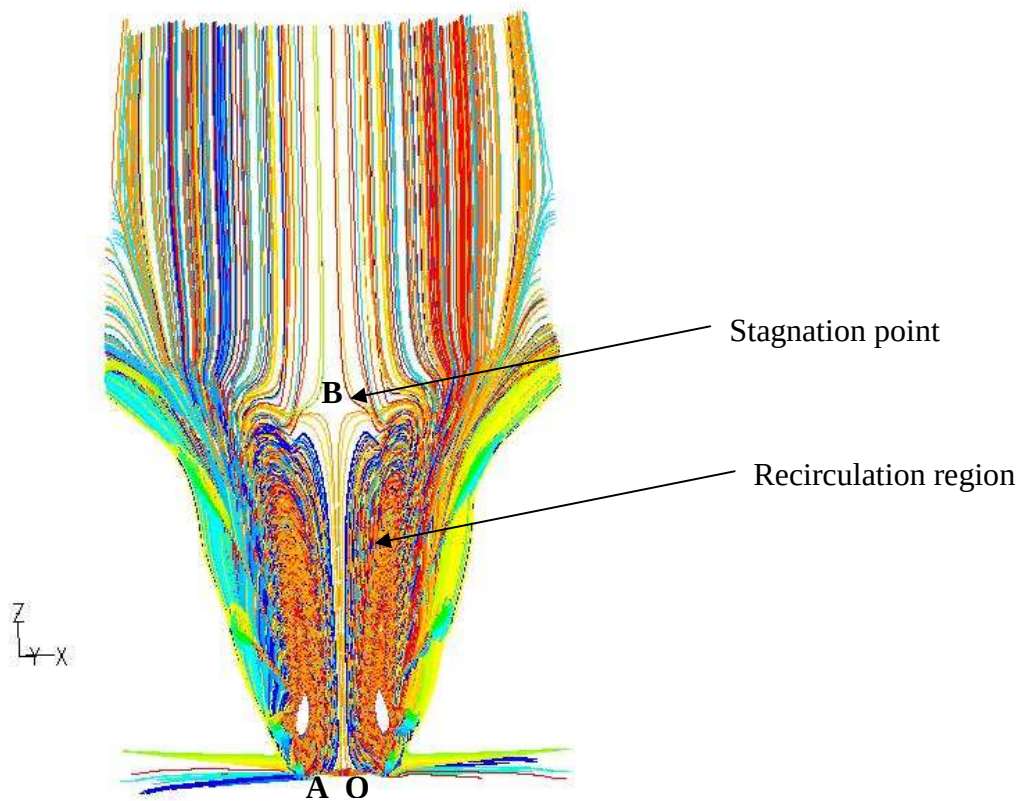


Figure 6. 17 Streamlines highlighting recirculation region in flow field with air flow rate at 3.5 g/s

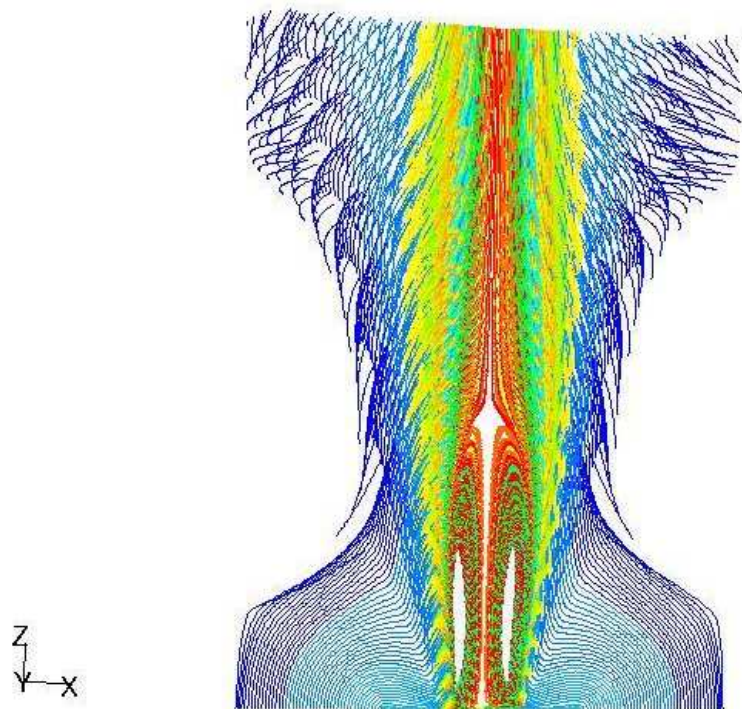


Figure 6. 18 Streamlines highlighting recirculation region in flow field with air flow rate at 3 g/s

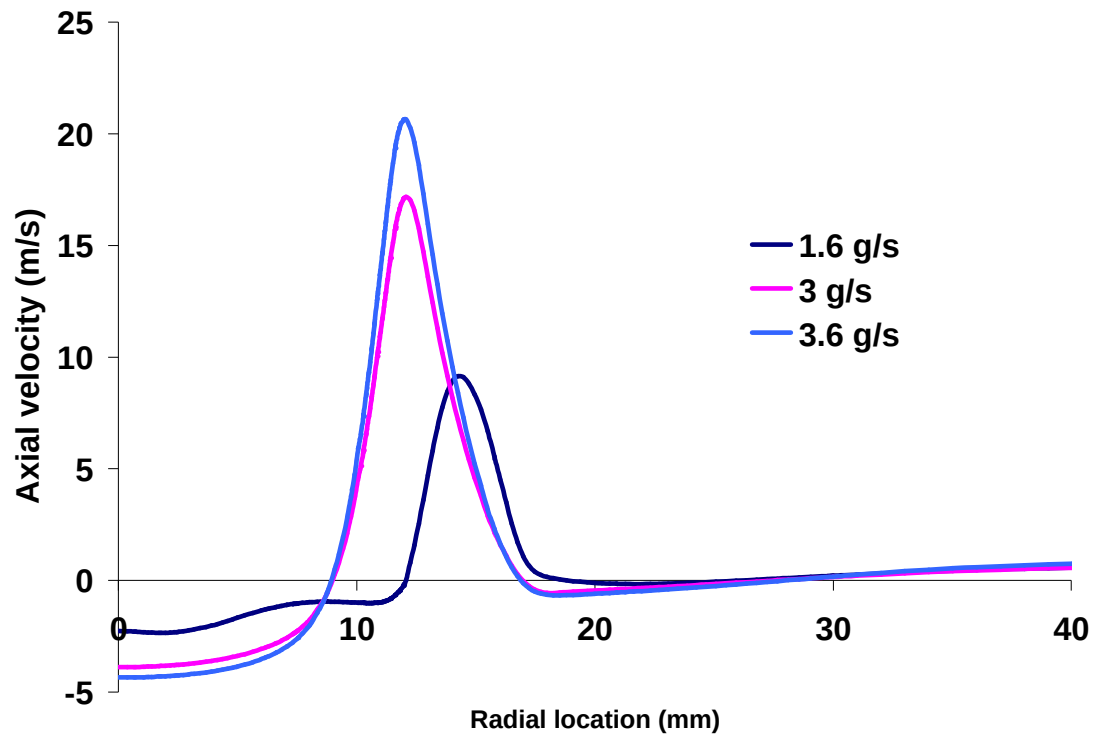


Figure 6. 19 Axial velocity profiles of cold swirling air at 10 mm downstream

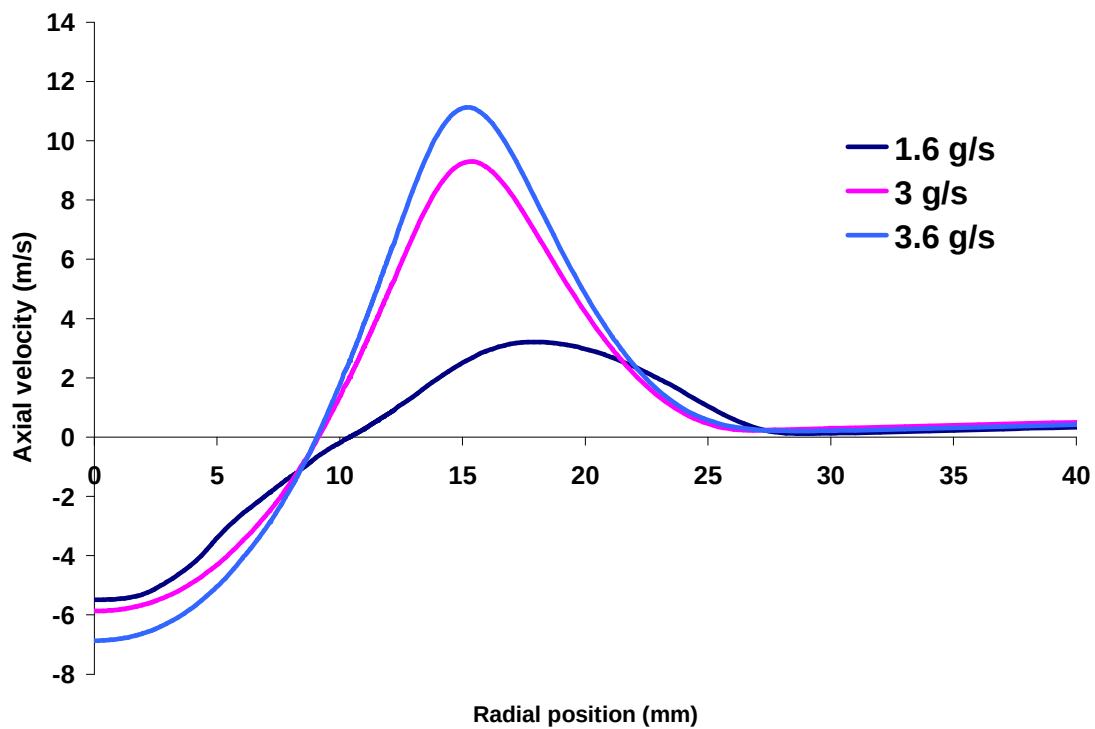


Figure 6. 20 Axial velocity profiles of cold swirling air at 30 mm downstream

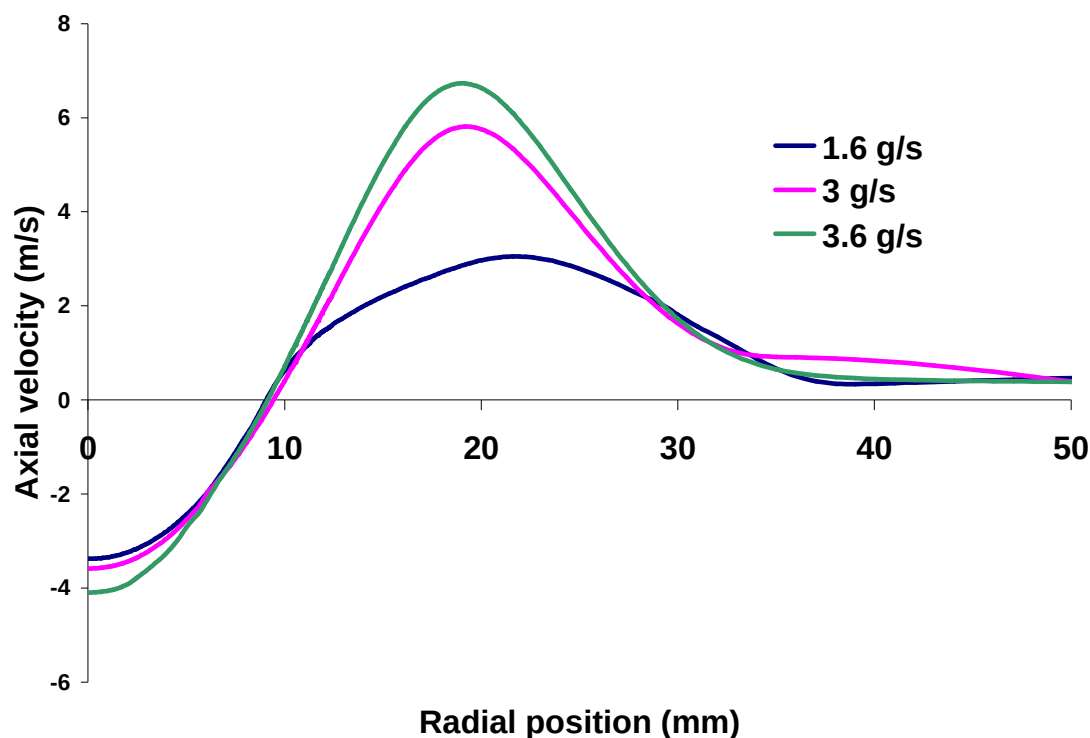


Figure 6. 21 Axial velocity profiles of cold swirling air at 50 mm downstream

Typical axial velocities at different mass flow rates are shown in the figure 6.19 to 6.21 at axial position varying between 1 cm and 5 cm from the swirler. The position of the maximum gradients in the axial velocity profiles coincide with the boundary of the reverse flow zone in every flow field and velocity gradients are the strongest close to the swirler exit.

Figure 6.19 to 6.21 show that the peak axial forward and reversed velocity is associated with the case with the higher mass flow rate and these velocities progressively decrease with the air mass flow rate.

To summarize, the calculated gas flow field show that the large recirculation zone, clearly evident in the PIV data, was well captured and the agreement between experimental data and numerical results was judged to be satisfactory in terms of forward and reversed flow zones values as well as the position and magnitude of the peak velocities using the RSM model, although the $k-\varepsilon$ model brings relatively accurate results in the region within the vicinity of the swirler.

For all the mean flow values considered, a recirculation region is observed as demonstrated by the numerical results with the axial velocity profiles. The upstream stagnation point is always located close to the swirler exit, while the downstream stagnation point depends on the air mass flow rate. The air jet spreads further out radially as the flow is moving downstream and the reverse velocities were observed to disappear further downstream at a distance depending on the air mass flow rate. The numerical results demonstrated that there is a direct effect of the air mass flow rate and Reynolds number on the size of the recirculation zone since an increase of air mass flow rate is seen to increase the strength of the recirculation zone.

The numerical simulations provided greater insight on the flow dynamics of the experimental configuration in addition to providing evidence of model validation. However, the 2 D nature of the PIV data is restrictive and the specification of the boundary conditions is incomplete, since small changes in these conditions can be the cause of large discrepancies in the flow field. Tangential velocity measurements should be made available as well as turbulence intensity profiles to have a more complete assessment of the experimental conditions, in order to fully validate the numerical results. Indeed, different tangential velocity profiles may modify the flow field (Ramos and Somer, 1985).

6.5 *Reacting Sprays*

6.5.1 Fuel Type

Whilst the experimental measurements in the AFTUR programme also included pure rapeseed oil, the reported simulations focus on the fuels, ethanol and Rix biodiesel (fatty acid methyl ester). Ethanol was found to be the most volatile, whilst rapeseed oil was the most viscous. The similarly high viscosity of the biodiesel relative to ethanol implies that it needs to be preheated, in order to bring down this parameter which has a strong influence on the Sauter mean diameter as illustrated in section 3.3 of the Fuel Properties chapter.

6.5.2 Initial and boundary conditions

Some of the boundary conditions correspond to measurement conditions, in others the air mass flow rate has been scaled with pressure at a fixed fuel rate. Scaling with pressure preserves the air velocity which has a significant influence on atomization. Simulations have been conducted both in an open combustion chamber and pressure rig for ethanol but only in pressure rig for Rix biodiesel. Boundary conditions in the open atmosphere and the pressure rig are summarized in table 6.2 and 6.3. The atmospheric ‘free condition’ rig offered several opportunities and advantages, for example:

- To establish the design criteria for the more complex high pressure rig.
- To have full optical access when familiarising with the measurement technologies.
- To investigate the constraints and implications when using a two-dimensional PIV system in a three dimensional flow.
- To investigate the geometrical, optical and flow rate restrictions when using PDPA in combusting sprays.
- To facilitate those measurements that are not possible (or extremely difficult to perform) in a pressure casing - such as PIV measurements in planes that are not vertical or hot wire velocity measurements close to the exit of the swirler.
- To produce comprehensive data under relatively simple flow conditions for evaluation of CFD computations.

	Unconfined ethanol simulations
Primary air mass flow rate	1.6 g/s
Fuel mass flow rate	0.36 g/s
Fuel temperature	293 K
Air temperature	293 K

Table 6. 2 Boundary conditions for ethanol in unconfined rig

	Ethanol					Biodiesel			
Pressure (atm)	1	2	3	5	10	1	2	3	10
Primary air mass flow rate (g/s)	1.6	3.2	4.8	8	16	3	6	9	30
Secondary air mass flow rate (g/s)	12	12	12	12	12	12	12	12	12
Fuel temperature (K)	288					414	430	430	430
Air temperature (K)	300					423	460	463	470
Fuel mass flow rate (g/s)	0.36					0.75			

Table 6. 3 Boundary conditions for ethanol and biodiesel in confined rig

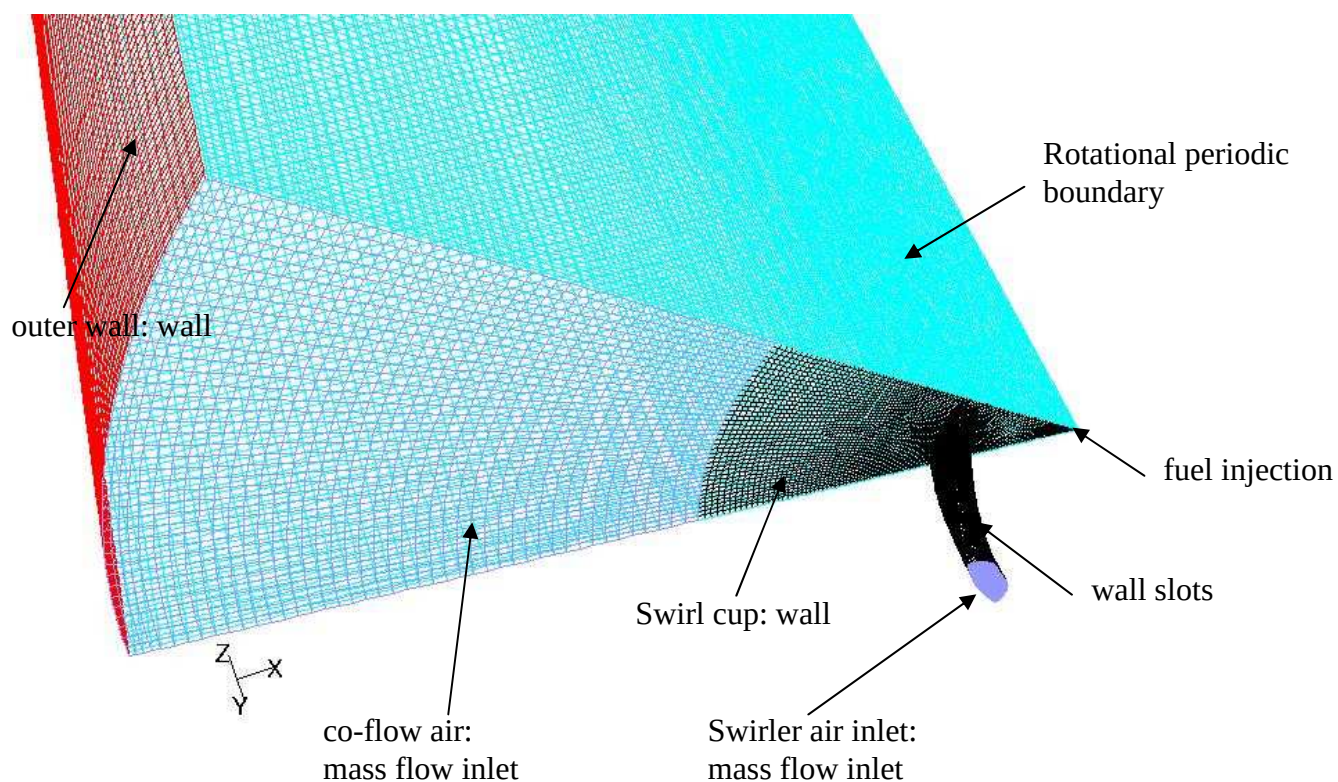


Figure 6. 22 Boundary conditions description

The boundary conditions set out in FLUENT are illustrated figure 6.22. The air inlet and co flow air boundary conditions, respectively the primary and secondary air flow have been designed as mass flow inlets, with the mass flow rate used as an input. The mass flow rate was varying according to the fuel type and operating pressure as seen figure 6.22. Different turbulence specification methods for the boundary conditions exist within FLUENT:

- k and ε
- intensity and length scale
- intensity and viscosity ratio
- intensity and hydraulic diameter

FLUENT documentation recommended that for flows downstream of turning vanes, which corresponds to the type of flow encountered in this study, the best option was to choose the intensity and hydraulic diameter method. The characteristic length of the flow opening has to be specified for the hydraulic diameter. The turbulence intensity at the primary and secondary air inlets were estimated at around 5% based on the following formula from an empirical correlation for pipe flows:

$$I = 0.16(\text{Re}_{DH})^{-1/8} \quad \text{Equation 6. 3}$$

with the Reynolds number defined as :

$$\text{Re} = \frac{UD}{\nu} \quad \text{Equation 6. 4}$$

The Reynolds number varied between 3000 and 6000 at 1 atm for the ethanol and biodiesel simulations, and could reach up to 54 000 for biodiesel at 10 atm, therefore the turbulence intensity was comprised between 4 and 6% as seen figure 6.23. A turbulence intensity of 1% or less is generally considered low and turbulence intensities greater than 10% are considered high.

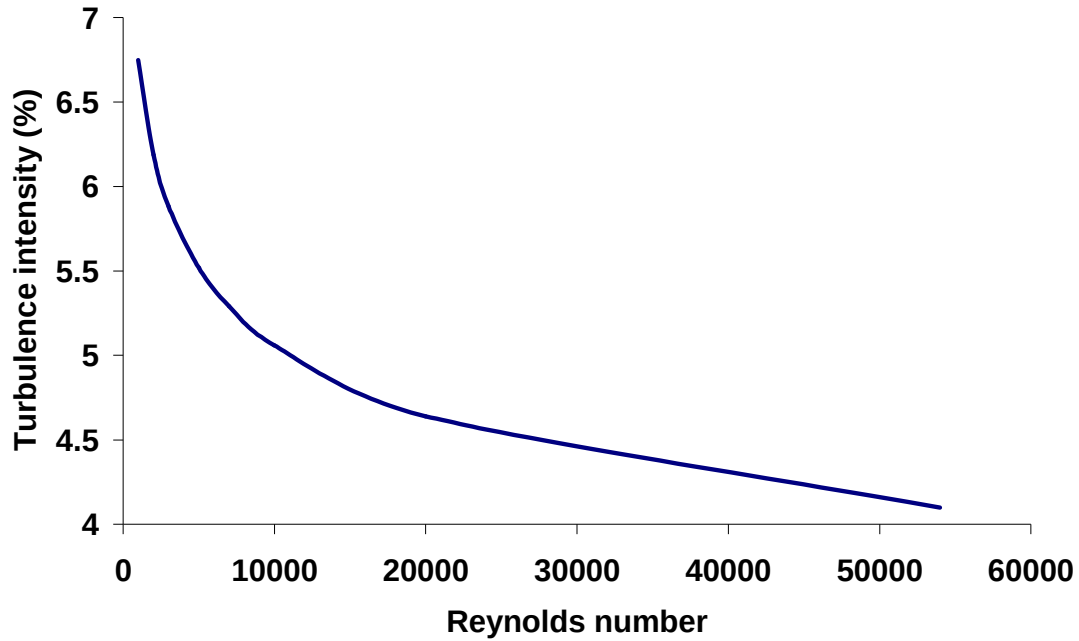


Figure 6. 23 Turbulence intensity as a function of Reynolds number

The air exit, where the air is extracted from, is set up as a pressure outlet. In the open configuration, the outer wall label is set up as a pressure outlet, and as a wall when the pressure casing is installed. The enclosure walls –labelled outer wall on figure 6.22 – are heated by radiation and convection from the hot gases inside the pressure rig. Therefore the uncooled liner temperature is determined based on a method of calculation described by Lefebvre (1998b) which yield a liner temperature of 1050 K.

When the discrete phase model is activated, a boundary condition has to be assigned to droplets which tend to hit the wall. The largest drops which managed to hit the wall formed a film once they touched the surface. The droplets are not reflected on the wall, since the experiments showed that the droplets do not bounce on the wall casing, there was a choice between “escape”, “wall-jet” or “trap” boundary condition. The wall-jet boundary condition is appropriate for high-temperature walls where no significant liquid film is formed and in high-Weber-number impacts where the spray acts as a jet but not for regimes where film is important. In the present simulations the Weber number is quite small as seen figure 4.9 therefore the choice is resumed to either escape or trap boundary condition. The “escape” boundary condition assumes that the droplet vanishes once it hits the wall while the “trap” condition assumes that the droplet immediately evaporates when it enters in contact with the wall.

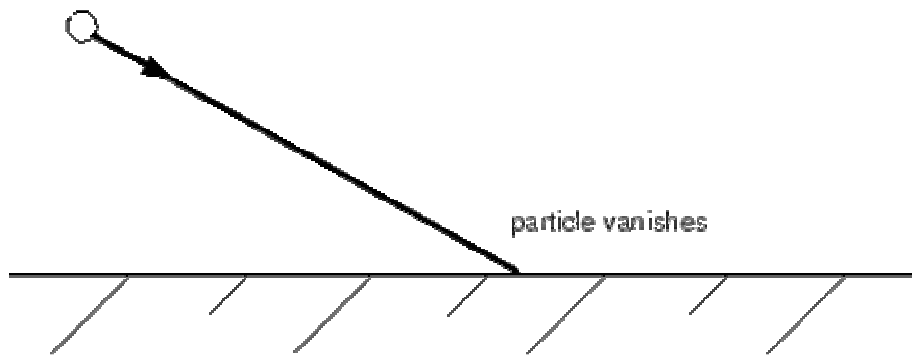


Figure 6. 24 Escape boundary condition

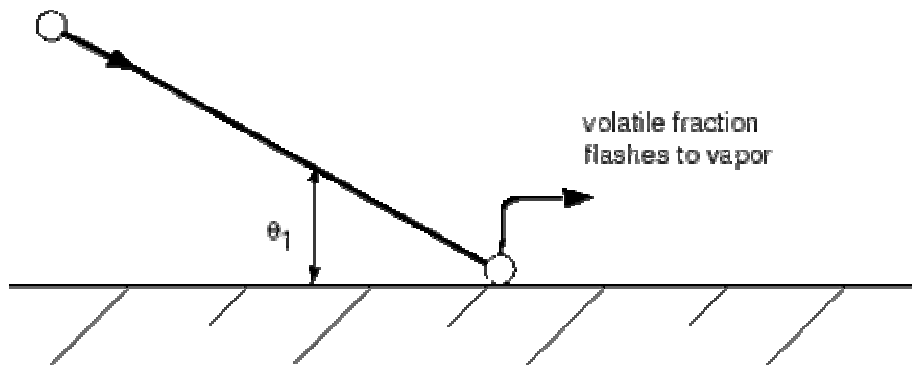


Figure 6. 25 Trap boundary condition

The “escape” boundary condition will have no influence on the flame structure since the droplet will vanish when in contact with the liner, while the “trap” boundary condition will produce some fuel vapour. Since the liner temperature is significant, droplet evaporation is likely to occur and cannot be neglected, therefore the “trap” boundary condition has been chosen.

6.6 Unconfined Turbulent Ethanol Spray Flame Study

For the reasons mentioned in section 6.5.2, a preliminary study was undertaken in an open laboratory environment. This case will be considered the pilot study in order to give a first assessment of the CFD code. The numerical results obtained are compared with the experimental data and a discussion ensues over the discrepancy between both sets of data.

The ethanol fuel and air are both assumed to be injected at a uniform isothermal temperature of 293K with a top hat profile for air. The fuel flow rate was set as in the

experimental conditions at 0.36 g/s with the air flow rate exiting the swirler at 1.6 g/s. These imply velocities of typically 20 m/s immediately downstream of the air swirler.

In this section, the gas temperature, Sauter Mean Diameter, gas axial velocity comparison between experimental and numerical work are presented. These parameters were measured at 7 different distances (5mm, 10 mm, 20 mm, and every 10 mm up to 60 mm) from the nozzle exit. At each distance, measurements were made in the radial direction to determine the spray characteristics.

To perform the simulation, a pure cold gas phase computation was performed using the RSM model and when convergence of the cold gas phase was reached after around 30 000 iterations, the liquid spray was injected. After the discrete phase is added to the simulation, convergence was assessed to be reached after 10 000 iterations. The convergence method is described in section 5.5.4. The multiphase flow computation was performed by injecting 6000 parcels distributed between 20 injection points over the 36 ° sector representing 1/10th of the full geometry of the domain. The spray was distributed between 6 particle streams regularly spaced by an azimuthal angle of 5 °, from 40° to 65°. The particles ranged from 5 µm to 60 µm, based on the experimental data, and were fitted to a Rosin-Rammler distribution, which was described by 10 size classes of different diameters. The spray initial conditions are resumed in table 6.4. The droplets were injected every 20 gas phase iterations. This parameter might be increased in problems where there is a high discrete phase mass loading or a larger grid size. Indeed, the value of the number of gas phase iterations between updates of the discrete phase trajectory calculations must be high enough to permit convergence before the next discrete phase injection. In the case where the residuals for the gaseous phase have not relaxed sufficiently, then it would be necessary to increase the value of this parameter. If the value is too low, then the gaseous phase will not have sufficient time to converge before the next discrete phase iteration and convergence will be too difficult to reach.

The number of parcels – in this case 6000 – is obtained by multiplying the number of particle streams by the number of diameter (or size classes) and the number of tries.

Spray parameters	
Cone angle	40, 45, 50, 55, 60, 65 °
Number of particle streams	20
Velocity magnitude	30 m/s
Total mass flow rate	0.36 g/s
Minimum diameter	5 μm
Mean mass diameter (MMD)	52.8 μm
Maximum diameter	60 μm
Spread parameter	4
Number of tries	5
Number of diameters	10

Table 6. 4 Spray initial conditions for ethanol in open atmosphere

20 particle streams x 6 angles (40, 45, every 5° up to 65°) x 10 diameters x 5 tries = 6000 parcels. As mentioned in section 5.5.2, increasing the number of tries would improve the statistical accuracy of the solution but to the detriment of computational time, which is an important factor for the completion of this study.

6.6.1 Gas Velocity profile

Comparison between the gas axial velocity profile PIV measurements and the CFD calculations are presented from figure 6.26 to figure 6.31. The axial velocities exiting in the immediate vicinity of the swirler at a height of 5 mm show a positive axial velocity of close to 20m/s, value which is accurately predicted by the simulations. The velocity profiles show a large recirculating region in the central region of the flow, extending from the nozzle exit towards a region around 10 cm downstream of the spray nozzle. The strongest recirculation has a peak axial velocity of around 8 m/s, at 20 mm from the spray nozzle and the swirl gradually decays as the fluid flows downstream.

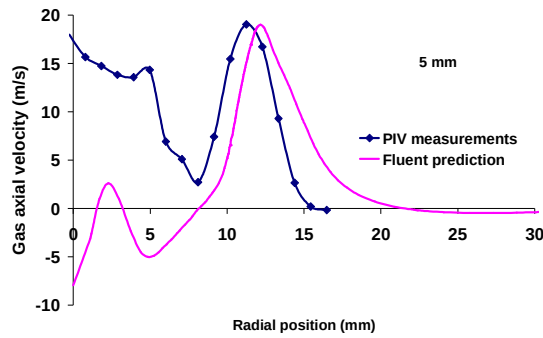


Figure 6.26 Gas axial velocity profile at 5 mm

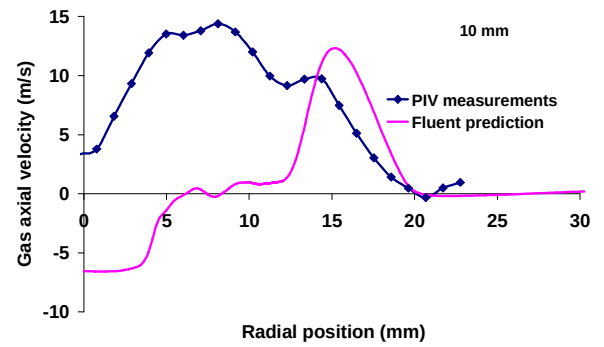


Figure 6.27 Gas axial velocity profile at 10 mm

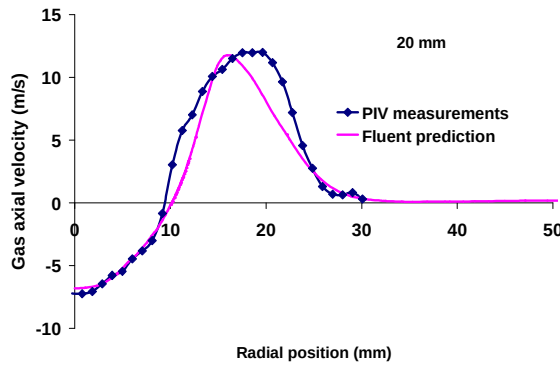


Figure 6.28 Gas axial velocity profile at 20 mm

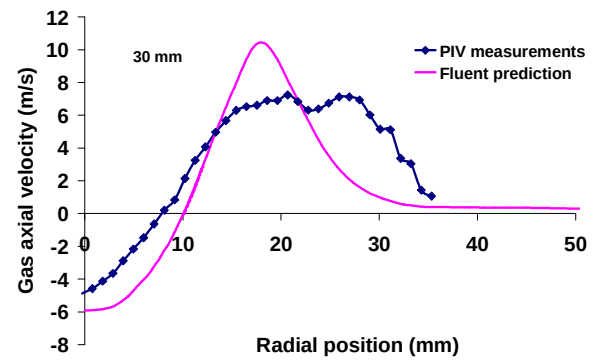


Figure 6.29 Gas axial velocity profile at 30 mm

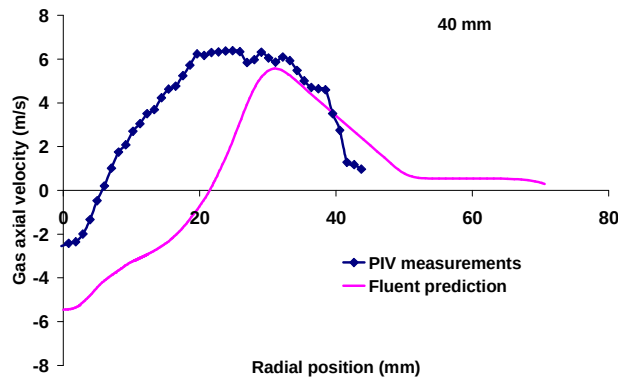


Figure 6.30 Gas axial velocity profile at 40 mm

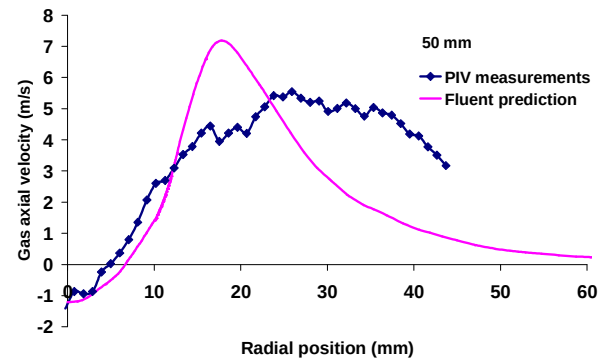


Figure 6.31 Gas axial velocity profile at 50 mm

In general, the results obtained numerically are in good agreement with the experimental data. However the calculation fails to capture the gas axial velocity in the immediate neighbourhood of the injector (cf. figure 6.26 and 6.27) where the predicted recirculation is stronger than observed experimentally and it appears that the observed axial peak velocities close to the centreline are not predicted by the simulation. These positive velocities could be generated by the seed material but it could also come from fine droplets from the spray, which would then be injected into the flow with sufficient momentum to have a substantial effect on the continuous phase. However the two way coupling between the spray and the gas phase does not appear to have a significant effect on numerical results. It is probably due to the fact

that the major hypothesis of Lagrangian methods is to impose a low volume fraction of the liquid fuel. It is evident that, close to the injector, where the liquid phase is dense, this hypothesis is not valid, with the discrepancy observed between the PIV measurements and the FLUENT predictions in the vicinity of the injector. A solid cone simulation was carried out in order to see if the spray would significantly modify the gas axial velocity profile in the vicinity of the atomizer.

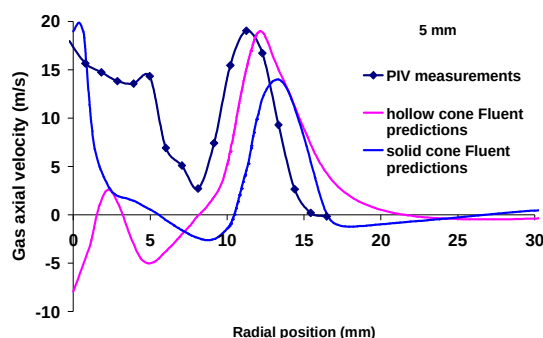


Figure 6.32 Comparison between a hollow and solid cone simulation with the PIV measurements at 5 mm

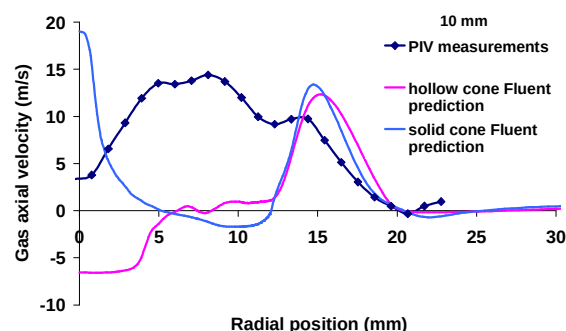


Figure 6.33 Comparison between a hollow and solid cone simulation with the PIV measurements at 10 mm

Fine droplet with a maximum SMD of 5 μm were injected on the spray centreline. Figure 6.32 and 6.33 illustrate a comparison between a hollow and solid cone simulation with the PIV measurements at 5 and 10 mm from the atomizer. At 5mm, the solid cone shows some positive velocities on the spray centreline but the simulation fails to capture the strong impact of the spray further out radially. Again at 10 mm, the impact of the spray on the centreline is clearly visible but is significantly overpredicted. Moreover, the simulation shows some significant discrepancy all along the radial direction. Therefore it can be concluded that the impact of the spray on the gas phase in the Lagrangian approach is not well predicted.

On the other hand, the predictions compare favourably with the experimental data as the flow moves further downstream, from a distance of 20 mm onwards. Indeed, while the positive axial velocity is slightly overpredicted at 30 mm and 50 mm and the width of the air jet underpredicted, the strength of the recirculation is accurately captured by the simulation. As demonstrated in the cold swirling flow section, the RSM model used in this study is more suitable to predict strongly swirling flows than the k- ϵ turbulence model.

6.6.2 Temperature profile/Flame structure

The computed structure of the ethanol spray flame in the open is shown in figures 6.34 to figure 6.39 with the spray initial conditions described table 6.4, which gives the radial profiles of gas temperature and a comparison between the numerical results and the thermocouple measurements at different axial positions. At 1 cm, the temperature peak at the centreline is underestimated by around 250 K. As mentioned in section 4.4.5 from the Experimental Study, the experimental errors coming from the thermocouple are estimated to be of around 50 K at most, so they are not believed to be solely responsible for the discrepancies observed. The poor agreement suggests that fuel-rich burning is evident within the cone and this is facilitated by the fact that ethanol is a highly volatile fuel. Figure 6.40 suggests that the fuel burns on the rich side of stoichiometry. In fact, the stoichiometric mixture fraction is at 0.11 while the predicted mixture fraction at 1 cm is close to 0.4.

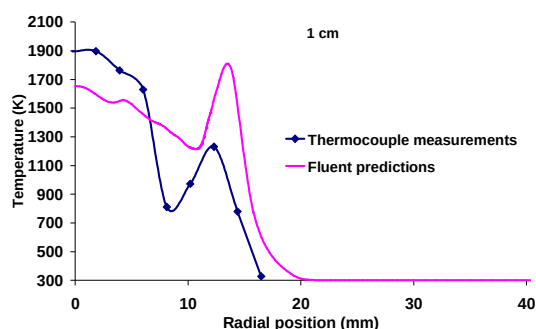


Figure 6. 34 Temperature profile at 1 cm

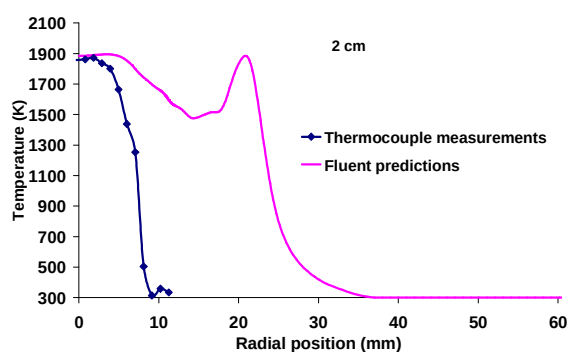


Figure 6. 35 Temperature profile at 2 cm

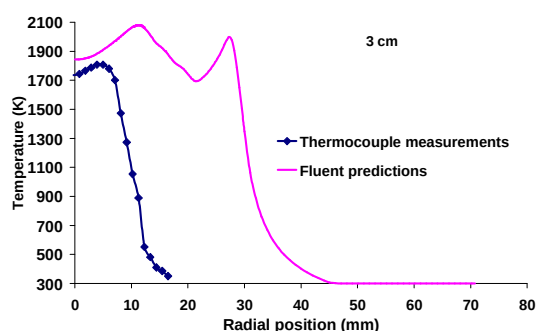


Figure 6. 36 Temperature profile at 3 cm

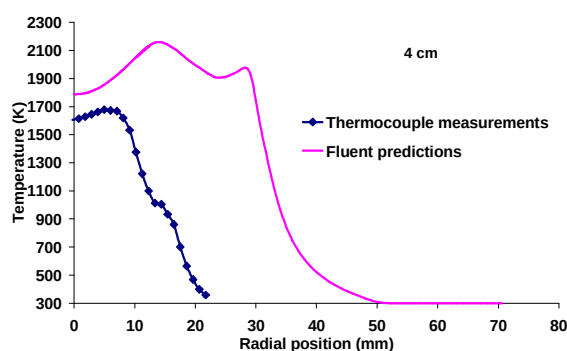


Figure 6. 37 Temperature profile at 4 cm

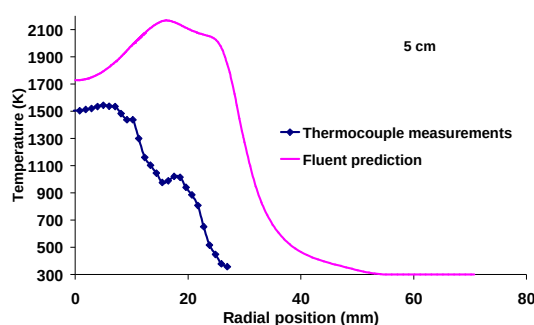


Figure 6.38 Temperature profile at 5 cm

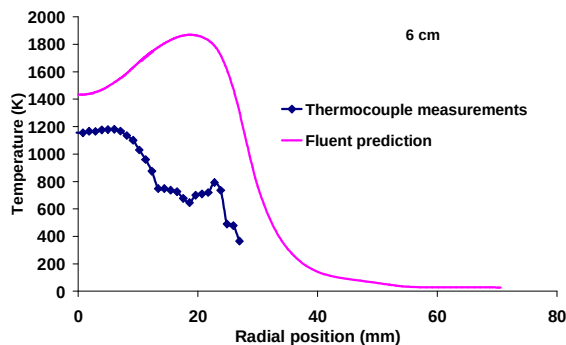


Figure 6.39 Temperature profile at 6 cm

The most likely explanation for the fact that the fuel is too rich too burn close to the nozzle is due to early vaporization and consequent rich mixing of fuel vapour with the air as the convection effects due to the significant initial relative velocity between the spray and the gas phase added to the effect of increased gas temperature further enhances the vaporization rate, which causes the mixture fraction to increase very rapidly along the spray. As a result, the vaporization rate is greatly enhanced, rendering the mixture increasingly fuel rich. Also, as mentioned in section 5.5.3 of the Computational Study, the Ranz-Marshall correlation used by default in the FLUENT model overpredicts the vaporization rate and can produce inaccurate results, especially for low Reynolds number. Also ethanol is known to be a volatile fuel which tends to exacerbate the flaws of the evaporation model since it starts evaporating at around 271 K at 1 bar and its boiling point is 351 K. Early vaporization leads to a large accumulation of fuel vapour in the vicinity of the nozzle. As a result, the temperature is predicted to be well below stoichiometric temperature and severely underpredicted close to the nozzle. In a realistic situation, the region in the vicinity of the atomizer would be expected to correspond to a fuel (vapour) lean condition because the initial spray region is dense and relatively cold.

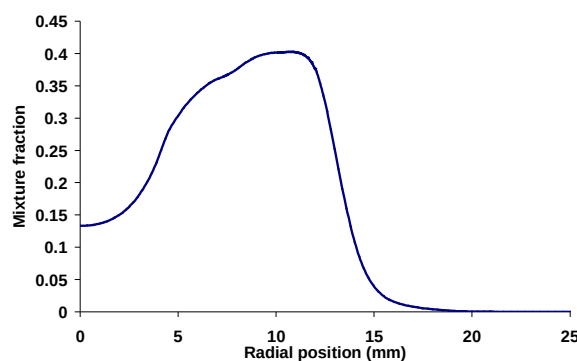


Figure 6.40 Predicted mixture fraction at 1 cm

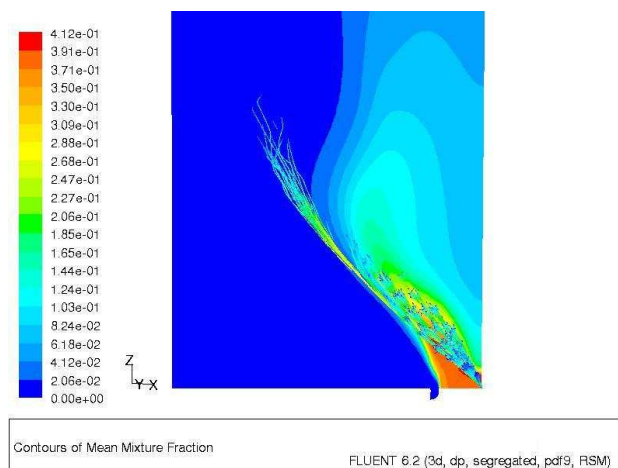


Figure 6.41 Mixture fraction field superposed with spray trajectories

At 1 cm, the CFD predictions show some interesting features such as double peaks in temperature. This feature has been discussed in the literature (Aggarwal and Chitre, 1992; Presser et al. 1988) and it seems that the first peak close to the centreline where the maximum temperature reaches 1654 K, stems from the combustion of quickly evaporated small ethanol droplets while the simulation identifies the second temperature peak located further out radially as the location of the main reaction zone. In that region, the maximum temperature is predicted to be higher than on the centreline, reaching 1806 K. Therefore unlike the thermocouple measurements, the main reaction zone is shifted radially outward of the spray centreline. The same observation applies at 2 cm downstream of the fuel atomizer. The peak temperature corresponds to the location immediately above which some droplets complete vaporization as illustrated figure 6.42.

Further downstream, the simulation predicts that the peak temperature is also located at the same radial location. However, the experiments consistently show that the flame peak temperature is located on the spray centreline. Although the flamelet model will always predict burning if the mixture fraction is within the range $0 < Z < 1$, it would have been expected that the spray would cool the gas phase region along its path in a more significant manner, since it would locally act as a heat sink on the ambient air, as the droplets would be evaporating but not combusting in this region. However it appears that it is not well predicted in the present simulation, and this results in a significant overprediction in the flame width.

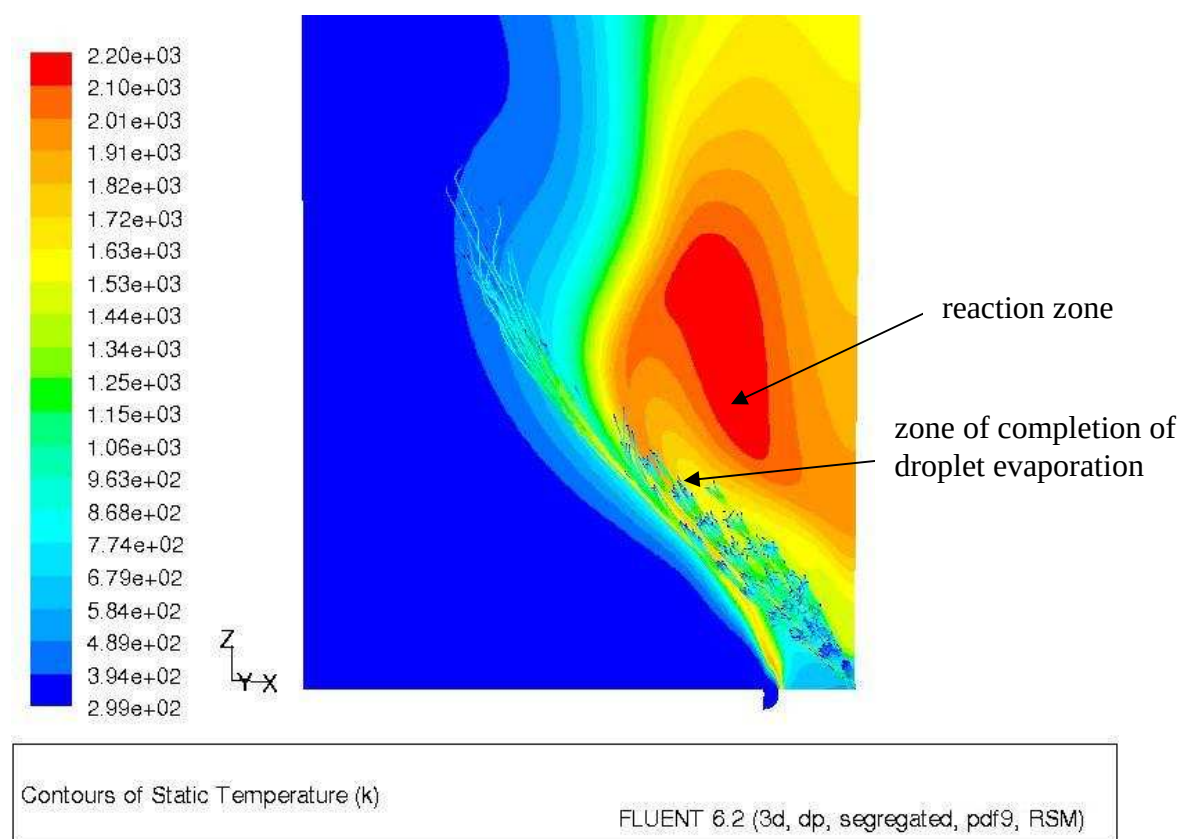


Figure 6.42 Temperature field for an unconfined ethanol flame. The reaction zone is located immediately above the zone of droplet evaporation.

The temperature overprediction might be a result of rapid droplet vaporization. In fact, as the droplets evaporate and vanish, they do not penetrate deep into the pressure rig and therefore do not act as a significant heat sink. Indeed, the liquid fuel penetration may be an indirect measure of the size of the fuel drops in the combustion chamber and of the rate of vaporization of the fuel. If the droplet Sauter mean diameter is correctly predicted at around 10 and 20 mm from the atomizer, this would imply that the droplet initial sizes affected at the spray nozzle is not the source of the discrepancy. Then it would probably demonstrate that the evaporation rate is too strong and the spray does not act as a significant heat sink due to underprediction of the droplet penetration.

Given the range of processes occurring in this initial region, the strategy adopted was that of prescribing an initial distribution at zero height and matching its evolution to the downstream measurement, especially 1 and 2 cm downstream, where the liquid fuel is estimated to be in the shape of spherical droplets. At 5 mm, although ethanol is

not a very viscous liquid, droplet still have ligament like structure so droplet information at this height has to be discarded. Therefore a hypothetical distribution has to be defined at the injector orifice which would match the droplet size at 10 mm and further downstream. The spray combustion computations involve empirical inputs for the initial droplet size distribution based on:

- the MMD or mass mean diameter
- the minimum $D_{\min}$ and maximum diameter $D_{\max}$
- the spread parameter n

Simmons (1977) directly related the MMD with the SMD and found that drop size distribution after primary breakup satisfied the universal root normal distribution with $MMD/SMD = 1.2$. To ensure that the droplets have reached their spherical shape, PDPA measurements were considered at a height of 2 cm, and the droplet SMD at this location is around 44 microns, consequently the droplet $MMD = 52.8$ microns.

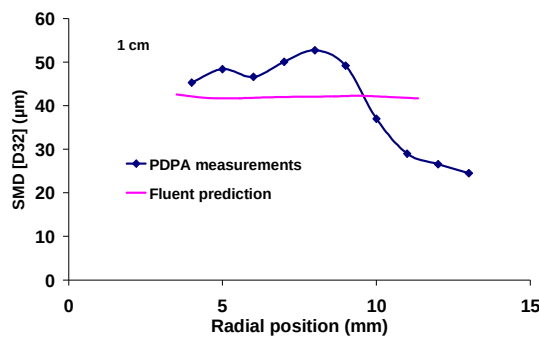


Figure 6. 43 SMD at 1 cm

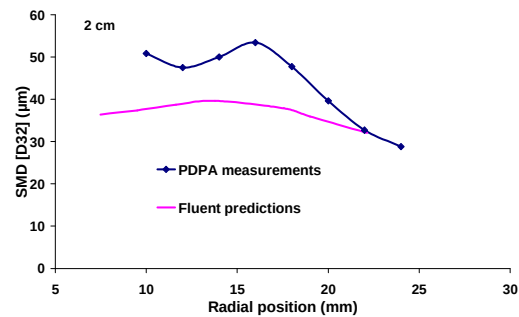


Figure 6. 44 SMD at 2 cm

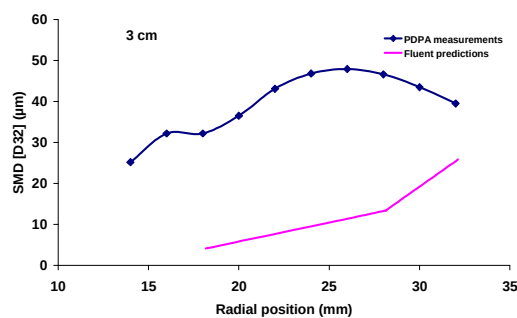


Figure 6. 45 SMD at 3 cm

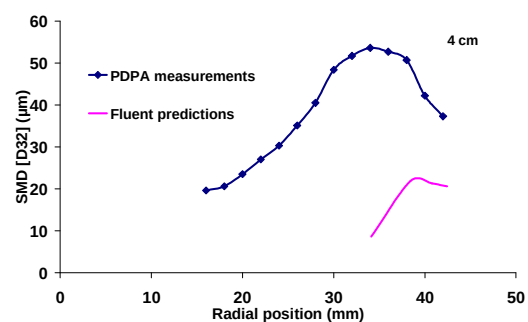


Figure 6. 46 SMD at 4 cm

Figure 6.43 shows the profile of the SMD at 1 cm and it appears that the droplet SMD and the radial spread of the spray are accurately predicted, however as the spray moves further downstream, there is a large underprediction of the droplet SMD,

especially from an axial distance of 3 cm, seen figure 6.45. Moreover, the radial spread of the spray in the simulation is significantly more reduced as the spray moves further away from the fuel atomizer, implying that the droplets particularly on the inner edges have already completely vaporized, unlike what is observed in the experiments. Consequently it can be concluded that the predicted droplet evaporation is stronger than is observed experimentally. The resulting reduced penetration also highlights the fact that it will provoke a high centreline fuel concentration.

In order to improve the droplet evaporation for the present study, several approaches exists:

- change the evaporation model
- change the droplet initial size

However, as it will be mentioned in the Discussion section, options to change the evaporation model within FLUENT appears to be a rather extremely limited, as more sophisticated models imply the representation of temperature gradients within the droplets, which is not possible to achieve with FLUENT. The droplet size distribution as well as the modification of the fuel temperature will rather be investigated in the section 6.7.1 where the confined rig is more representative of conditions encountered in gas turbine systems.

Besides the issue of the rapid fuel evaporation, temperature on the centreline seems to be accurately predicted. Therefore the strong evaporation rate will have an impact on the structure of the flame along the spray path, but temperatures elsewhere do not seem to be affected. Hence, whilst calculated temperatures on the centreline show a good agreement with the thermocouple measurements, the temperature further out radially are overpredicted seemingly due to an overprediction of the evaporation rate. The implication is that the spray flame structure is strongly influenced by the liquid-phase processes and cannot be simulated by the simple modification of the single phase models.

Moreover, it is expected that the swirling air has a significant influence on the flowfield and the structure of the flame and the dip in temperature observed experimentally coincides with the trajectory of the air coming out of the swirler. Local flame extinction on the outer edges of the swirler occurs because the strain rate

encountered in this area is beyond the critical strain rate for ethanol, which has been predicted by CHEMKIN to be around 500 s^{-1} and as a result, heat loss will be sufficient to quench the flame in this region.

Temperature profiles from flamelet calculations are shown with the corresponding strain rate at 1, 2 and 3 cm figure 6.47 to 6.49. FLUENT calculates the strain rate according to the formula proposed by Bray and Peters (1994):

$$a = \frac{\mathcal{E}}{k_{turb}} \quad \text{Equation 6. 5}$$

Figures 6.44 to 6.46 show that despite the fact that the strain rate is increased in the region above the swirler, the gas temperature increases instead of decreasing as it would have been expected and seen in the experiments (cf. figure 6.47 to 6.49), especially when conditions are close to extinction. Indeed, at 10 mm, at a radial location between 10 and 20 mm, the flow field shows that the strain rate is above 500 s^{-1} , and FLUENT predicts the peak temperature in this particular region. The highly strained regions at 20 and 30 mm also show that the FLUENT flamelet model fails to predict the flame local extinction and the simulation in the present state is unlikely to succeed locally if there is significant departure from equilibrium.

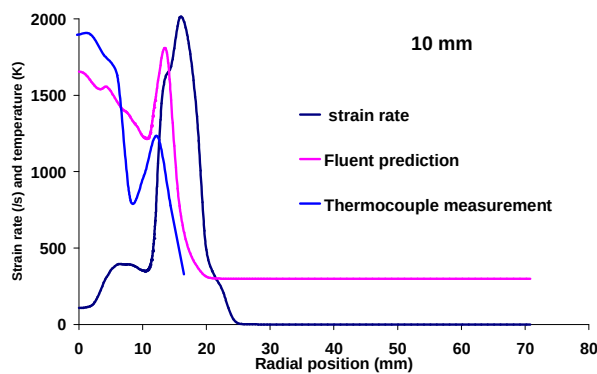


Figure 6. 47 Flame temperature versus strain rate at 10 mm

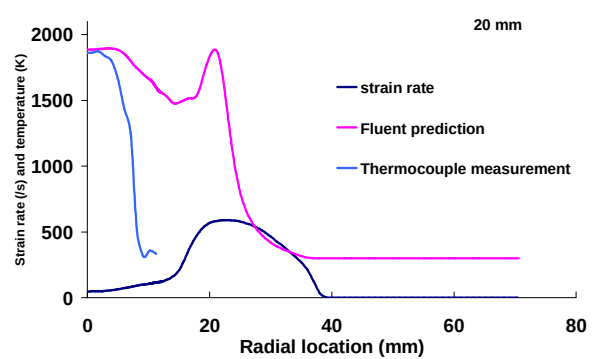


Figure 6. 48 Flame temperature versus strain rate at 20 mm

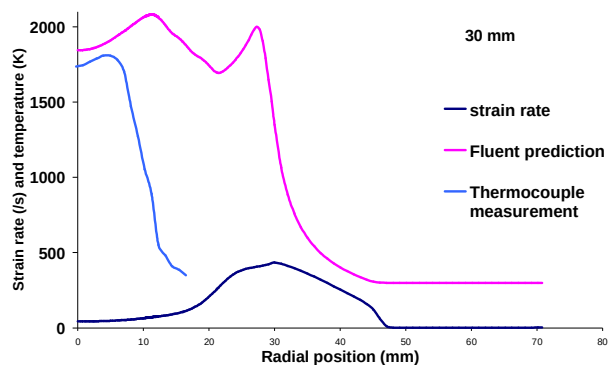


Figure 6.49 Flame temperature versus strain rate at 30 mm

The open flame simulations have shown that the temperatures are accurately predicted on the centreline but the spray evaporation rate seems to be overpredicted, which leads to an underprediction of the spray penetration. Moreover, despite the use of the flamelet model, FLUENT fails to predict local flame extinction. However, the atmospheric unconfined rig simulation is just a preliminary study to evaluate the accuracy of CFD predictions. In fact, numerical simulations in a confined pressure rig are of more interest since they describe conditions encountered in engineering gas turbine applications.

6.7 Ethanol Confined rig

Experimental data were compared with numerical results obtained for the ethanol spray flames in a confined rig. Compared to the previous simulation, the burner is enclosed within a pressure vessel, hence defining the degree of confinement of the flowfield and possibly having an influence on the flowfield structure. The temperature of the walls might also affect the radiative heat flux, but the coflowing air stream is believed to isolate the flame from the influence of the wall. Moreover, ethanol flames are not very luminous and radiation will play a minor effect on the flame structure.

The approach used in the present work was to adjust the initial droplet parameters in order to match the experimental measurements made 10 and 20 mm downstream from the nozzle. The original distribution was generated by 10 different classes with a diameter class width of about 5 microns each. Droplet diameters were varying from 5 to 60 μm , with the droplet SMD estimated at 44 and the spread parameter at 4.

The injected spray is assumed to comprise 7 conical streams, spread every 5 degrees from a half angle of 40 degrees to 70 degrees, based on the experimental data. The number of tries was kept to 5 therefore the total number of parcels injected in the flow field was 7000 for the cases under consideration (7 cone angles x 20 particle streams x 5 tries x 10 size classes). The spray initial conditions are summarized table 6.5. At 1 atm, the reported ethanol mass flow rate and air mass flow rate were 0.36 g/s and 12 g/s respectively as described in table 6.3.

Spray parameters	Value
Cone angle	40, 45, 50, 55, 60, 65, 70 °
Number of particle streams	20
Velocity magnitude	30 m/s
Total fuel mass flow rate	0.36 g/s
Minimum diameter	5 μm
Sauter mean diameter	44 μm
Mean mass diameter (MMD)	52.8 μm
Maximum diameter	60 μm
Spread parameter	4
Number of tries	5
Number of diameters	10

Table 6. 5 Spray initial conditions for ethanol in confined rig at 1 atm

The temperature plots are shown on figures 6.50 to 6.52 and the temperature field is displayed figure 6.53. As for the open flame observation, a likely explanation for the temperature underprediction around the spray at 1 cm is due to the fact that the fuel is too rich to burn as shown figure 6.54. In fact, the evaporation rate is overestimated in this region, due to the use of the Ranz-Marshall correlation. Indeed, the droplet Sauter mean diameter, although correctly predicted at 1 cm downstream of the spray nozzle, as illustrated figure 6.56, is significantly underpredicted after 3 cm figure 6.57, which implies a more rapid evaporation rate than observed with the experiments. As a whole, the predictions indicate a region in the vicinity of the atomizer where strong

evaporation and rich fuel mixture keep the temperature low. Further work is needed to address this problem.

As illustrated figure 6.50, at a height of 10mm, between 5 and 10 mm from the centreline, a cool region is visible due to the strong quenching action of the droplets, following by a significant rise in temperature, due to the turbulent convective transfer of heated products from the flame. Although the value of the dip in temperature seems to be well predicted, the experimental data show that it occurs further out radially, and is much more localized. This would imply that the spray trajectory is not well estimated. Indeed, figure 6.58 and 6.59 show that the predicted spray inner edge is located closer to the centreline than what is observed with the PDPA measurements. As a result, the angle spread of the spray will be varied to see its effect on the flame structure in section 6.3.2.

At 30 mm, the centreline gas temperature is well predicted but the peak flame temperature at this location is located further out radially, when the thermocouple measurements show that the temperature has already started decreasing. As noticed for the open flame simulation, by invoking the strain rate effects (cf. figure 6.60), the peak temperature is emphasized, which is the opposite of what would be expected. In fact, as the strain rate is increased due to the high turbulence levels encountered in some regions of the pressure rig, the flame should depart from equilibrium conditions and if it is increased beyond the extinction strain rate, the flame should extinguish.

The droplet trajectories for the spray are shown figure 6.55 with the temperature field. It can be clearly seen that the droplets enter the combustor with straight trajectories and droplet evaporation is completed when the spray reaches the flame front, 3 cm downstream of the spray nozzle. In fact, hot products drawn from downstream by the recirculation zone and entrained on the inner edge of the spray provide sufficient enthalpy to vaporize the spray and initiate combustion. However, the droplets on the outer edge of the spray, do not travel through the flame front and consequently continue their straight trajectory and penetrate further downstream in the pressure vessel before being decelerated by the drag forces and ultimately following the gas flow, but the simulation shows no wall wetting by the spray, as it appears that all the droplets have already vaporized before hitting the wall. However, large droplets pass

through the flame and penetrate the air jet coming out of the swirling, having a sufficiently strong impact to deflect the air jet, as a result broadening the recirculation zone as seen in a comparison between cold and reacting flow figures 6.61 and 6.62.

It takes about 1 ms for the smallest droplet to evaporate and 5 ms for the biggest one to do so. The droplet residence time is increased with the reversed flow generated by the swirlers, consequently enhancing mixing between the fuel and incoming air. The Reynolds number rapidly falls from a value of around 20 towards unity as the droplets reach the flame front. The reduction in the droplet Reynolds number is expected, as the drag effect tends to reduce the relative velocity between the droplets and the gas phase, and the evaporation process will reduce the droplet diameter, which by consequence decreases the Reynolds number.

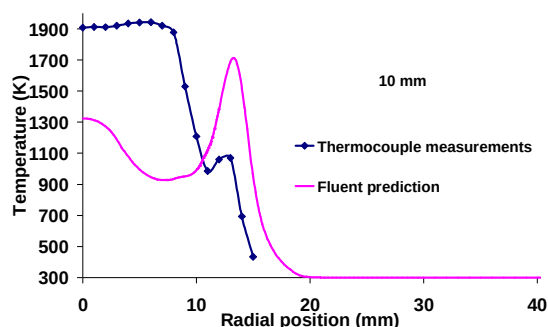


Figure 6. 50 Temperature predictions at 10 mm

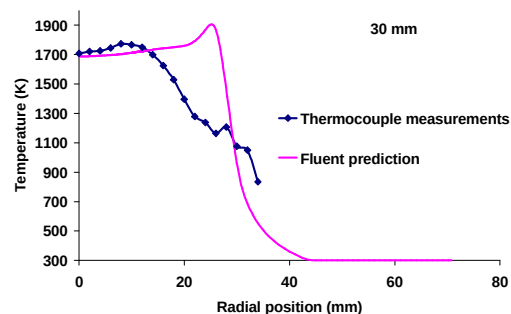


Figure 6. 51 Temperature prediction at 30 mm

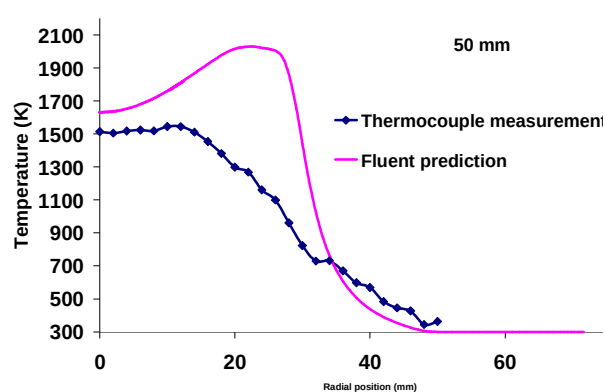


Figure 6.52 Temperature prediction at 50 mm

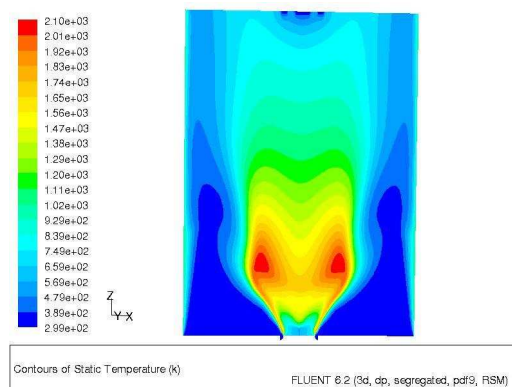


Figure 6.53 Temperature field

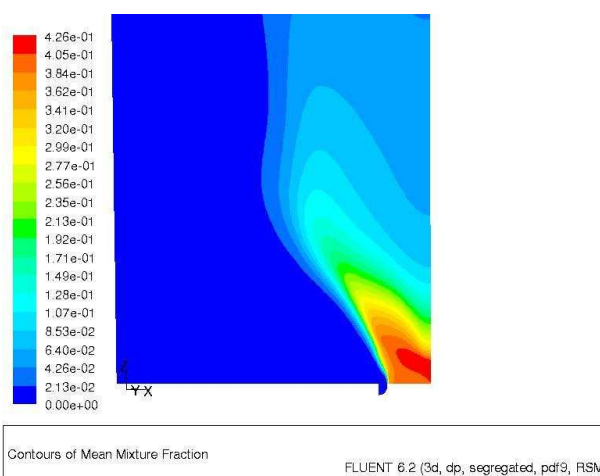


Figure 6.54 Fuel mixture fraction

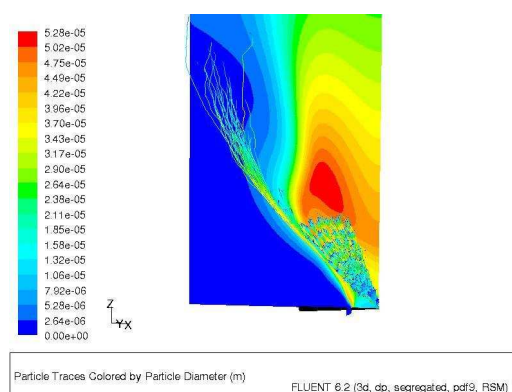


Figure 6.55 Flame temperature field and spray trajectory

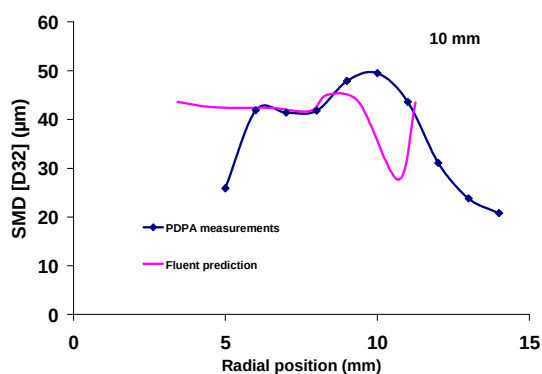


Figure 6.56 Droplet Sauter mean diameter at 1 cm

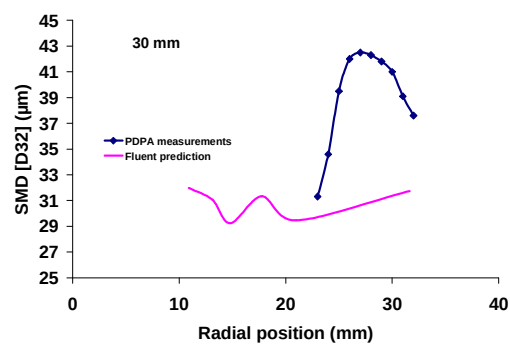


Figure 6.57 Droplet Sauter mean diameter at 3 cm

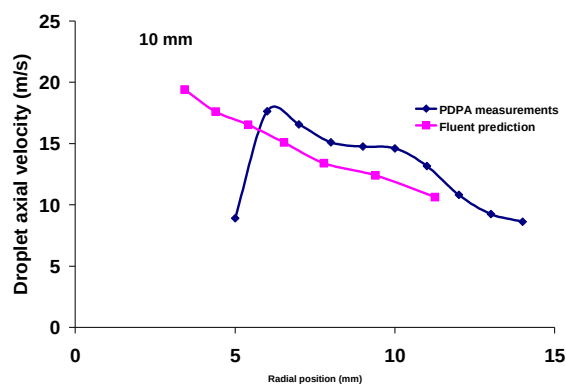


Figure 6. 58 Droplet axial velocity at 1 cm

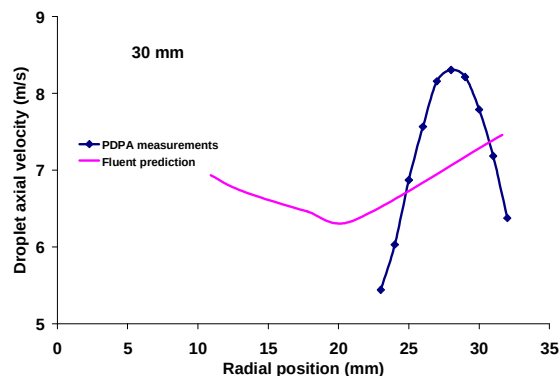


Figure 6. 59 Droplet axial velocity at 3 cm

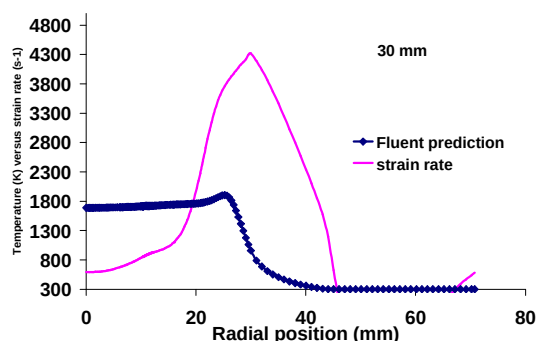


Figure 6. 60 Temperature (K) versus strain rate

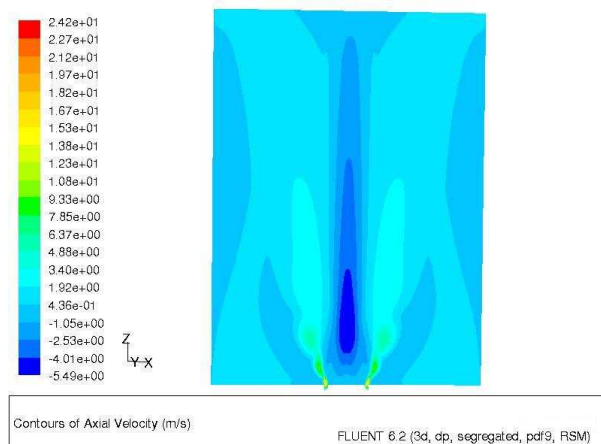


Figure 6. 61 Cold flow axial velocity contours

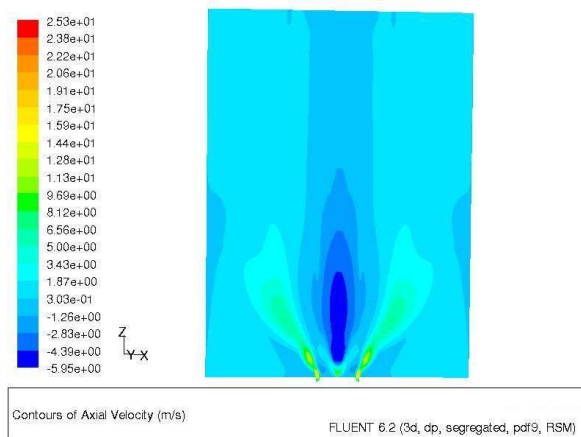


Figure 6. 62 Reacting flow axial velocity contours

The droplet visibly have a higher velocity than the gas phase initially as illustrated figure 6.63 but after their initial acceleration they begin to decelerate, as they travel through the gas phase, until they reach momentum equilibrium by rapidly settling

with the gas phase velocity, dropping from a maximum axial velocity of 20 m/s at 10mm to 7 m/s at 30 mm.

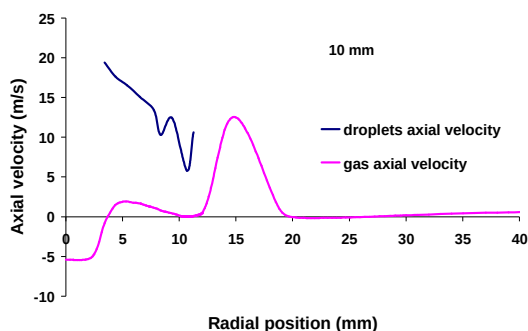


Figure 6. 63 Droplet and gas axial velocity at 10 mm

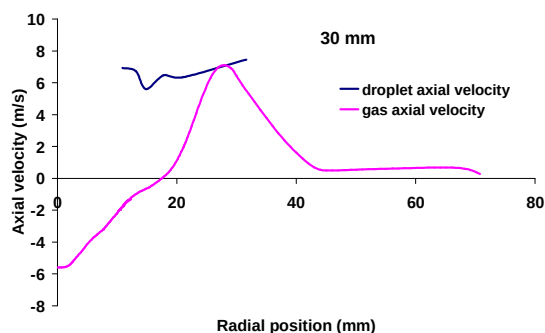


Figure 6. 64 Droplet and gas axial velocity at 30 mm

6.7.1 Droplet size distribution

Improvement in results cannot be accomplished without very accurate measurement of the droplet initial conditions as close as possible from the nozzle exit. However, one major challenge is the difficulty, even with nowadays technology, to make droplet measurements in the vicinity of the spray nozzle due to the high droplet number density and the fact that the liquid fuel is not at the stage of spherical droplets before at least 10 mm. The problem is further exacerbated by the difficulty of Lagrangian models to accurately model high volume fractions. However, this region is particularly crucial since it will determine how the spray will behave further downstream. Pressure swirl atomizers produce sprays which contain droplets of a wide range of sizes or polydisperse sprays and complex physical phenomena are involved in the present model, such as primary breakup, droplet evaporation and combustion processes which much be accurately determined, further complicating an accurate prediction of the initial droplet boundary condition. As a result, it is necessary to investigate the effect of the initial droplet size distribution on the spray flame structure.

Indeed, the structure of spray flames is highly dependent on the initial droplet size since it is a factor determining atomization quality, which in turn is (Lefebvre, 1984; Lefebvre, 1985) one of the main factors determining combustion performance. Kom and Sharma (2002) demonstrated that the combustion efficiency increases for all fuels when the initial SMD is increased from 25 μm to 50 μm , but a further increase from 50 to 75 μm , will negatively though slightly, affect the combustion efficiency. Combustion efficiency is considered to be high when it is close to 100 percent and is a result of proper atomization, leading to low emissions pollutants such as CO and NOx emissions. Khalil and Whitelaw (1977) observed that a significant shortening of the flame length was observed as the SMD was increased from 50 μm to 100 μm .

One major concern will be how to use the experimental data in order to convert them into initial conditions for the CFD model and to minimize uncertainty in the droplets initial conditions specifications. Detailed drop size distributions were fitted to a Rosin-Rammler distribution. The Rosin-Rammler distribution function is based on the assumption that an exponential relationship exists between the droplet diameter, d , and the mass fraction of droplets with diameter greater than d , Y_d and is described as follow:

$$Y_d = e^{-(d/\bar{d})^n} \quad \text{Equation 6. 6}$$

As defined in section 6.6.2, several parameters may be changed in the Rosin-Rammler distribution:

- the minimum and maximum droplet diameter to be considered in the size distribution
- the mean mass droplet diameter MMD
- the spread parameter n , with n representing an exponent measuring the spread of the distribution.
- the number of size classes, i.e. the number of diameters in each distribution

The parameters which are of more interest are believed to be the mean diameter and the spread parameter.

Different droplet size histograms have been compared as listed in table 6.6. One parameter was changed at a time compared to see its effect on the flame structure.

When the mean diameter was increased, the maximum diameter was arbitrarily increased to 80 μm . All the results will be compared to case 1.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8
Spread parameter	4	4	4	3	5	4	4	4
Minimum diameter (μm)	5	1	5	5	5	5	5	5
Mean diameter (MMD) (μm)	44	44	44	44	44	53	72	36
SMD (μm)	36	36	36	36	36	44	60	30
Maximum diameter (μm)	60	60	60	60	60	80	80	60
Number of size classe	10	10	5	10	10	10	10	10

Table 6. 6 Run cases with different droplet size distribution

For case 2, the droplet minimum diameter has been reduced from 5 μm to 1 μm . The number of size classes has been reduced from 10 to 5 for case 3, while the spread parameter was changed respectively to 3 and 5 for case 4 and 5. Finally the SMD was modified respectively to 44, 60 and 30 μm in case 6, 7 and 8.

6.7.1.1 Influence of minimum droplet size

The minimum droplet size detected by the PDPA devices was around 5 microns, so this analysis is performed to give an indication of how sensitive the results are if the PDPA device could take measurements as low as 1 micron.

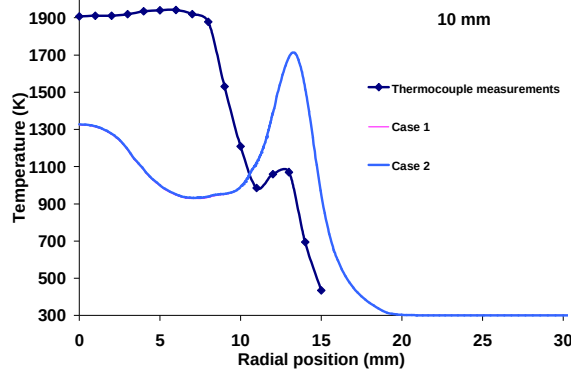


Figure 6. 65 Comparison between $D_{min} = 1 \mu$ and $D_{min} = 5 \mu m$ at 10 mm for ethanol confined rig at 1 atm

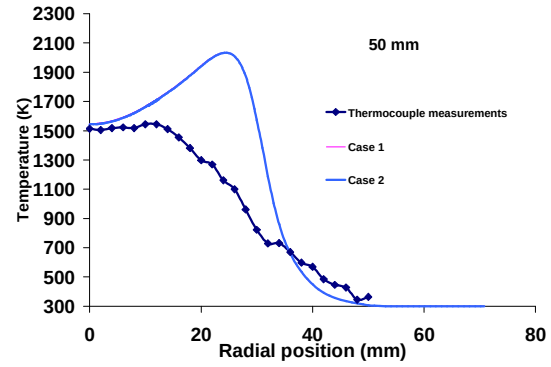


Figure 6. 66 Comparison between $D_{min} = 1 \mu$ and $D_{min} = 5 \mu m$ at 50 mm for ethanol confined rig at 1 atm

The flame temperature profiles, seen figure 6.65 and 6.66, show no variation from the flame with a 5 microns minimum diameter. This demonstrates that whether or not the real minimum droplet size is $5 \mu m$ or not, this has no significant influence on the flame properties. In fact, it has been mentioned in the past (Jasuja and Tam, 1992) that while bigger droplets affect combustion performance, ignition characteristics are influenced by the early availability of droplets of small size. However, spray ignition is beyond the scope of this study, unlike combustion performance.

6.7.1.2 Influence of number of size classes

The effect and sensitivity of FLUENT to the number of size classes specified on the numerical predictions have been analysed. Increasing the number of droplet diameter from 5 to 10, which in fact corresponds to increasing the number of droplet size classes from 4 to 9, does change the droplet size distribution as seen figure 6.67. The spread parameter as well as the Sauter mean diameter have been kept constant, with $n=4$ and $SMD = 36 \mu m$. A detailed description of the fuel mass fraction for 5 and 10 droplet diameters is respectively given table 6.7 and 6.8. By varying the number of size classes, these solutions explored the effect of varying the fuel split between the size ranges.

Size range	Fuel mass fraction
5 μm – 17 μm	0.074
17 - 28.9 μm	0.266
28.9 μm – 40.9 μm	0.413
40.9 μm – 52.8 μm	0.247

Table 6. 7 Droplet size distribution for 5 size classes

With 5 droplet diameters, the fuel proportion of small droplets is larger than when 10 droplet diameters are set, which would mean that more fuel is expected to evaporate from the droplet surface. Fuel mass fraction for 10 size classes is given below (table 6.8).

Size range	Fuel mass fraction
5 μm – 10.3 μm	0.008
10.3 μm – 15.6 μm	0.023
15.6 μm – 20.9 μm	0.055
20.9 μm – 26.2 μm	0.099
26.2 μm – 31.6 μm	0.149
31.6 μm – 36.9 μm	0.189
36.9 μm - 42.2 μm	0.199
42.2 μm – 47.5 μm	0.170
47.5 μm – 52.8 μm	0.115

Table 6. 8 Droplet size distribution for 10 size classes

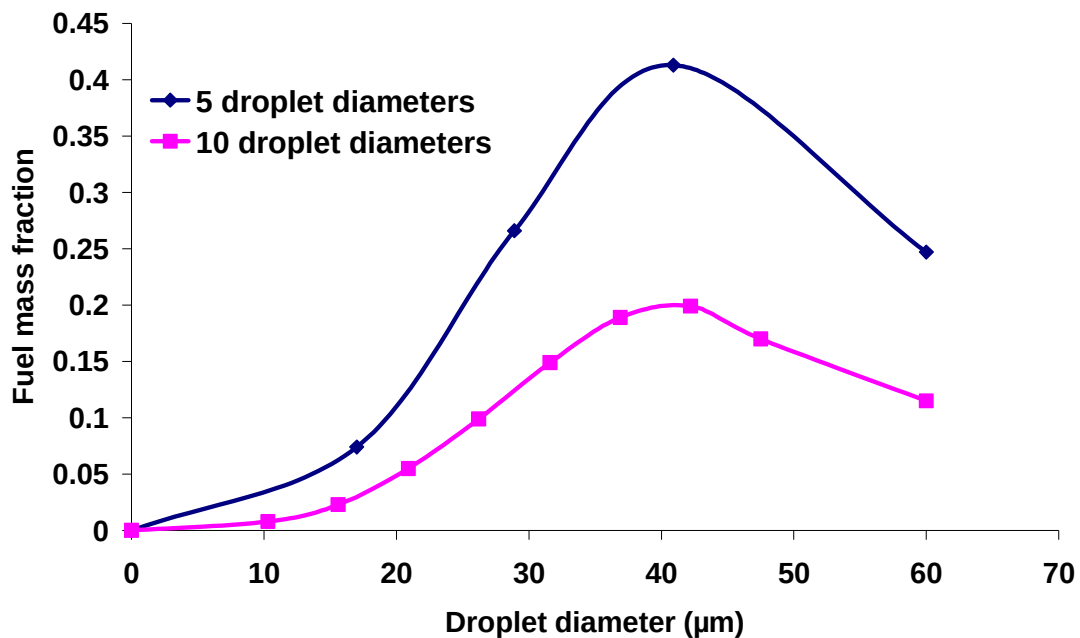


Figure 6. 67 Droplet size distribution for 5 and 10 droplet diameters

However, it does not appear to have a significant influence on the results. In fact, there is little difference between the temperature fields obtained at different heights as

illustrated figure 6.68 to 6.70, despite the fact that the fuel split differs in a non negligible manner between 5 and 10 droplet diameters, which would imply that FLUENT is not very sensitive to the number of size classes. The greater percentage of fuel in the smaller size ranges with 5 droplet diameters should result in a richer central core in the vicinity of the atomizer. This suggests that fuel mixing is not the main parameter compared to others in changing the spray flame structure.

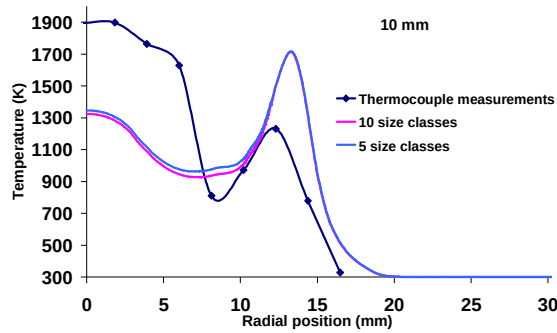


Figure 6. 68 Comparison between 5 and 10 size classes at 10 mm

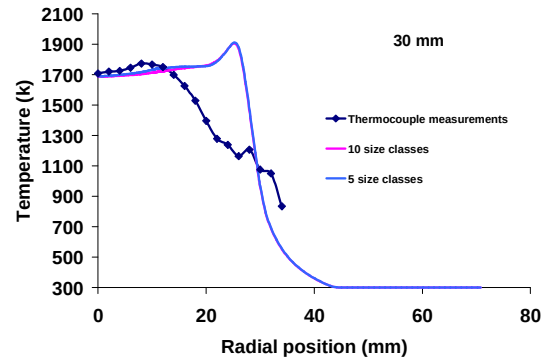


Figure 6. 69 Comparison between 5 and 10 size classes at 30 mm

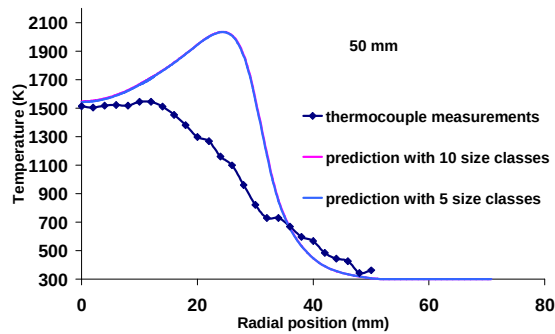


Figure 6. 70 Comparison between 5 and 10 size classes at 50 mm

6.7.1.3 Influence of spread parameter

The spread parameter was varied from 3 to 5 to see its influence on the flame structure. The spread parameter is a constant used in the Rosin-Rammler distribution function described equation 6.6 and is determined experimentally. Its value for pressure swirl atomizers (used in this study) usually varies between 3 and 5. Figure 6.71 shows that the higher the spread parameter, the larger the proportion of small droplets, consequently producing larger amount of vapour with a lower spread parameter. Although the temperatures are quite similar at 10 mm, significant differences are observed from a height of 30 mm. Since the spray with a spread

parameter $n = 3$ produced a smaller proportion of fine droplets, smaller amount of fuel vapour was then generated, which resulted in fuel lean conditions. In fact, spray evaporation is facilitated by the presence of a large proportion of fine droplets over larger ones. Less fuel lean conditions were encountered for the spray with a spread parameter $n = 5$, due to the larger presence of smaller droplets. As a result, 30 and 50 mm downstream from the spray nozzle, the stoichiometric conditions were most closely met for the case with $n = 5$ and the spray with $n = 3$ was burning at much leaner conditions than the case for $n = 5$ as illustrated figure 6.75 and 6.76. As a result, initial drop size distribution that produce smaller amounts of fuel vapour will result in cooler flames. Due to the difference in fuel distributions, the temperature profiles shown figure 6.73 and 6.74 display some noticeable differences in terms of peak temperature. As a result, 50 mm downstream of the spray nozzle, FLUENT predicted spray flames for $n = 3$ with temperatures more than 200 K lower than for the case with $n = 5$ (cf. figure 6.74).

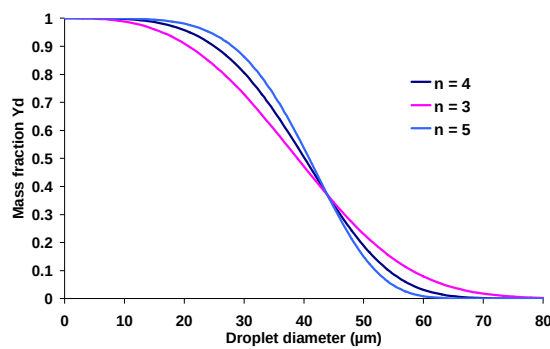


Figure 6. 71 Rosin-Rammler curves with $n = 3, 4$ and 5

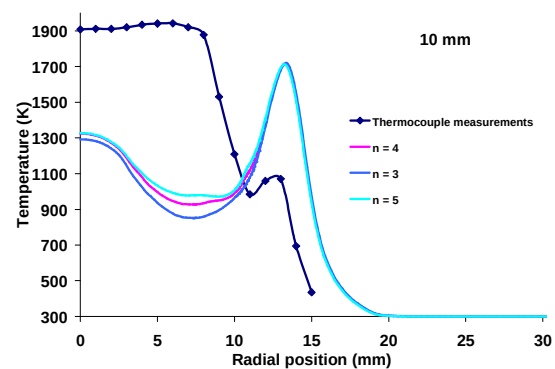


Figure 6. 72 Comparison for different spread parameters at 10 mm

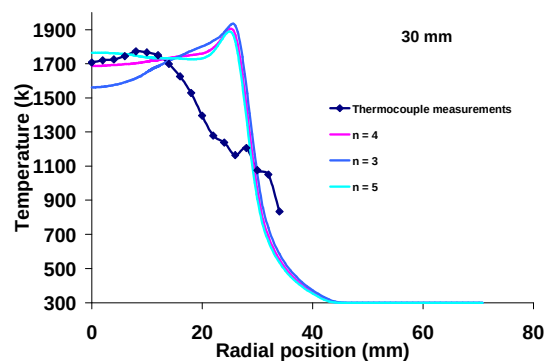


Figure 6. 73 Comparison for different spread parameters at 30 mm

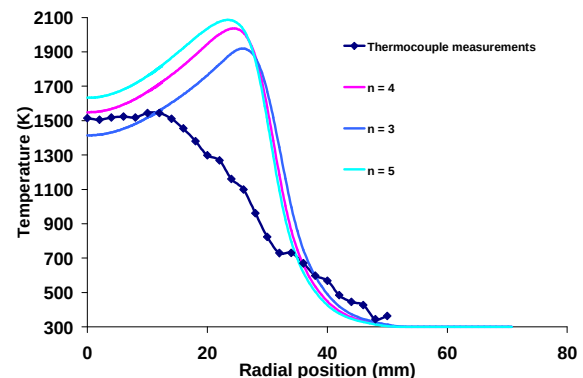


Figure 6. 74 Comparison for different spread parameters at 50 mm

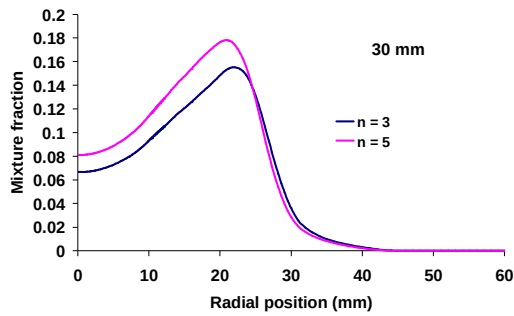


Figure 6.75 Mixture fraction comparison for $n = 3$ and $n = 5$ at 30 mm

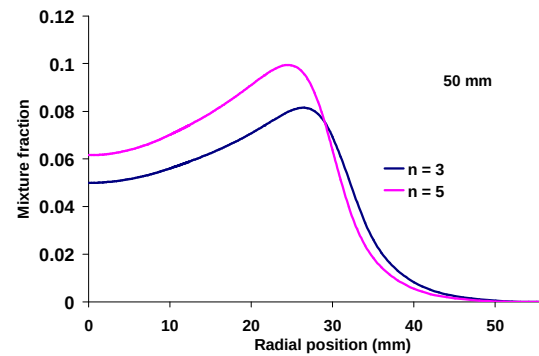


Figure 6.76 Mixture fraction comparison for $n = 3$ and $n = 5$ at 50 mm

6.7.1.4 Influence of Sauter mean diameter

The Sauter mean diameter, which represents the volume/surface ratio of the spray, is the most widely used parameter to describe the quality of “fineness” of an atomization process. This definition of mean drop size has special significance for heat and mass transfer application, especially in the field of spray combustion (Lefebvre, 1989). As seen in section 3.3 of the Fuel Properties chapter, the Sauter mean diameter depends on different fuel properties, such as surface tension and viscosity, fuel flow rate and injection pressure as well as air ambient density. In order to assess the influence of initial conditions on the flame structure, the initial Sauter mean diameter (SMD) of the spray was modified. The spread parameter was maintained at $n = 4$, while the SMD was varied from 36 to 60 μm . The results are summarized from figure 6.77 to figure 6.84.

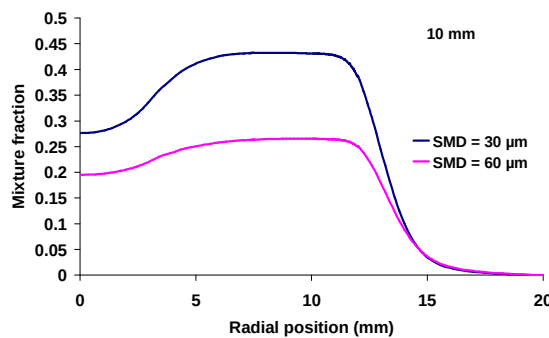


Figure 6.77 Mixture fraction profile at 10 mm for SMD = 30 to 60 μm

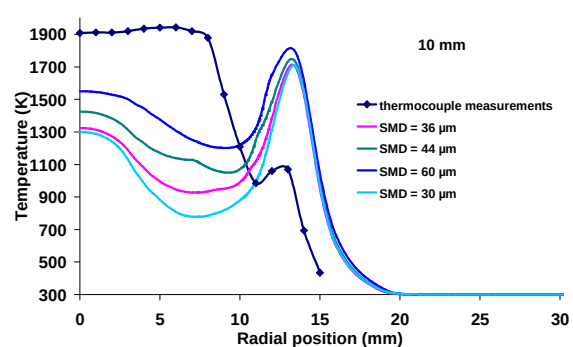


Figure 6.78 Temperature profile comparison at 10 mm for SMD = 30 to 60 μm

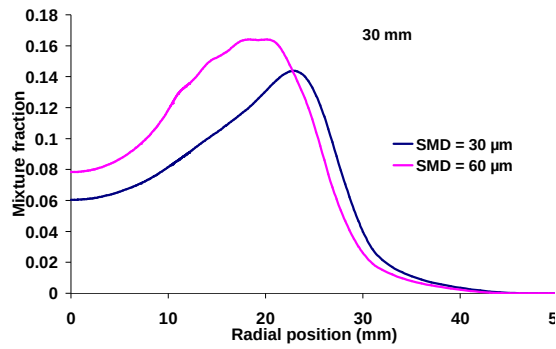


Figure 6.79 Mixture fraction profiles at 30 mm for SMD = 30 and 60 μm

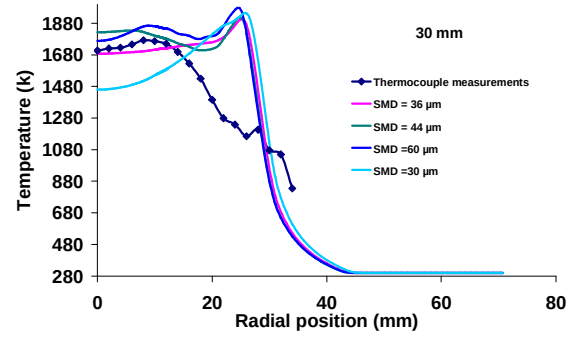


Figure 6.80 Temperature profile comparison at 30 mm for SMD = 30 to 60 μm

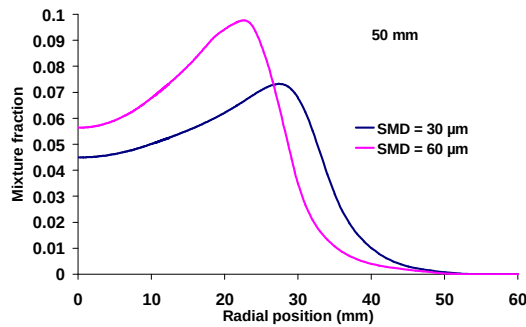


Figure 6.81 Mixture fraction profiles at 50 mm for SMD = 30 and 60 μm

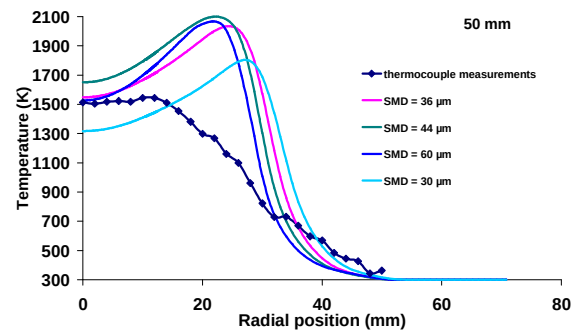


Figure 6.82 Temperature profile comparison at 50 mm for SMD = 30 to 60 μm

At a distance of 10 mm downstream of the spray nozzle, as fine droplets with SMD = 30 μm are injected, the vaporization is greatly enhanced due to their larger surface area and consequently the mixture becomes fuel rich, as illustrated figure 6.77 leading to a lower flame temperature. For the case where the SMD = 60 μm , the larger droplets are less subject to evaporation, and the mixture becomes less fuel rich, (cf. figure 6.77), leading to a flame temperature higher by 250 K compared to the case for SMD = 30 μm (cf. figure 6.78). Further downstream, the initially larger droplets for SMD = 60 μm have become smaller due to the evaporation process and therefore a significant amount of fuel vapour is generated while for initial SMD=30 μm most of the small droplets have already vaporized, leading to a very lean mixture, as seen figure 6.79 and 6.81, ultimately leading to a lower flame temperature compared to the case where SMD = 60 μm (cf. figure 6.82). In all cases, the maximum value of temperature occurred at the same height.

The combustion of these larger droplets (SMD = 60 μm and $D_{\text{max}} = 100\mu\text{m}$) may result in the formation of hot spots on the liner as illustrated figure 6.83 if there is no

wall cooling. With the larger drop size distribution, 32% of the fuel has hit the wall, which corresponds to a significant proportion of unburnt fuel, and consequently a reduced maximum local temperature. Therefore the exit temperature distribution of the exhaust stream can be adversely affected if too many large droplets hit the wall. For this reason, sprays with smaller SMD are preferred to optimize the temperature distribution.

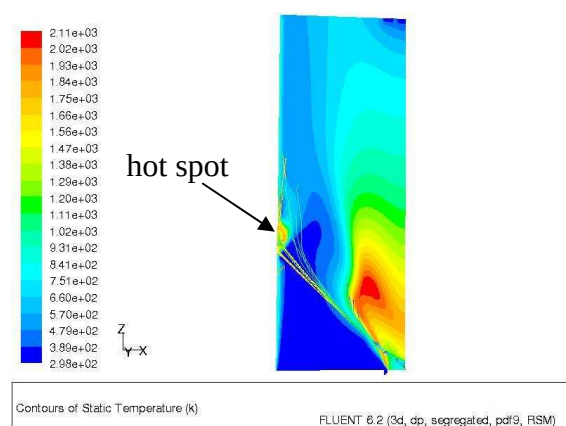
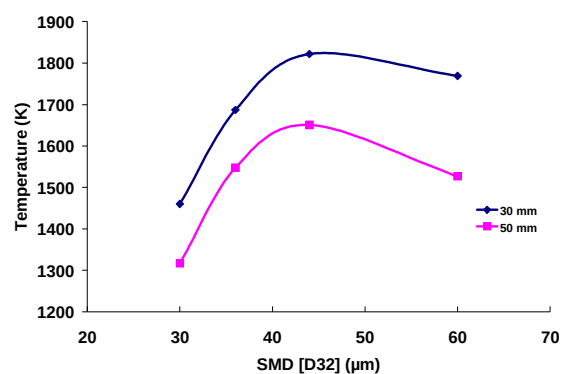


Figure 6.83 Hot spots on the rig casing with higher SMD **Figure 6.84** Maximum centreline temperature 30 and 50 mm downstream

On the other hand, the case whose SMD = 44 μm leads to the highest flame temperature, 30 and 50 mm downstream of the spray nozzle, compared to the other droplet size distributions. Therefore, it can be concluded that the maximum local temperature increases when the initial SMD is increased from 30 μm to 44 μm, but a further increase from 44 to 60 μm, will negatively affect the maximum lo, as shown figure 6.84. Indeed, with the lower range of SMD, the droplets will undergo significant evaporation but their residence time is too short for the droplet to burn, therefore lowering the maximum local temperature. When the SMD is increased the droplet penetrate further in the pressure rig, as illustrated figure 6.55 and burning is more complete, since the residence time is prolonged in the main reaction zone. However when the droplet size is further increased, the droplet will pass through this primary zone and travel further (with possible wall wetting as seen figure 6.83) without vaporizing in a region where a large proportion of the droplet will evaporate in a cold environment, resulting in poor mixing, and consequently lower reaction rates, therefore burning will become less effective, reducing the flame temperature. Therefore it appears that there is an optimum SMD for spray combustion, which is around 44 μm in this study.

However, as mentioned in section 6.7, the drop size distribution was based on experimental data. Section 4.4.2 described that a certain level of uncertainty is likely to be present, such as droplet size overprediction by as much as 15 % due to fuel temperature and consequently modification of the refractive index, or a high droplet rejection rate due to the presence of several droplets in the probe sample area in dense sprays. In case the initial droplet size distribution defined for the simulation underestimates the real spray characteristics, this would affect the reliability of the simulations by modifying the flame structure. Varying the mean particle diameter would modify the fuel mass fraction, therefore the mixture fraction. The larger droplets would undergo less evaporation, consequently a less fuel rich region in the vicinity of the fuel atomizer, resulting in a higher flame temperature, which would give a closer match to the experimental data in that region. However, as the larger droplets evaporate, they will obviously become smaller and release more fuel vapour, leading to a higher flame temperature compared to initially smaller droplets and therefore causing a longer flame length. But the main effect of the measurement uncertainty would be more important in the vicinity of the fuel nozzle, where the flame temperature is highly sensible to the spray initial conditions. Moreover, it is not possible to rely on cold spray measurements, which would remove the uncertainty linked to the modified refractive index, since combustion is present in the immediate vicinity of the fuel nozzle.

To summarize, FLUENT predicts a strong sensitivity to the initial conditions, therefore to the initial liquid phase properties, which is reflected on the spray flame structure.

6.7.2 Influence of the spray angle spread

The influence of the variation of the spray angle has been tested. While keeping the same initial droplet size distribution, the fuel mass flow rate and boundary conditions, the spray angle spread was varied from 30 degrees to 20 degrees and finally 1 degree, respectively making a half angle spread from 40 to 70 degrees (cf. figure 6.85), to a spray angle ranging from 40 to 60 degrees (cf. figure 6.86) and a single spray angle of 45 degrees illustrated figure 6.87.

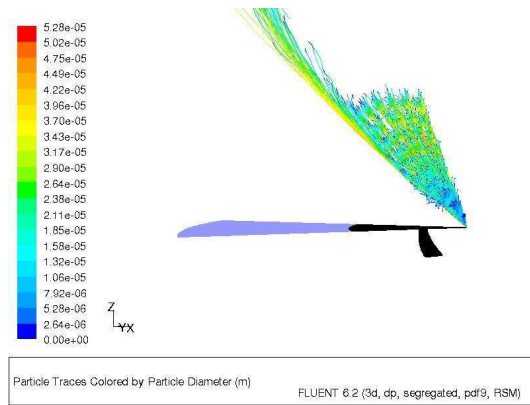


Figure 6.85 30 degrees spread, 40 to 70 degrees

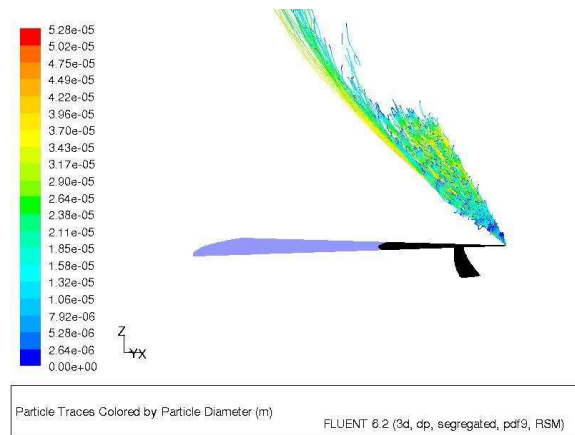


Figure 6.86 20 degrees spread, 40 to 60 degrees

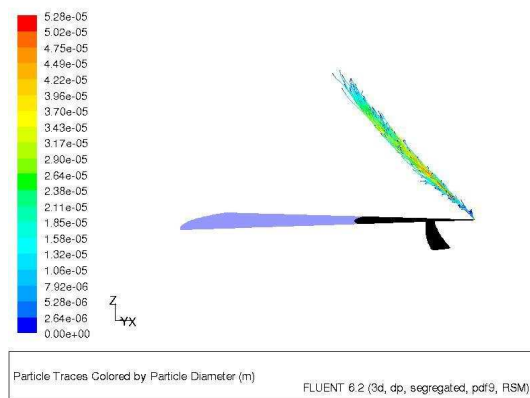


Figure 6.87 Single spray stream at 45 degrees

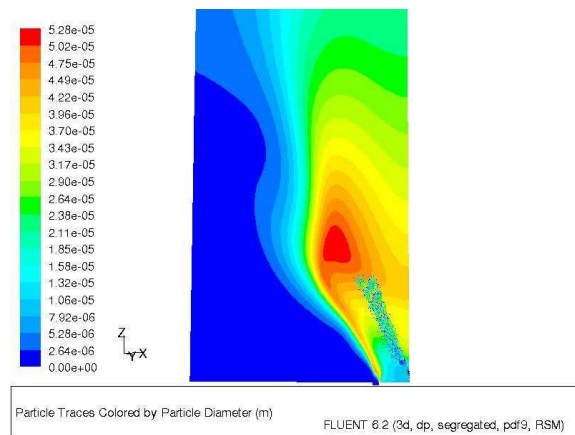


Figure 6.88 65 and 70 degrees spray streams with ethanol temperature field at 1 atm

There is a significant discrepancy between the temperature profile obtained with the spread angle of 1 degree compared to a spread of 30 degree, especially in the vicinity of the spray nozzle. In fact, the fuel vapour diffuses more radially with a spread of 30 degrees towards the spray centreline and as it has already been mentioned the mixture is fuel rich in the vicinity of the fuel nozzle due to the overestimation of the evaporation rate. But reducing the spray angle spread tends to significantly reduce the mixture fraction near the spray nozzle as seen figure 6.92. The mixture fraction with a single spray stream is reduced to a value close to stoichiometric conditions and the gas temperature is significantly higher on the spray centreline at a height of 10 mm, consequently there is a better agreement between the thermocouple measurements and the numerical prediction. Moreover, the single spray stream narrows the width of the cool region compared to 20 and 30 degrees spray angle variation, due to the cooling

effect of the spray along its trajectory, although the radial spread is still overpredicted. However, the cool region temperature is overpredicted by nearly 400K. If the width of the cool region is already overpredicted with a single stream, it is obvious that the discrepancy will only grow when the spread angle will be further increased. When the spray angle variation is changed from a single stream to a spray ranging between 40 and 60 degrees, the temperature is still overpredicted, but this time the discrepancy has reduced to 160 K while increasing further the spray angle to 30 degrees (40 to 70 degrees) leads to a satisfactory agreement in terms of cool region temperature although this region is located further inside radially in the simulation. Therefore, it can be concluded that the fuel vapour diffuses more than what is observed experimentally.

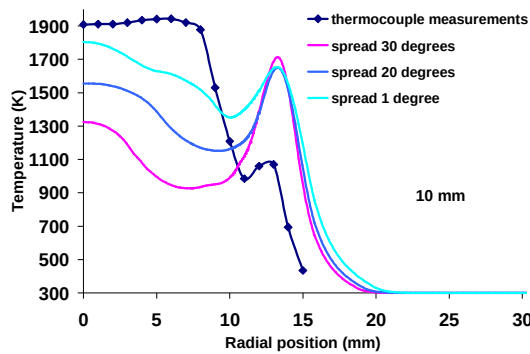


Figure 6.89 Temperature profile comparison between 1 and 30 degrees at 10 mm

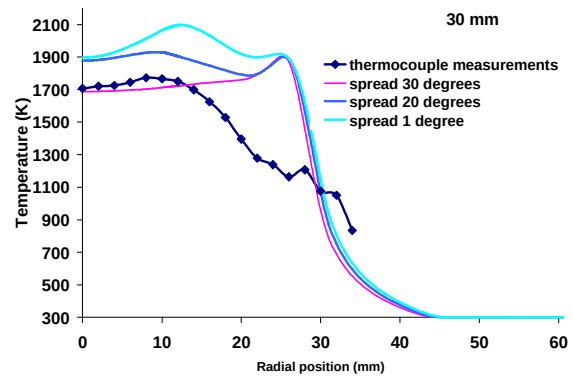


Figure 6.90 Temperature profile comparison between 1 and 30 degrees at 30 mm

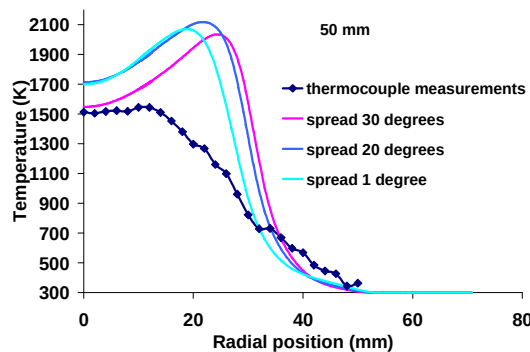


Figure 6.91 Temperature profile comparison between 1 and 30 degrees at 50 mm

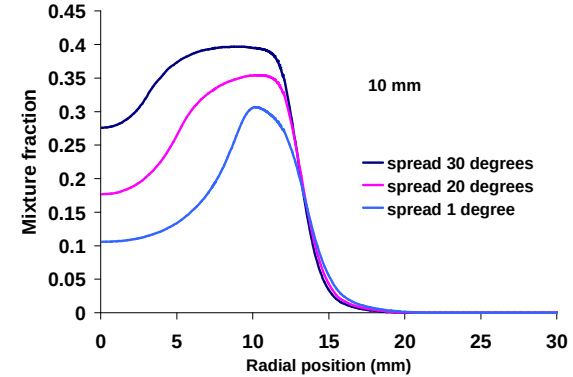


Figure 6.92 Mixture fraction comparison for spread of 20 degrees, 30 degrees and single stream

However, further downstream the temperature seems to be significantly overpredicted by nearly 200 K when the spray angle spread is reduced to 20 degrees or a single stream as seen figure 6.90 and 6.91. Therefore it can be concluded that the spray streams at 65 and 70 degrees are directly responsible for bringing down the

temperature close to the centreline since the discrepancy is not as significant between the spray streams and the 30 degrees spray variation angle. In fact, it is known that the spray acts as a heat sink and consequently brings down the temperature along its trajectory. Figure 6.88 shows that the 65 and 70 degrees angle are on the inner side of the main reaction zone, and the fuel vapour diffuses toward the spray centreline, therefore cooling down the temperature in this region. .

The influence of the radial spread of the spray becomes even more obvious if it is assumed that the spray takes the form of a semi-solid cone. Indeed, it is believed that some the positive axial velocity near the fuel atomizer is due to the presence of very small droplets which are not detected by the PDPA, since their size might be lower than the minimum size range of the device. So the numerical model was set up in such a manner that the spray possessed a spread angle ranging from 40 degrees to 90 degrees, but no spray streams were set up between 70 and 90 degrees, which is why the cone has been labelled as semi-solid. The fuel flow rate proportion at 90 degrees was arbitrarily assumed to be at around 1% of the total fuel mass flow rate. However, even using 5 μm droplets lead to an extreme cooling down of the flame, displacing it further downstream as illustrated figure 6.93 with the temperature field and figure 6.94 which showed a spectacularly fuel rich region since the mixture fraction was closed to unity.

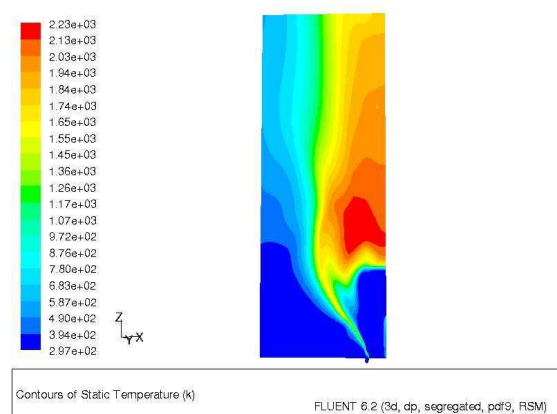


Figure 6. 93 Solid cone temperature contours with ethanol in confined rig at 1 atm

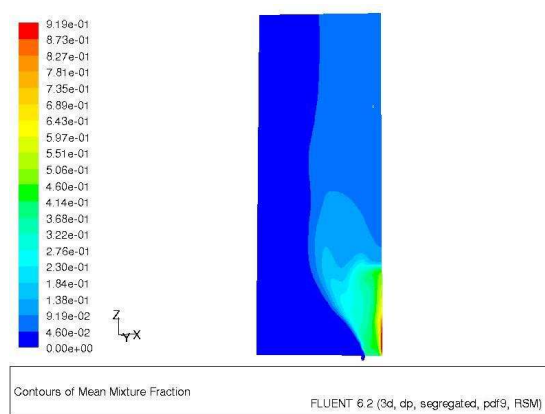


Figure 6. 94 Solid cone mixture fraction contours with ethanol in confined rig at 1 atm

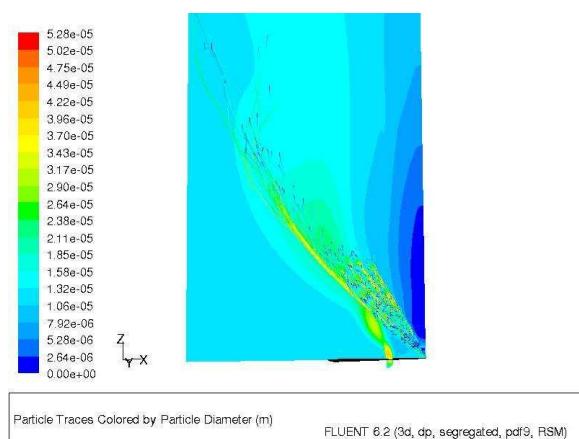


Figure 6.95 Spray trajectory and recirculation zone with ethanol in confined rig at 1 atm

From this section, it can be concluded that:

- narrowing down the spray spread angle from 30 to 20 degrees leads to a closer agreement to the centreline temperature in the vicinity of the spray nozzle
- the particle streams at 65 and 70 degrees are responsible for the lower temperature on the spray centreline compared to the other cases where the spread angle is narrowed down
- in the cool region corresponding to the spray trajectory, the fuel vapour diffusion is overpredicted and finally,
- extending the spray to a semi-solid cone, despite assumptions based on the experimental data, leads to an unrealistic flame, since flame evaporation rate and fuel diffusion are overpredicted.

While it is preferable that the spray half angle does not go beyond 60 degrees, which is approximately outside the edge of the recirculation zone (cf figure 6.95), care has to be taken so that the spray half angle does not go below 40 degrees. Indeed, for instance if the spray half angle is set at 30 degrees, the droplet might penetrate too far in a cool region beyond the reaction zone, where poor mixing will occur, resulting in a low rate of evaporation and the fuel might burn in the zone above the coflowing air, or even in the vicinity of the wall as seen figure 6.83, resulting in a lower maximum local temperature and eventually a significant proportion of unburnt fuel. Therefore, it can be concluded that there is a range of spray injection angles at which optimum temperature distribution is reached.

6.7.3 Droplet/droplet interaction

Droplet droplet interaction are still poorly understood in reacting sprays and it is important to know whether FLUENT is capable of providing a qualitative prediction of the effect of droplet spacing on the spray flame structure.

Indeed, real life sprays are known to involve a large number of droplets and it is believed that the spray behaviour will be quite different from isolated droplets evaporation (Sirignano, 1983; Labowsky, 1978; Labowsky, 1976; Labowsky, 1980; Imaoka and Sirignano, 2005; Raju and Sirignano, 1990) due to the effects of droplet spacing (Labowsky, 1976; Labowsky, 1980; Imaoka and Sirignano, 2005; Raju and Sirignano, 1990). Fuel droplet vaporization and burning rates are known to be influenced by the presence of neighbouring droplets even at large separations (Labowsky, 1978), which can significantly affect the combustion efficiency and the soot and pollutant formation (Klimenko and Bilger, 1999; Labowsky, 1980). Hence it is important to account for droplet interactions for spray combustion calculations. However, to the author's knowledge, no investigator has included the effect of droplet spacing on spray vaporization and combustion in numerical simulations, which obviously considers a serious neglect, especially for dense spray applications, encountered in industrial applications.

In order to study the effects of droplet spacing, FLUENT simulations have been conducted where the number of particle streams is initially set at 20 for one sector of 36° , and then decrease to 5 and finally increase to 40. The droplet spacing was uniform and was varied between 0.9° and 7.2° as illustrated figure 6.96-6.98.

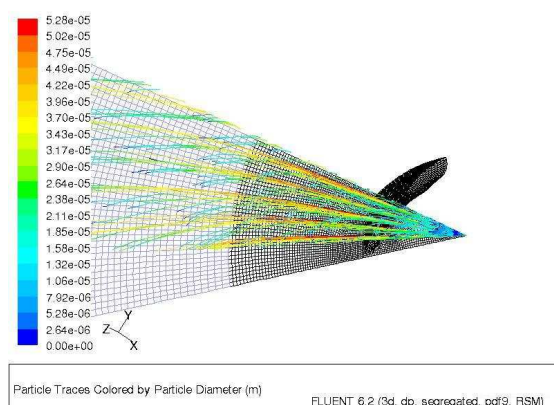


Figure 6.96 5 streams representation with ethanol in confined rig at 1 atm

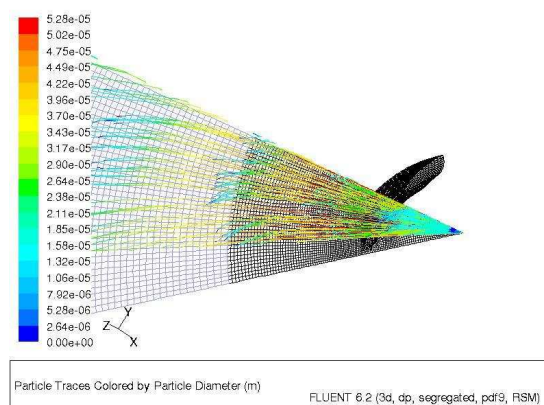


Figure 6.97 20 streams representation with ethanol in confined rig at 1 atm

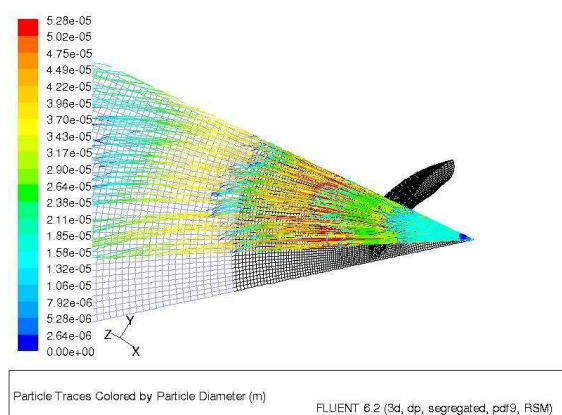


Figure 6.98 40 streams representation with ethanol in confined rig at 1 atm

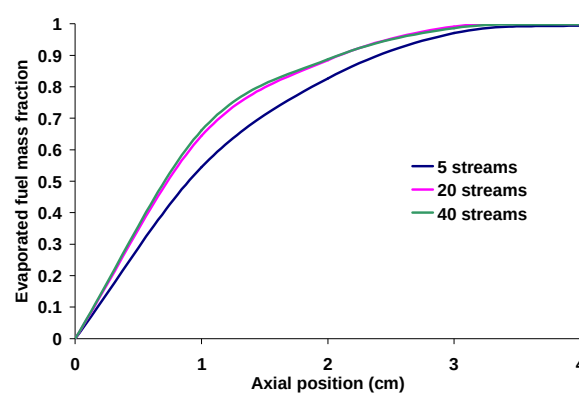


Figure 6.99 Evaporated fuel mass fraction

The numerical simulations show that the droplet evaporation rate may be significantly affected by the droplet interactions. This effect is shown figure 6.99 where as the number of particle streams is increased, the evaporation rate is reduced, and stronger evaporation is predicted when there are reduced interactions. The mixture fraction is consistently lower in the case of strongly interacting droplets with 20 and 40 droplets streams as compared to 5 streams confirming that the mixture is leaner when the number for particle streams is significant as illustrated figure 6.100, 6.101 and 6.102.

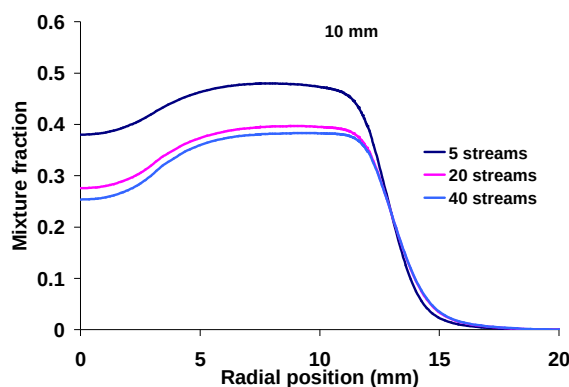


Figure 6.100 Mixture fraction at 10 mm for 5, 20 and 40 streams streams with ethanol in confined rig at 1 atm

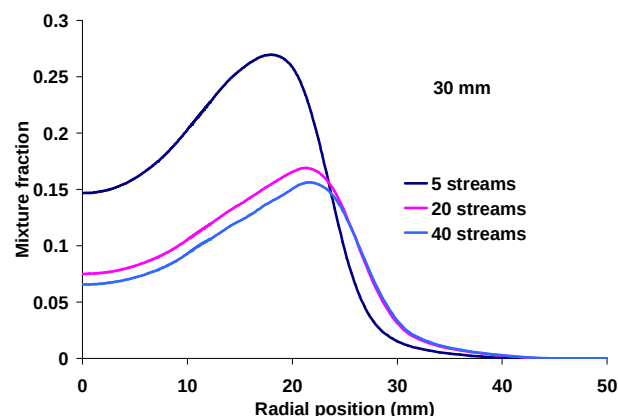


Figure 6.101 Mixture fraction at 30 mm for 5, 20 and 40 streams streams with ethanol in confined rig at 1 atm

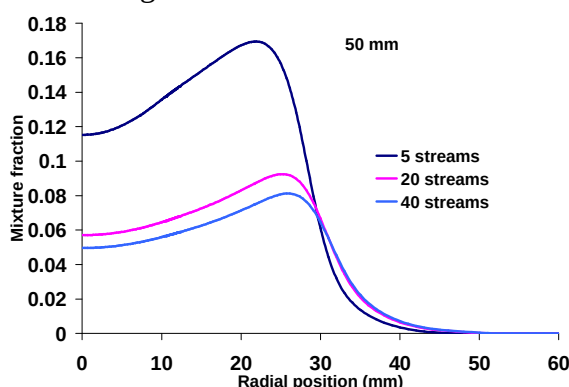


Figure 6. 102 Mixture fraction at 50 mm for 5, 20 and 40 streams streams with ethanol in confined rig at 1 atm

It is in agreement with the findings of several researchers. Labowsky (1976) and Sirignano (1983) demonstrated that droplet evaporation rates decrease as the number of interactions increases even for large spacings, and also spray vaporization rates are lower than isolated droplets. Indeed, a decrease in droplet spacing leads to an increase in local fuel vapour mass fraction and the local environment will be cooled by the presence of droplets, which as a consequence will reduce the heat transfer to the droplets therefore decreasing the local ambient temperature as illustrated figure 6.104 and 6.105. There is a discrepancy ranging from 50 and 150 K if 20 particle streams rather than 40 are considered but between 40 and 5 particle streams the temperature difference can be as high as 700 K (cf figure 6.105). At 10 mm downstream of the spray nozzle, the temperature is higher with 40 streams than the other cases (cf. figure 6.103) because although consistently leaner than the other cases, it is burning under fuel rich conditions, as illustrated figure 6.100, and consequently closer to stoichiometric conditions than the simulations with 20 and 5 streams.

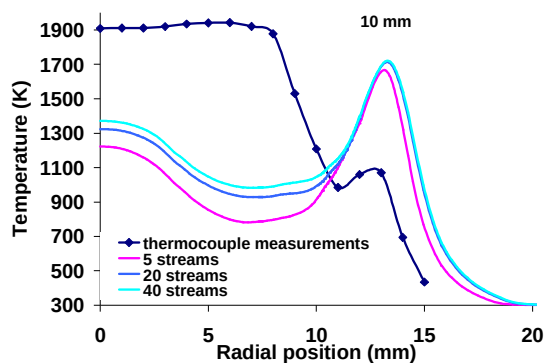


Figure 6. 103 Temperature profile at 10 mm for 5, 20 and 40 streams with ethanol in confined rig at 1 atm

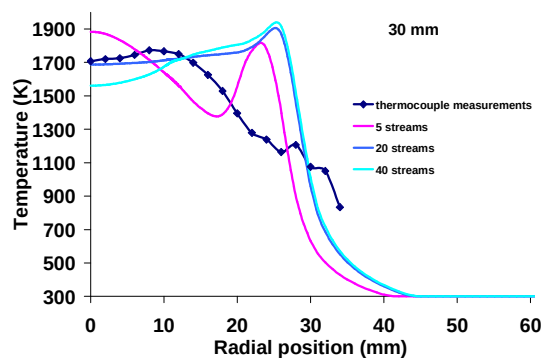


Figure 6. 104 Temperature profile at 30 mm for 5, 20 and 40 streams with ethanol in confined rig at 1 atm

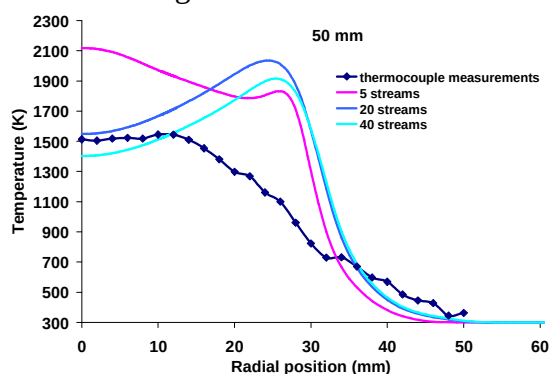


Figure 6. 105 Temperature profile at 50 mm for 5, 20 and 40 streams with ethanol in confined rig at 1 atm

Therefore, in order to correctly predict the spray behaviour it is important to know the number of particle streams forming the spray since it can make a difference of several hundred Kelvin in the temperature prediction. Indeed, a typical droplet in an industrial or even laboratory scale pressure rig cannot be treated as an isolated droplet since it will be strongly influenced by neighbouring droplets. In a convective situation, a droplet even at a distance of several tens of droplets diameters can significantly influence a neighbouring droplet if it is in its wake (Sirignano, 1999).

This sensitivity analysis demonstrated that FLUENT is sensitive to the number of particle streams in the spray and does not consider the spray as an ensemble of isolated droplet but rather takes into account the influence of the neighbouring droplets. Thus, FLUENT exhibits a strong coupling between the droplet droplet interaction, the evaporation rate, and the temperature field.

The combustion process and spray calculations are therefore very sensitive to droplet initial conditions. As a result, setting up proper initial droplet conditions is one of the most challenging tasks for any spray combustion system because it will have a significant impact on the spray flame structure and also influence pollutant emissions predictions. Too large droplets will have a negative influence on the combustion performance, added to the wall wetting problem that may be encountered, whereas too small droplets will result in early evaporation without combustion. Hence a good compromise has to be found for the droplet size distribution in order to achieve high maximum local temperature.

6.7.4 Influence of Air/Fuel ratio

Flame stability is strongly affected by the air/fuel ratio and the stoichiometry, therefore the mass flow rates of the main carrier will have a significant effect on the spray flame structure. Indeed, the purpose of imparting swirl to incoming primary air is to create a recirculating flow in the region close to the nozzle, in order to increase the fuel residence time and as a result enhance the evaporation rate and mixing of the fuel with air with a required flame stabilisation. However on the other hand it will reduce the droplet penetration in the primary zone, which will affect the effectiveness of the droplet vaporization.

The sensitivity of the primary air flow rate on the flame structure is investigated in this section. A case where the primary air mass flow rate was arbitrarily doubled while keeping the same droplet size distribution, fuel flow rates and boundary conditions has been tested. The spray initial conditions are summarised as follow:

Spray parameters	
Cone angle	40, 45, 50, 55, 60, 65, 70 °
Number of particle streams	20
Velocity magnitude	30 m/s
Total fuel mass flow rate	0.36 g/s
Minimum diameter	5 μm
Sauter mean diameter	44 μm
Mean mass diameter (MMD)	52.8 μm
Maximum diameter	60 μm
Spread parameter	4
Number of tries	5
Number of diameters	10

Table 6.9 Spray initial conditions for ethanol in confined rig at 1 atm with double air flow rate

The case with 3.2 g/s primary air flow rate will be called case 2, while the lower swirling air flow simulation will be labelled case 1. The flame structure has been dramatically modified by an increase in air flow rate as seen figure 6.106. In fact, increasing the air mass flow rate leads to a stronger recirculation zone and the flame is largely anchored in a narrow region comprised between the fuel atomizer and the swirler slot and therefore the flame length has considerably shortened because of the impact of the recirculation zone due to vortex breakdown. The flame stabilized just above the atomizer. The peak flame temperature has substantially decreased from a value of around 2100 K for case 1 to slightly less than 2000 K in case 2, and a faster decay in temperature with downstream distances has been observed. The peak temperature is located off the centreline, suggesting a hollow reaction zone. One of the reason for the falling off in the performance of the swirl burner at high mass flow rate is that combustion is complete before the end of the reverse flow zone, some cold products are recirculated, thus reducing the heat release.

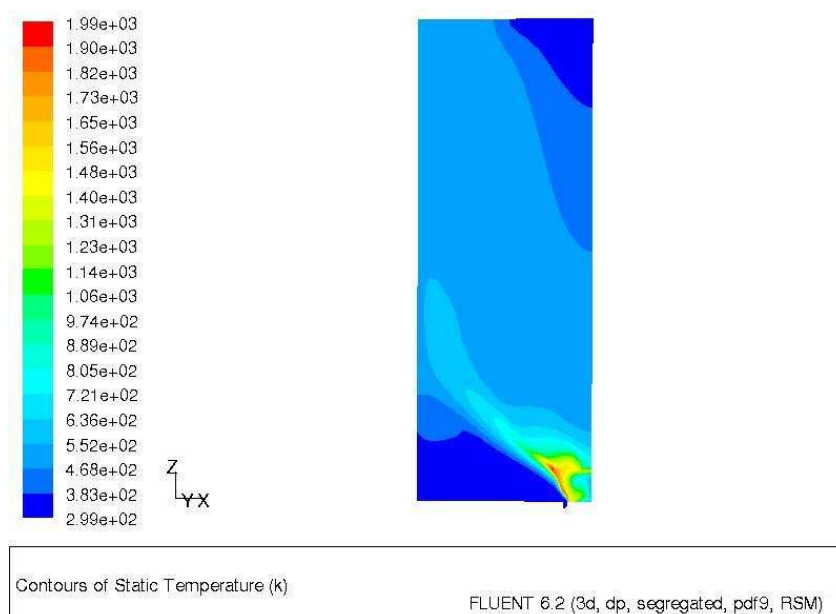


Figure 6. 106 Flame temperature field with 3.2 g/s

The increase in the air mass flow rate resulted in a greater radial expansion of the air jet, since the air momentum is doubled in case 2 and consequently the air jets hit the wall, unlike case1 and the peak velocity is located much further out radially than for case 1. The velocity field for case 2 is shown figure 6.108, and compared to case 1, displayed figure 6.107. The strong heat release in the immediate vicinity of the nozzle resulted in greater axial momentum, eliminating the recirculation zone, and further downstream the central recirculation zone was therefore generally weaker than for case 1, due to the greater contribution of the spray to the gas momentum. The heat release with the reacting spray results in an acceleration of the gas, and therefore the peak axial velocity resulting from the reacting spray was increased compared to the cold flow as seen figure 6.109 and 6.110.

The narrow flame region resulted in weaker heat release and consequently tends to lower the evaporation rate as illustrated figure 6.112. Therefore, despite the fact that the initial conditions are the same, the slow evaporation of the droplets yield larger droplet size (cf. figure 6.113 and 6.114) than for case 1 when the droplet move further downstream.

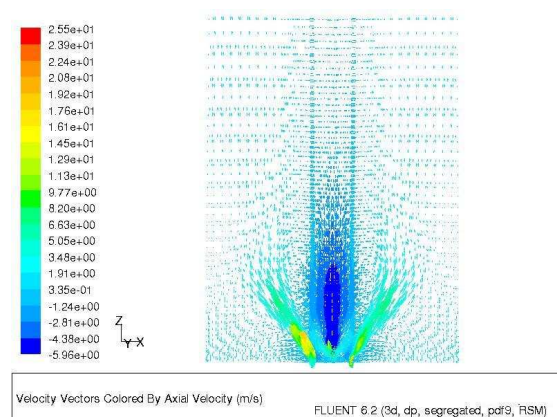


Figure 6.107 Velocity contours at 1.6 g/s for ethanol in confined rig at 1 atm

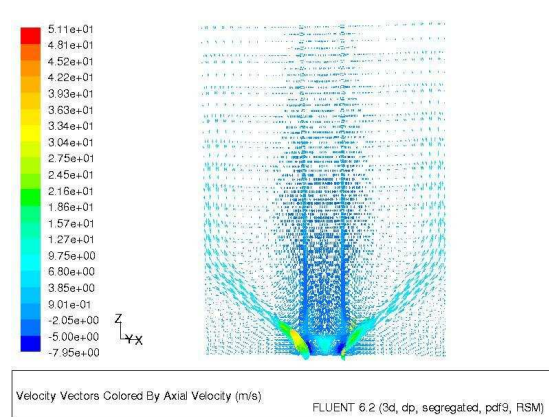


Figure 6.108 Velocity contours at 3.2 g/s for ethanol in confined rig at 1 atm

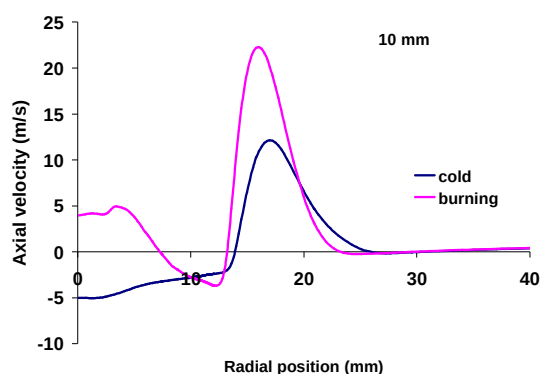


Figure 6.109 Axial velocity profiles at 3.2 g/s for cold and reacting flow at 10 mm for ethanol in confined rig at 1 atm

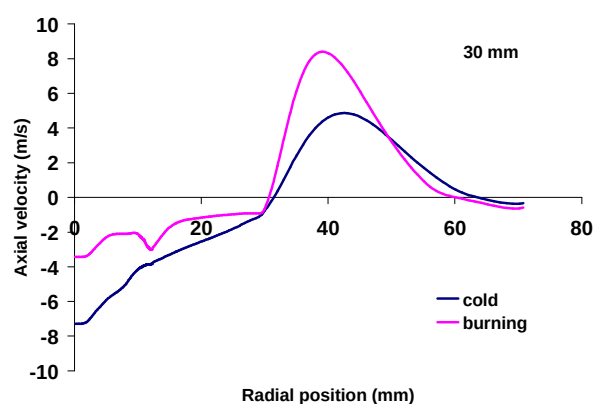


Figure 6.110 Axial velocity profiles at 3.2 g/s for cold and reacting flow at 30 mm for ethanol in confined rig at 1 atm

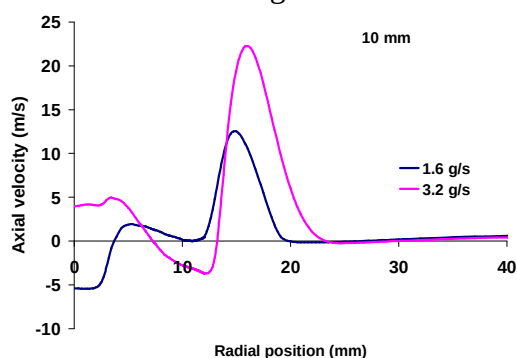


Figure 6.111 Comparison of axial velocity profiles between case 1 and 2 at 10 mm

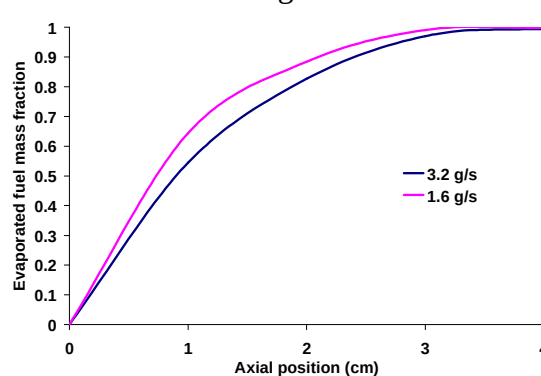


Figure 6.112 Evaporated fuel mass fraction

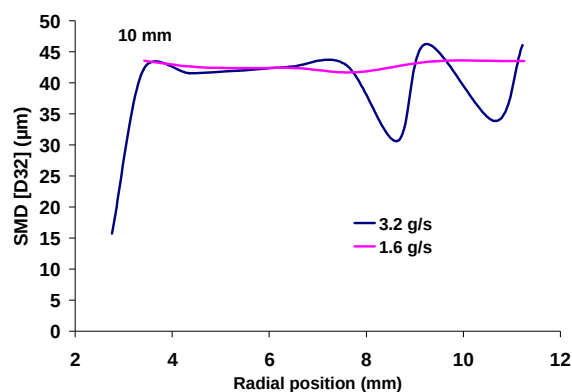


Figure 6. 113 Droplet SMD at 10 mm for case 1 and 2

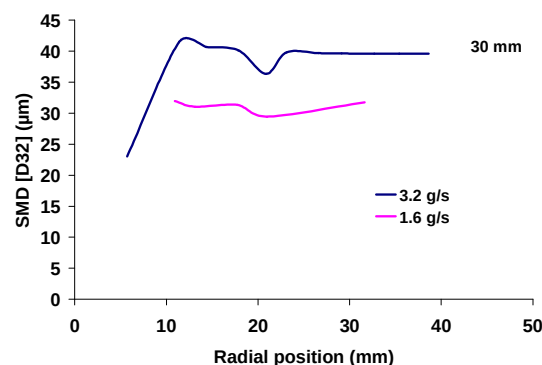


Figure 6. 114 Droplet SMD at 30 mm for case 1 and 2

The results showed that the peak temperature is significantly lower compared to case 1 due to an increase in the air fuel ratio, with more recirculating air cooling the gas temperature. Moreover, due to an increase in swirling air flow rate, the flame length has been significantly reduced. It seems obvious to say that if the mass flow rate is increased further, the central recirculation zone may create a flame flashback. Since no experimental data is given for increased primary air flow rate, there is no possibility of judging the numerical predictions given by FLUENT.

6.7.5 Ethanol combustion at higher pressure

High pressures are commonly encountered in industrial gas turbines, therefore it is important to get a clearer understanding of the evaporation and combustion process under such conditions.

Because of increased pressures, the spray atomization and vaporization characteristic will be very different from those encountered at lower pressures. In section 2.3.4 of the Literature Review, it is mentioned that the increased operating pressure will increase the evaporation rate and a rise of temperature of up to 200 K higher than those encountered at 1 atm can be expected. The higher evaporation rate will result in a decrease in spray penetration. Moreover as the pressure is raised, the gas ambient density increases making it more difficult for the spray to significantly penetrate the ambient gas.

Although no spray flame data for ethanol is available for this study, no quantitative assessment will be provided here, but it is still possible to qualitatively assess the capability of FLUENT to predict the spray behaviour under increased pressures.

Ethanol spray flames have been modelled at an operating pressure of 2, 3, 5 and 10 atmosphere. The pressure range can be divided into two regimes, the moderately high pressure regime, for pressure less than 0.75 of the critical pressure of the fuel, and the critical/supercritical regime. In the moderately high pressure regime, the transport properties are quasi independent of pressure and the relative gas density is relatively small compared to the fuel density. The critical pressure for ethanol is estimated at 63 atm, therefore the range of pressures for this study will be well within moderately high pressures.

In order to be able to see the effect of pressure, it has been judged preferable to keep the same operating conditions as the ones used under 1 atm, i.e. keeping the same initial droplet conditions (velocity, droplet size distribution, fuel flow rate) and the velocities have been kept the same as for 1 atm therefore it was necessary to scale the pressure accordingly. Therefore, the primary air flow rate was doubled at 2 atm, tripled at 3 atm, and multiplied by 10 under 10 atm, respectively to 3.2 g/s, 4.8 g/s and 36 g/s. The boiling point was set according to the pressure, whose data are presented on table 3.12.

FLUENT does predict that the evaporation rate is stronger with pressure, since the droplet SMD, set at the same initial conditions for all pressures, is also displaying the same values at 10 mm (cf. figure 6.122) but is lower at 50 mm, seen figure 6.124. This observation is confirmed when a closer look is taken at the evaporated fuel mass fraction, figure 6.121, where the simulation at 3 bar clearly displays a stronger evaporation rate than for the lower pressures.

On the other hand, it is clear that the increased evaporation rate is not strong enough at such pressure to significantly affect the spray penetration. Indeed, the droplet axial velocities are quite similar 10 mm, 30 and 50 mm downstream of the spray nozzle, as shown figure 6.118 to 6.120. At higher pressures, it will be expected that the evaporation rate will significantly reduce the spray penetration and the spray would

have completely vaporized in the primary zone, reducing the combustion heat release. Indeed the reduced combustion heat release is due to the droplet reduced penetration in the primary zone. On the other hand, the spray is shifted closer to its centreline as the pressure is raised.

Although the temperatures are quite similar for all pressures 10 mm downstream of the spray nozzle, there is a significant temperature drop further downstream for the higher pressures, which is the result of a much shorter flame due to the higher air mass flow rate, enhanced rates of mixing, heat transfer and reaction kinetics.

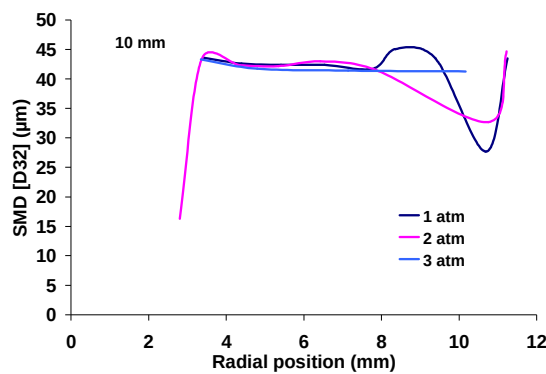


Figure 6.115 SMD at 1,2 and 3 atm at 10mm

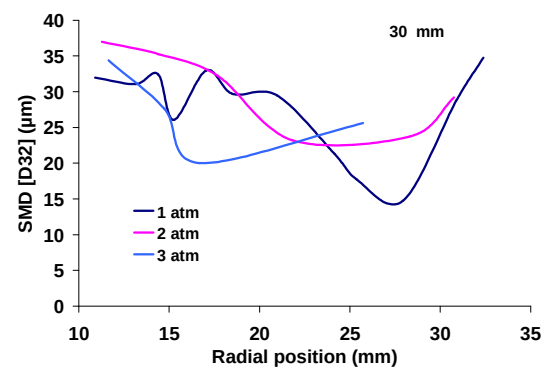


Figure 6.116 SMD at 1,2 and 3 atm at 30mm

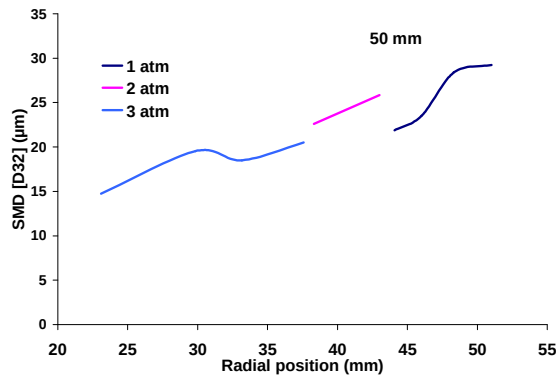


Figure 6.117 SMD at 1,2 and 3 atm at 50mm

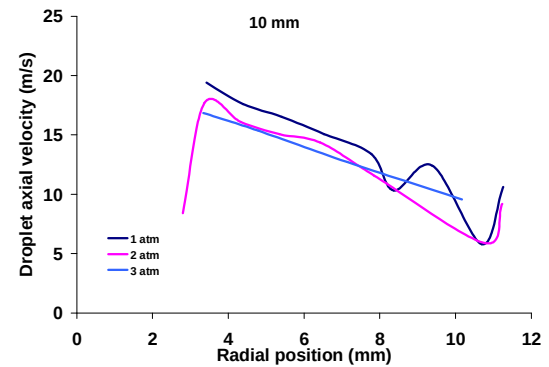


Figure 6.118 Droplet axial velocity at 1,2 and 3 atm at 10mm

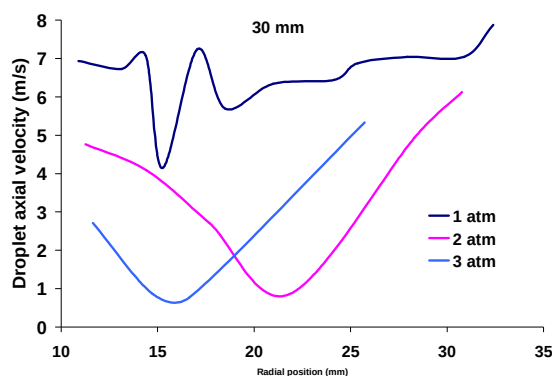


Figure 6.119 Droplet axial velocity at 1,2 and 3 atm at 30mm

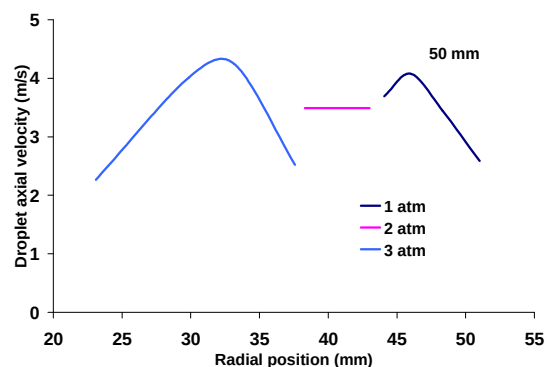


Figure 6.120 Droplet axial velocity at 1,2 and 3 atm at 50mm

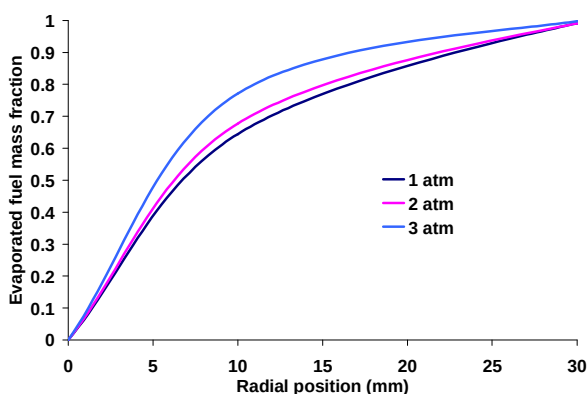


Figure 6.121 Evaporated fuel mass fraction

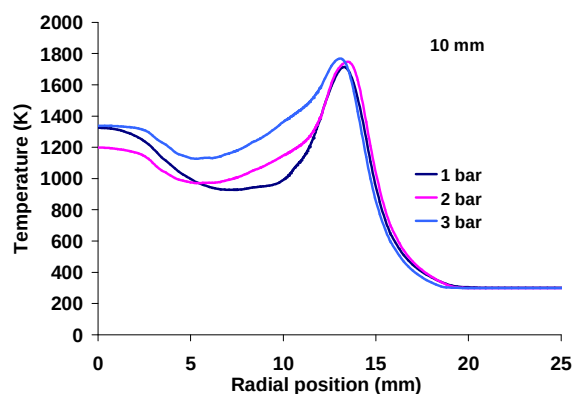


Figure 6.122 Temperature profile at 1,2 and 3 atm at 10mm

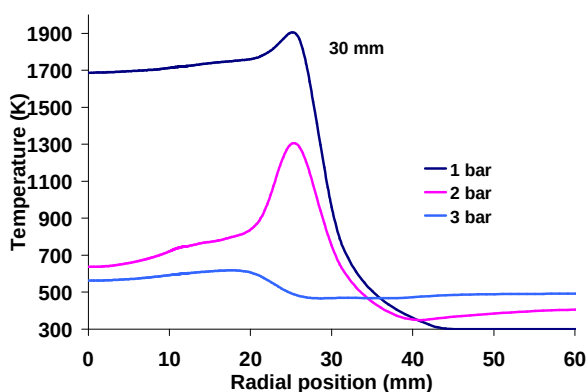


Figure 6.123 Temperature profile at 1,2 and 3 atm at 30mm

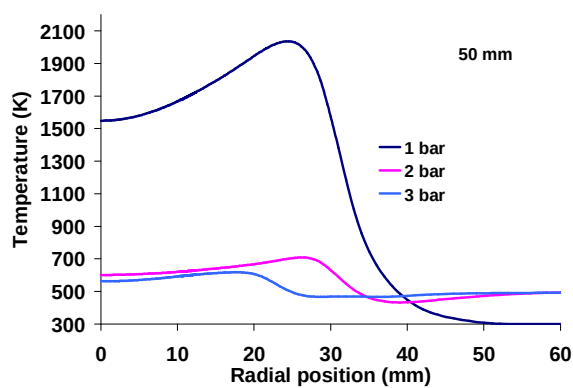


Figure 6.124 Temperature profile at 1,2 and 3 atm at 50mm

At 10 atm, the effect of the ambient pressure is quite significant. Indeed, FLUENT predicts that an increase in pressure from 1 to 10 bar reduced the droplet penetration considerably as illustrated figure 6.125. In fact, the droplets travel up to a distance of

20 mm downstream of the spray nozzle. This can be attributed to the high drag forces acting on the droplets due to the higher density of the high pressure environment in the pressure rig. Then, the droplet are entrained in the recirculation zone between the fuel atomizer and the swirler, and while passing above the swirl slots, they are again accelerated and get carried away by the swirling jet, which is very strongly deflected radially as seen figure 6.126, due to the high primary air mass flow rate of 16 g/s. The droplets impingement on the walls would be a detrimental event to the combustion heat release. Indeed, this would imply that part of the fuel atomized in the pressure rig remains unburnt, where the objective is obviously to burn the fuel completely. On the other hand, one would expect the combustion heat release to be low, since the air fuel ratio is critically high. Usually, an increase in air pressure is accompanied with an increase in fuel flow rate, and in this case, would have resulted in a high spray velocity, therefore the spray would be less likely to be carried away towards the walls.

ERRATUM: there is a considerable amount of doubt on the spray penetration and wall wetting, since it is expected that droplet secondary breakup will occur at 10 atm but the author has realised lately that it should have been included. Moreover, the latent heat of vaporization is significantly decreased at 10 atm but its value has been maintained constant for this particular pressure, therefore the results obtained at 10 atm should be treated with extreme caution.

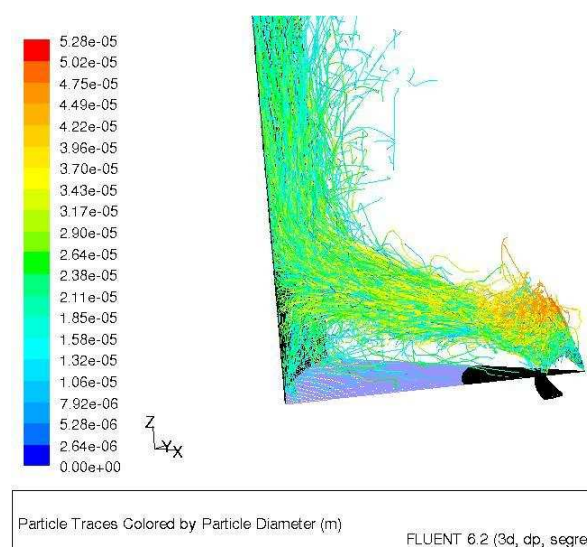


Figure 6. 125 Spray trajectory at 10 atm

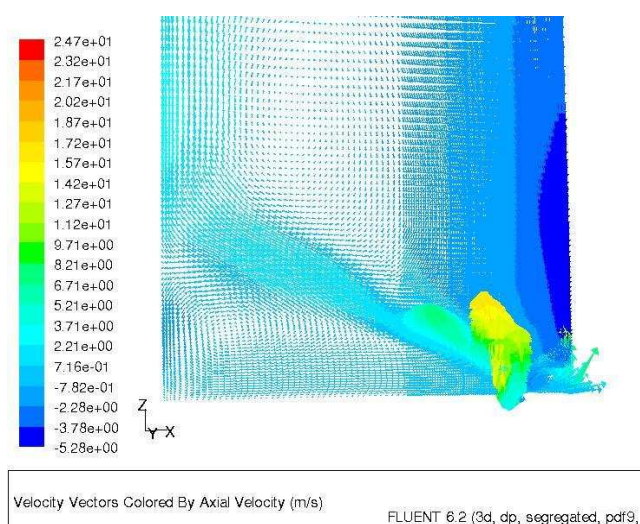


Figure 6. 126 Axial velocity vectors

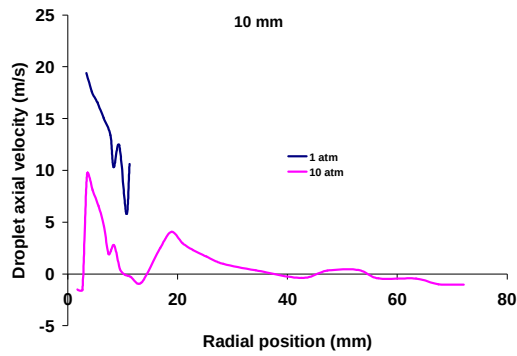


Figure 6.127 Droplet axial velocity profile at 1 and 10 atm at 10 mm

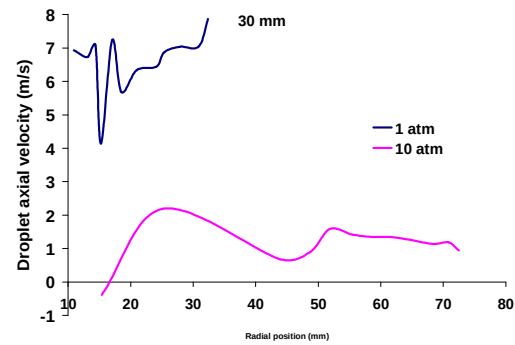


Figure 6.128 Droplet axial velocity profile at 1 and 10 atm at 30 mm

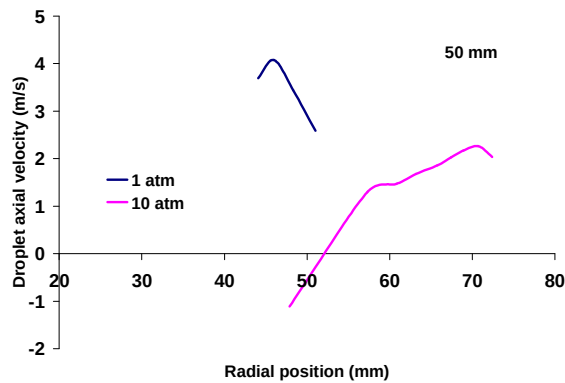


Figure 6.129 Droplet axial velocity profile at 1 and 10 atm at 50 mm

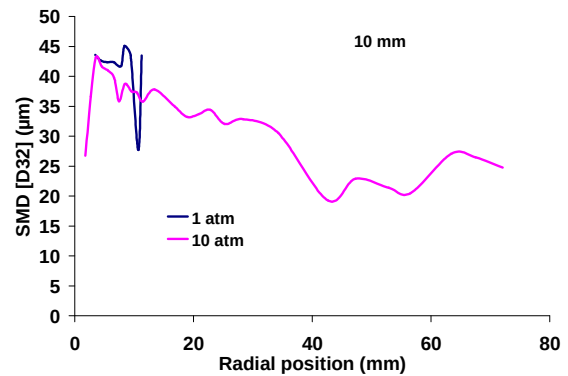


Figure 6.130 SMD at 1 and 10 atm at 10 mm

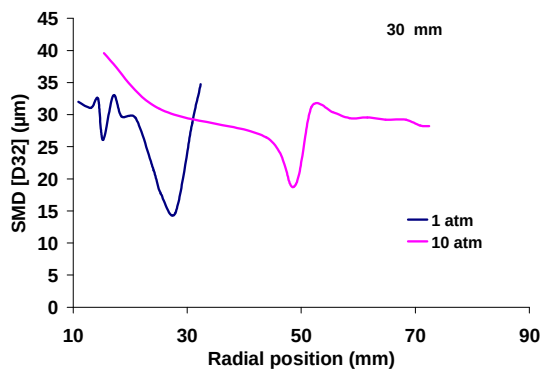


Figure 6.131 SMD at 1 and 10 atm at 30 mm

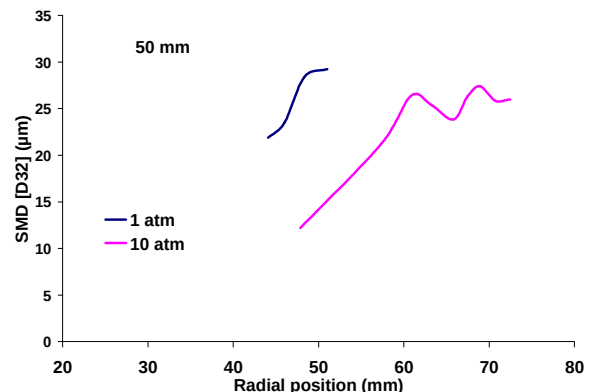


Figure 6.132 SMD at 1 and 10 atm at 50 mm

FLUENT predictions on the effect of air pressure on the mean axial velocities revealed low mean velocities (1-2 m/s) near the outer edges of the spray at 10 atm as seen on figure 6.127 to 6.129. The numerical results revealed negative velocities, which imply the existence of a recirculating airflow pattern cornered on the lower part of the casing walls. The existence in close proximity of low velocity, both negative and positive flows could mean that droplet collision and coalescence occurs at 10 atm, which could account for the observed large drop sizes seen figure 6.131. These phenomena are not encountered at the lower pressures simulated in this study but clearly seems to be occurring at 10 atm. At 50 mm, the spray is dominated by the

smaller droplets which are carried away by the swirling air jets. The figures clearly showed that an increase in air pressure can lead to fuel impingement on the walls, therefore it would be necessary to increase the fuel flow rate to avoid such occurrences. In fact, generally, when gas turbines operate under higher pressures, the pressure is increased at the same time as the fuel flow rate to maintain the air fuel ratio. However, this has not been tested here, since the main goal of this section was to see whether FLUENT accurately accounts for pressure effects on the spray, even though it is not thermodynamically meaningful for industrial applications.

The figures obtained clearly show that increases in fuel-air momentum ratio on spray dimensions has important practical applications, one obvious example being the risk of fuel impingement on the liner walls at high fuel flow rates. In general, this influence of fuel air momentum ratio on spray structure is beneficial to combustion performance. For example, a reduction in fuel flow rate at constant pressure causes the fuel to be associated with a smaller volume of air. Also, an increase in fuel flow rate at constant pressure is accompanied by an increase in the amount of air participating in combustion. The effect of this additional air is generally to reduce the local fuel-air ratio and flame temperature, thereby alleviating problems of exhaust smoke at high combustion pressures.

Changes in ambient pressure modify the general anatomy of a spray flame. As the pressure is raised, the flame length is shortened and well as its width. A pressure increase shortens the flame and reduces its width, due to enhanced rates of mixing, heat transfer and reaction kinetics.

6.8 Biodiesel

While ethanol reaction mechanisms do exist, there is no detailed kinetics which have been published for biodiesels. Therefore, a surrogate reaction mechanism had to be chosen and the methylbutanoate detailed kinetics was selected as the source for generating the flamelet libraries as explained in section 5.5.4.

As described in table 6.3, the primary air flow was set at 3 g/s at 1 atm while the fuel was injected with a mass flow rate of 0.75 g/s and the secondary air flow was

maintained at 12 g/s. The primary air temperature and the fuel were preheated respectively at a value of 150 °C and 141°C.

Based on the PDPA data in section 4.6.1 and 4.6.2 in the Experimental Study, it seems that the spray forms a hollow cone describing an angle spread of 25 degrees between 40 and 65 degrees but the PIV data (see section 4.6.3) seem to imply that some fine droplets located in the centre of the spray dominate the flow up to a height of approximately 10 mm, therefore the assumption that the spray forms a hollow cone is not valid. However, FLUENT tends to overpredict the influence of small droplets on the centerline as seen earlier with ethanol in section 6.8.2, therefore the spray will be described as a hollow cone only.

The convergence procedure used for the ethanol simulations described section 5.5.4 was used for the biodiesel study. The angle spread of 25 degrees was equally spaced every 5 degrees, therefore 6 angles were defined, each comprising 20 particle streams. Since the PDPA measurements displayed the same range of values than for the ethanol PDPA measurements, the droplet size distribution was conserved. Consequently, the droplets ranged from 5 μm to 60 μm , and a Rosin-Rammler distribution was assumed for the spray, which was described with 10 size classes of different diameters and the droplets were injected every 20 gas phase iterations. The number of tries was maintained to 5 and as a result, 6000 parcels distribution were introduced into the domain. Based on the experimental data, the injection pressure was at 147 psi, which corresponds to an exit fuel velocity of 33.42 m/s. The spray initial conditions at 1 atm are summarized in table 6.10.

Spray parameters	
Cone angle	40, 45, 50, 55, 60, 65 °
Number of particle streams	20
Spray injection velocity	33.42
Total mass flow rate	0.75 g/s
Minimum diameter	5 μm
Mean mass diameter (MMD)	52.8 μm
Maximum diameter	60 μm

Spread parameter	4
Number of tries	5
Number of diameters	10

Table 6. 10 Spray initial conditions for biodiesel spray at 1 atm

The computed results for the biodiesel spray flame are compared with the experimental data. Gas temperature comparisons are shown in figures 6.133, 6.142 and 6.143, respectively at 10, 30 and 50 mm. At 10 mm, the temperature on the centreline is correctly predicted but further out radially, the heat loss due to the droplet impingement on the thermocouple is underpredicted by a significant margin of around 800 K. The PDPA data shows that the volume flux figure 6.133 peaks further out radially than the minimum value encountered in the cool region. Consequently, it would seem that the turbulent dispersion of fine droplets on the inner edge of the spray would induce significant evaporation, explaining the location of the minimum temperature. Therefore to resolve this, it was decided to change the droplet size distribution by using smaller droplets on the inner edge of the spray. The droplet SMD was reduced to 20 μm instead of 36 μm used previously. The modified droplet size distribution is summarized in the following table:

Spray parameters	Previous drop size distribution	New drop size distribution	
Cone angle	40, 45, 50, 55, 60, 65 °	40, 45, 50, 55	60, 65 °
Number of particle streams	20	20	20
Spray injection velocity	33.42	33.42	33.42
Minimum diameter	5 μm	5 μm	5 μm
Mean mass diameter (MMD)	52.8 μm	52.8 μm	24 μm
Maximum diameter	60 μm	60 μm	40 μm
Spread parameter	4	4	4
Number of tries	5	5	5
Number of diameters	10	10	10

Table 6. 11 Modified spray initial conditions for biodiesel spray at 1 atm

The newly set droplet size distribution gave a satisfactory agreement with the PDPA SMD measurements, as illustrated figures 6.134 to 6.136 and the droplet axial velocity profile was well predicted (cf. figure 6.138 and 6.139). However the temperature was subsequently further underpredicted from the cool region to the centreline, as seen figure 6.133. Moreover, the width of the cool region which is narrower in the experiments than showed with the FLUENT simulations, was further overpredicted with the reduced droplet size due to the increased presence of fuel vapour as droplet vaporization goes preferably to the finer ones.

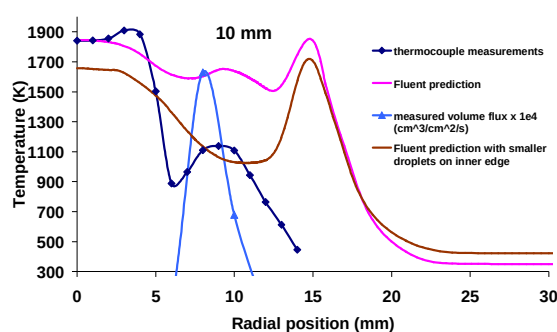


Figure 6.133 Temperature profile for biodiesel at 10 mm and 1 atm with initial and modified droplet size distribution with smaller droplets on the inner edge

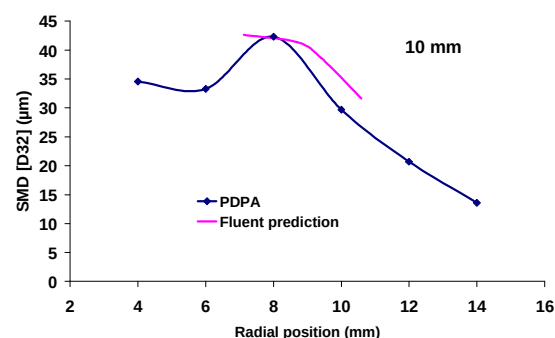


Figure 6.134 Droplet SMD at 10 mm

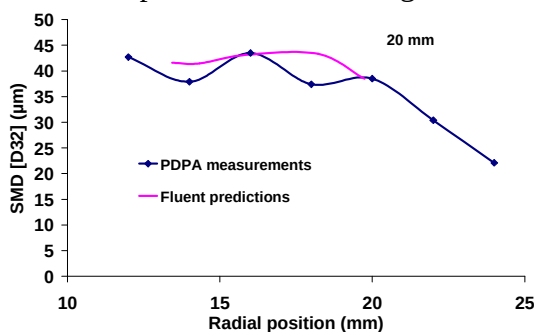


Figure 6.135 Droplet SMD at 20 mm

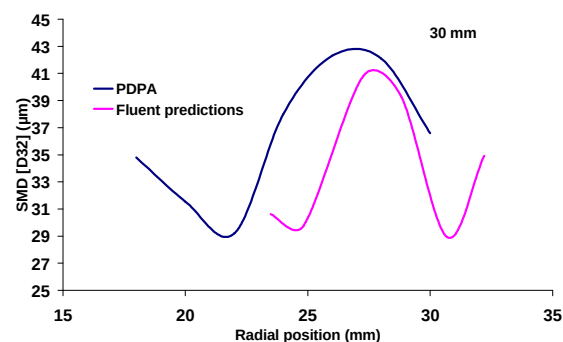


Figure 6.136 Droplet SMD at 30 mm

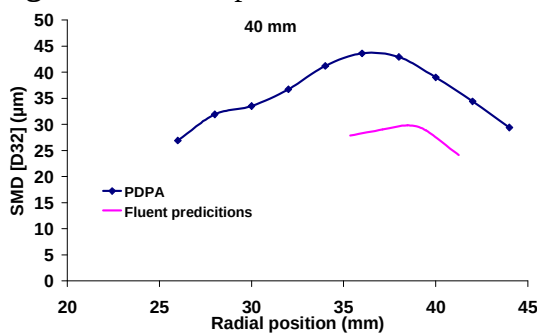


Figure 6.137 Droplet SMD at 40 mm

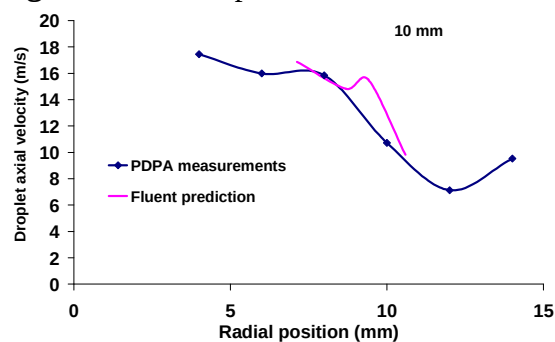


Figure 6.138 Droplet axial velocity at 10 mm

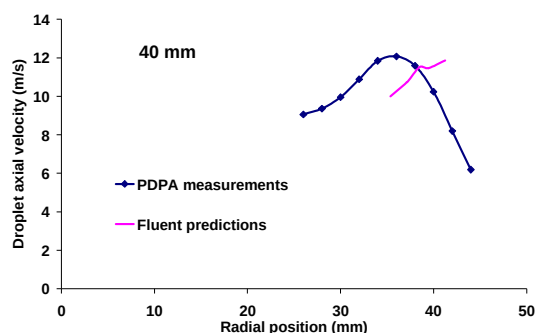


Figure 6.139 Droplet axial velocity at 40 mm

The presence of a local peak temperature further out radially on the lean side of the flame is not observed in the experiments. In fact, at this location, the flame should be quenched by the strongly swirling air jet. Indeed, the calculations with CHEMKIN showed that the flame was extinguished for the methylbutanoate reaction mechanism for any value beyond 550s^{-1} . Consequently, the extinction flamelet was chosen with a strain rate of 600s^{-1} . However, even though the strain rate in the flow field is way beyond this value as seen figure 6.140, the flame is not strained out. Actually, the FLUENT predictions show the presence of a local flame when it is the contrary that should have happened therefore the FLUENT flamelet model fails to predict local flame extinction.

In fact, when the strain rate is beyond the flame critical value, the coupling between temperature distribution and strain rate is lost. The FLUENT documentation provided some information when it mentions that extinguished flamelets are excluded from the flamelet library but there is no given explanation for this. Therefore instead of adding extinguished flamelets, the choice was reported on highly strained, partially extinguished flamelets so that none of the flamelet can be excluded from the flamelet library.

The strain rate in the first 5 mm downstream of the swirler was predicted to be slightly below 6000s^{-1} ; therefore it was decided to define a flamelet with this value of strain rate. The flamelet was artificially generated in order to match the temperature encountered in the experiments in the highly strained region, as seen figure 6.141. However, instead of decreasing the flame temperature, assigning a partially extinguished flamelet seemed to have exacerbated the problem since the temperature is even higher. Eventually a strain rate of $600\,000\text{s}^{-1}$ was assigned, which is the

highest strain rate encountered in the whole domain, and the local flame temperature was even higher, increasing from a maximum predicted value of 1718 K with the highest strain rate set at 6000 s^{-1} to 1851 K. It was concluded that this approach was not satisfactory. Consequently, the main case displayed figure 6.133, 6.142 and 6.143 was based on a maximum strain rate of $600\ 000\text{ s}^{-1}$ with a partially extinguished flamelet since there was a good agreement on the centreline with the thermocouple measurements, and also because all the flamelets used all presented a sharp peak in the normally extinguished region. Figure 6.144 displays the flame temperature 10 mm downstream of the swirler with the different flamelets with extinction strain rate at 600 s^{-1} , 6000 s^{-1} and $600\ 000\text{ s}^{-1}$ as well as a single flamelet at 600 s^{-1} . The figure clearly shows that changing the extinction strain rate does not improve the numerical prediction in the outer region where the experiments show that the flame is quenched.

Although these results appear to demonstrate that the strain rate is taken into account, it is necessary to ensure that strain rate alone can be responsible for heat loss in the flame. In fact, there are two major reasons for heat loss to occur in the spray flame:

- the effects of aerodynamic strain
- the cooling effect of evaporating spray

Therefore, it was decided to separate the sources of heat loss by modelling a gaseous flame in a simple geometry. Assuming that the fuel was injected at a velocity of 30 m/s in a cylindrical combustor shown in figure 6.145. A small nozzle in the center of the combustor introduces methylbutanoate at 30 m/s while ambient air enters the combustor coaxially at 0.5 m/s. 2 cases were simulated, one with two flamelets, the first one at a strain of 10 s^{-1} while the second was partially extinguished at 100 s^{-1} . The other case was run with the partially extinguished flamelet set at 300 s^{-1} instead of 100 s^{-1} . Figure 6.146 exhibits a clear difference in peak temperature between both cases, with the partially extinguished flamelet set at 100 s^{-1} clearly displaying a lower flame temperature since the strain rate values showed that the flame was partially strained out, contrary to the other case where the strain rate in the flow field was consistently lower than 300 s^{-1} . Consequently it can be concluded that the effects of strain are taken into account in FLUENT but when the strain rate is beyond the flame critical value, the correlation of temperature and flamefront position with strain rate that is fundamental for this approach is lost.

Apart from the issue of local peak temperature in the highly strained region, the thermocouple measurements at 30 mm displayed figure 6.142 show that the main reaction zone is located further out radially from the spray centreline, unlike what is described in the experiments. The mixture fraction profiles displayed figure 6.147 show that FLUENT predicts a fuel rich region when the experiments show that the flame burns closer to stoichiometry 25 mm from the spray centreline and 30 mm downstream of the spray nozzle. Moreover, 50 mm downstream from the atomizer the temperature is overpredicted by 200 K on the spray centreline. In fact, figure 6.147 show that the mixture fraction has been maintained at nearly the same value on the centreline between 30 mm and 50 mm, so the computed mean mixture fraction spreads much further than desired while it would have been expected to be much leaner at such height. These results would imply two things:

- the turbulent fuel mass diffusion is overpredicted
- the evaporation rate is too strong

In fact, as a result of vaporization, the fuel vapour mass fraction reaches a maximum along the spray axis, so the coinciding fuel rich region. Further downstream, the effect of turbulent mass diffusion becomes the dominant factor, so the strong fuel mass fraction even 50 mm downstream. Another property that strongly affects droplet vaporization is the latent heat of vaporization. In fact, the higher the latent heat of vaporization, the lower the net energy transferred to the liquid to evaporate. The latent heat of vaporization for biodiesel is about 4 times lower than that of ethanol (respectively 217 612 J/kg and 855 237 J/kg). Therefore, although ethanol is much more volatile than biodiesel, it requires much more energy to vaporize and consequently, biodiesel is the easiest of both fuels to evaporate.

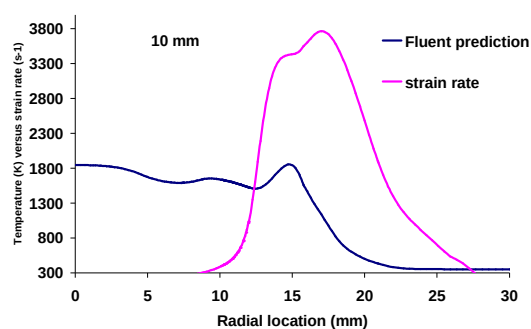


Figure 6. 140 Strain rate versus temperature at 10 mm

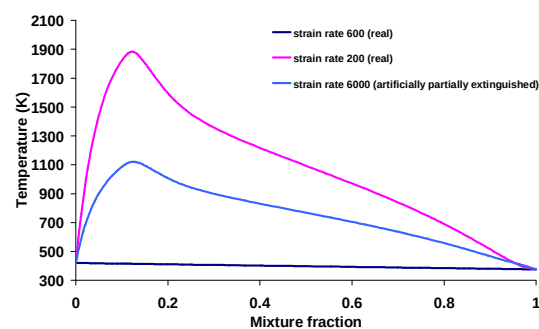


Figure 6. 141 Generation of the partially extinguished flamelet

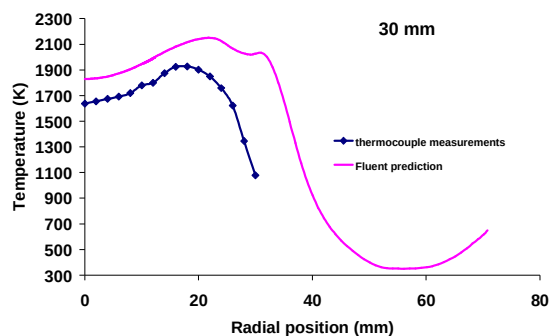


Figure 6. 142 Temperature profile at 30mm

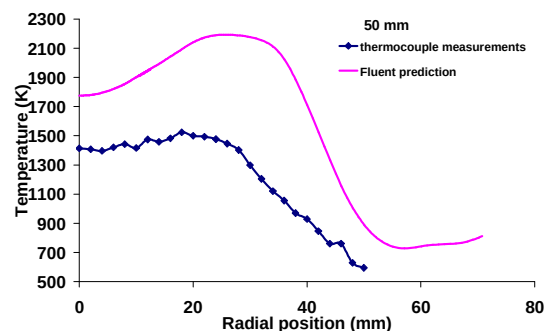


Figure 6. 143 Temperature profile at 50mm

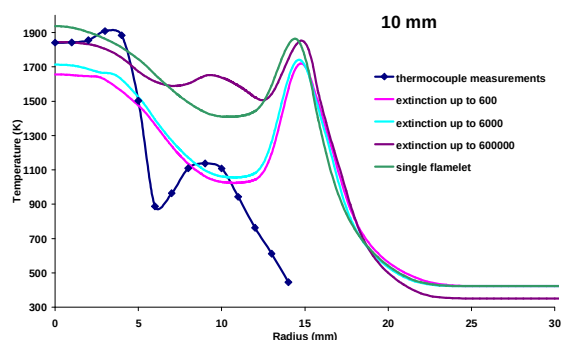


Figure 6. 144 Temperature profiles with different flamelets at 10 mm with extinction limits of 600 s^{-1} , 6000 s^{-1} , $600\,000 \text{ s}^{-1}$.

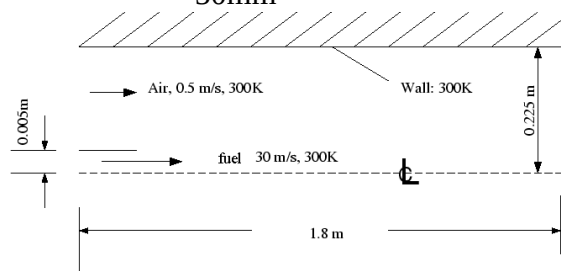


Figure 6. 145 Description of furnace in turbulent diffusion flame (FLUENT documentations)

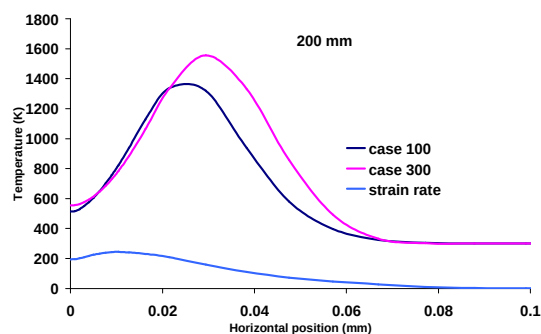


Figure 6. 146 Temperature profiles for gaseous flames with partially extinguished flamelets at 100 s^{-1} and 300 s^{-1}

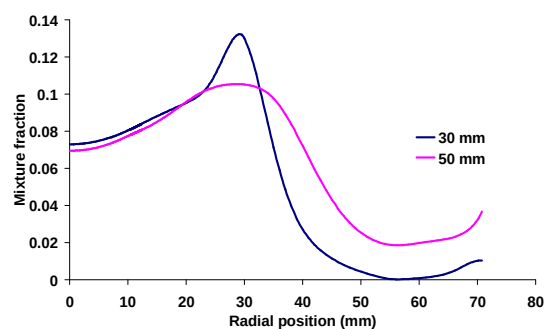


Figure 6. 147 Mixture fraction profiles at 30 and 50 mm

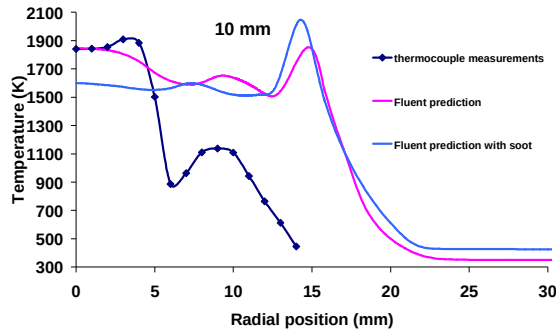


Figure 6. 148 Temperature profiles comparison with soot and radiation at 10 mm

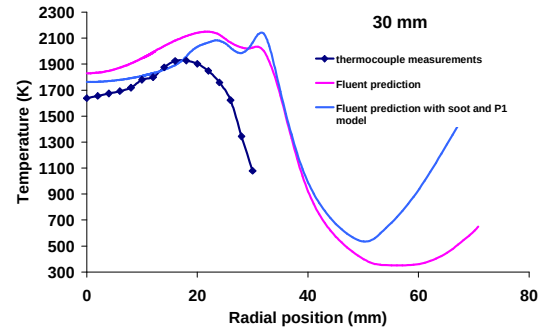


Figure 6. 149 Temperature profiles comparison with soot and radiation at 10 mm

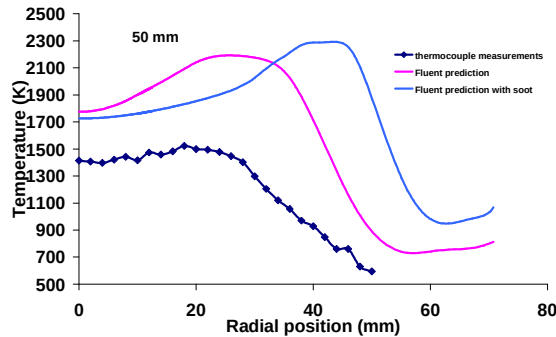


Figure 6. 150 Temperature profiles comparison with soot and radiation at 10mm

Another possible reason might be valid to describe the significant overprediction of the flame temperature in the downstream region. It could be the result of partially premixing between air and evaporating fuel, which would increase the volumetric heat release in the combustor.

Last but not least, the adiabatic nature of the simulation will result in a systematic overprediction of the temperature distribution. Although it has not been investigated in this study, radiation and soot calculations were implemented in the model to see their effect on the flame structure. The P1 radiation model was used and the wall emissivity was set to one. The results of the solutions can be compared with the previous solution and the thermocouple measurements, figure 6.149 to 6.150. There is a better agreement in the downstream regions compared to the solutions which did not include radiation. Indeed there is noticeable heat loss on the spray centreline, which can reach as much as 300 K in certain sections at 50 mm. Therefore the coupling of

soot and radiation with the turbulent reacting flow has reduced the overprediction of the temperature distribution and better agreement ensued. Unfortunately, this significant area of combustion could not be investigated more thoroughly and no soot measurements were taken to validate the numerical results. However, radiation and soot prediction are vast topics which could imply a whole research investigation by themselves. But clearly, an accurate predictive capability is required for flame radiation within spray flames, since the amount of heat loss by thermal radiation can be significant (respectively 20 and 40 % at 1 and 3 atm) and further increase as the ambient pressure is raised.

This section has demonstrated that the FLUENT laminar flamelet model is weak in predicting local flame extinction and is therefore not well suited to predict strongly non-equilibrium in turbulent flames due to aerodynamic straining by the turbulence. The flame temperature is overpredicted in the downstream region of the flame essentially because flame radiation and soot modelling are not invoked.

6.8.1 Influence of inlet air temperature

The effects of changing ambient temperature on the flame structure will be now considered. Figure 6.151 to 6.153 show the flame flow field with an air ambient temperature of 423 K instead of 288 K. The initial droplet size for both cases is the same as well as other boundary conditions in order to clearly identify the effect of air temperature on the gas temperature in reacting flows.

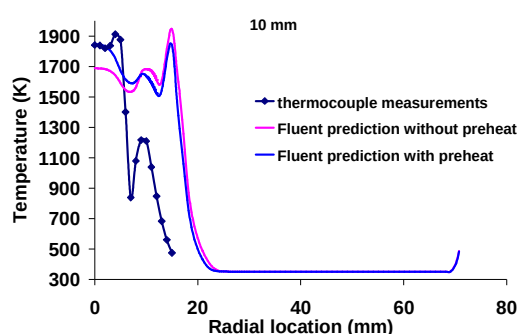


Figure 6. 151 Comparison between not preheated and preheated air temperature profiles with thermocouple measurements at 10 mm

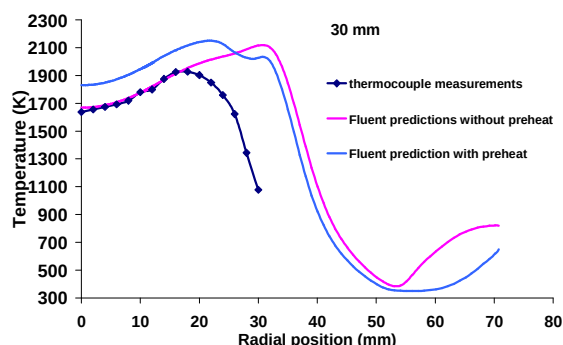


Figure 6. 152 Comparison between not preheated and preheated air temperature profiles with thermocouple measurements at 30 mm

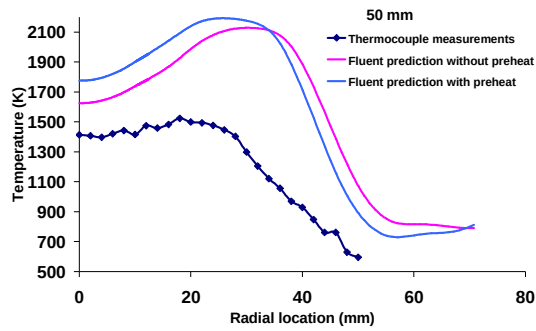


Figure 6. 153 Comparison between not preheated and preheated air temperature profiles with thermocouple measurements at 60 mm

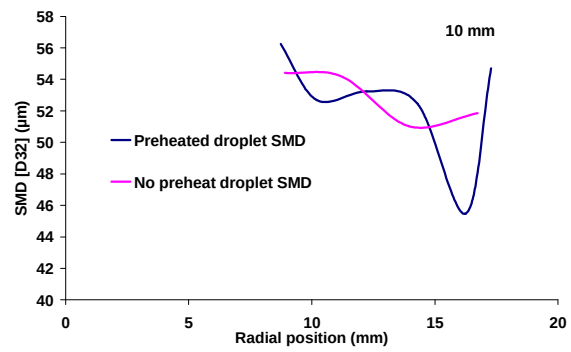


Figure 6. 154 Sauter mean diameter with preheated and not preheated air at 10 mm

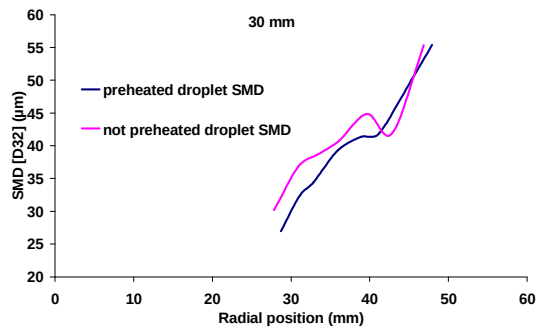


Figure 6. 155 Sauter mean diameter with preheated and not preheated air at 30 mm

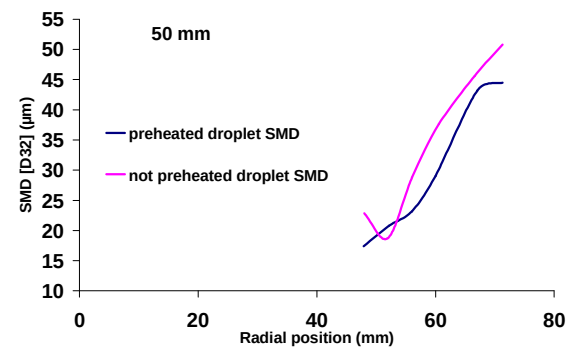


Figure 6. 156 Sauter mean diameter with preheated and not preheated air at 50 mm

Figures 6.151 to 6.153 show that the gas temperature is increased as a result of air preheating by an average of around 150 K on the spray centreline. The air temperature has been increased by 135 K, therefore the increase in gas temperature is significant.

The droplets Sauter mean diameter is not affected by the air preheating as illustrated figure 6.154 to 6.156. The air temperature would have to be more significantly increased to have an effect on the droplet Sauter mean diameter. Indeed, biodiesel boiling point is at 623 K and the droplet is at best heated to a temperature 200 K lower to its boiling point. On the other hand, if biodiesel was replaced by ethanol which is highly volatile with a lower boiling point of 351 K, the flame would have behaved liked a premixed flame since a significant portion of the fuel would have already vaporized before entering into contact with the swirling air as the air temperature would be beyond the liquid boiling point. The air preheating would have the most significant effect on the small droplets since they are the most subject to evaporation compared to the larger ones. The droplet penetration would increase as a result of an

increase in air temperature due to a reduction in the air density consequently leading to a drag reduction on moving droplets.

The axial velocity profile of the preheated air seen figure 6.157 to 6.159, display a slightly stronger recirculation and peak axial velocity, due to the lower gas density with the higher temperature, which results in more efficient mixing. The higher temperature distribution for the preheated air reflects the effects of improved mixing associated with the stronger recirculation zone.

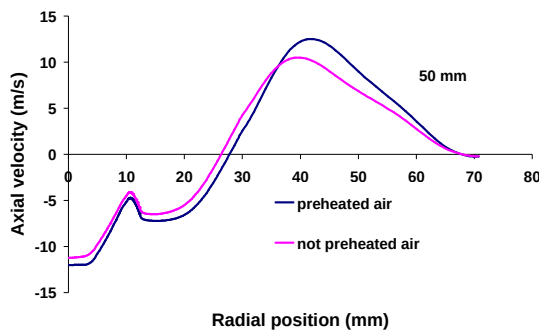


Figure 6. 157 Axial velocity profile comparison for preheated and not preheated air at 10 mm

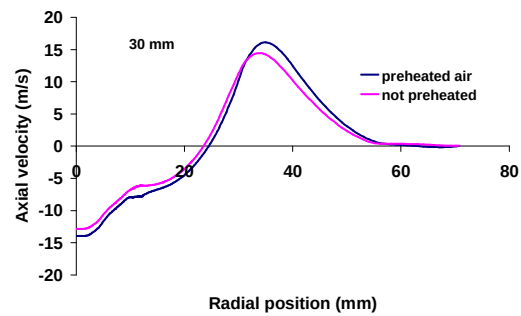


Figure 6. 158 Axial velocity profile comparison for preheated and not preheated air at 30 mm

6.8.2 Effect of droplet diameter

The influence of droplet size distribution on the spray flame development has been demonstrated to be of high importance for ethanol in section 6.8.1. Figure 6.159 to 6.161 show the influence of changing the Sauter mean diameter from 48 to 63 microns Varying the mean particle diameter in the Rosin-Rammler expression significantly modifies the mixture composition within the core of the spray flame.

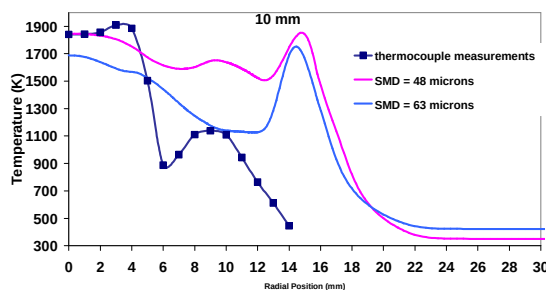


Figure 6. 159 Temperature profile comparison with SMD = 48 and 63 μm at 10 mm

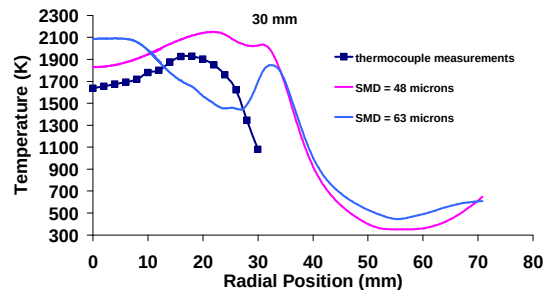


Figure 6. 160 Temperature profile comparison with SMD = 48 and 63 μm at 30 mm

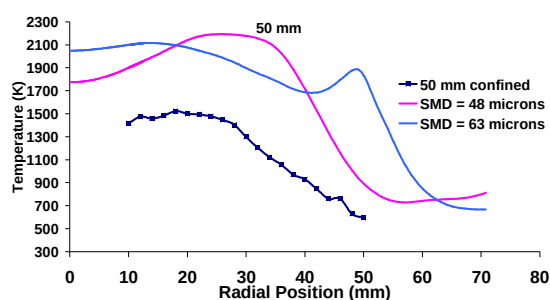


Figure 6. 161 Temperature profile comparison with SMD = 48 and 63 μm at 50 mm

The effect of the droplet size distribution model on the axial temperature predictions is also apparent. The temperature prediction is better at the centreline with SMD=48 μm and remains very good up to a height of 30 mm, however, beyond this point there is a substantial overprediction. The temperature prediction with SMD=63 μm , however deviate significantly from the thermocouple measurements, resulting in an underprediction of 170 K at 10 mm followed by an overprediction of order 700 K at a height of 50 mm.

6.8.3 Combustion at higher pressures

Biodiesel spray flames have been modelled at 2, 3 and 10 atm operating pressure. However, the critical pressure will not be exceeded for the Rix biodiesel since it has been determined to be at least 12 atm in section 3.1.3 of the Fuel Properties chapter.

As mentioned in the literature review, a rise in pressure will be accompanied by an increase in evaporation rate, which is likely to reduce the fuel penetration in the pressure rig. Contrary to the investigation of ethanol combustion at higher pressure, this time the operating conditions will not be kept the same, since some experimental data have been taken to determine the operating conditions at up to 3 atm unlike the ethanol experiments which were all conducted under atmospheric pressure. To keep the same trend up to 10 atm, the data obtained have been extrapolated and the following trend is obtained:

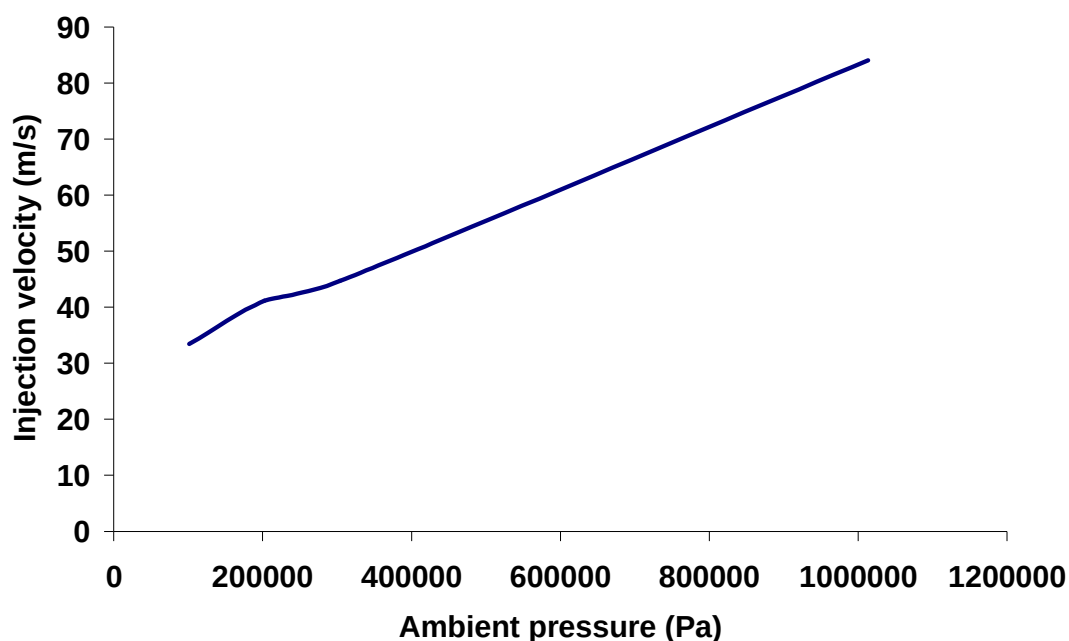


Figure 6. 162 Initial Injection velocity as a function of injection pressure

Consequently the injection velocities were set according to the different operating pressures as described in table 6.12. As the droplets velocities increase with pressure while the air velocities remain constant since they are scaled with pressure, it is important to know if secondary breakup might not be a likely occurrence, therefore the Weber number needs to be estimated and breakup will occur only if $We > 12$:

Ambient pressure	1 atm	2 atm	3 atm	10 atm
Injection velocity	33.43 m/s	41.16 m/s	44.66 m/s	84 m/s
Estimated Weber number	2.97	3.87	6.85	81.05

Table 6. 12 Estimation of injection velocities with ambient pressure and Weber number

Therefore breakup is certain to occur only beyond 10 atm unlike what was said section 5.8 of the Computational Study. Figure 6.163 to 6.165 show that the flame has considerably shortened with an increase in pressure due to enhanced rates of mixing, heat transfer and reaction kinetics.

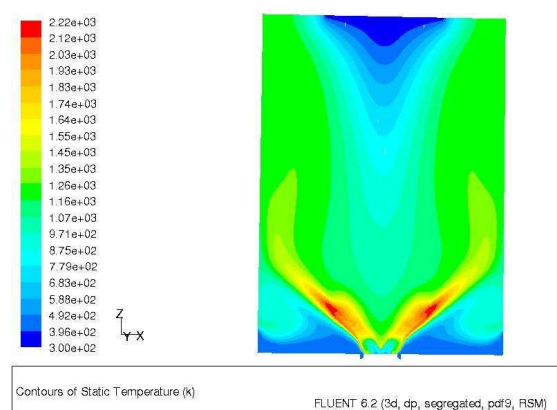


Figure 6.163 Temperature field at 2 atm

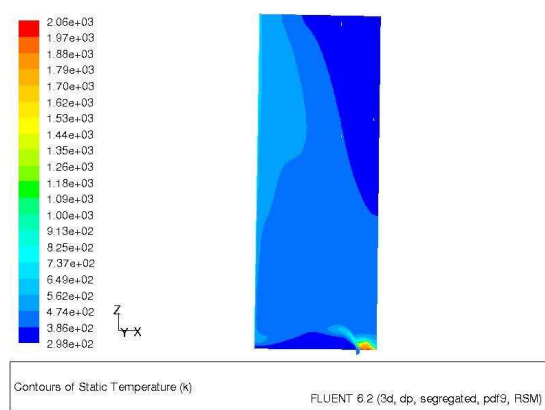


Figure 6.164 Temperature field at 3 atm

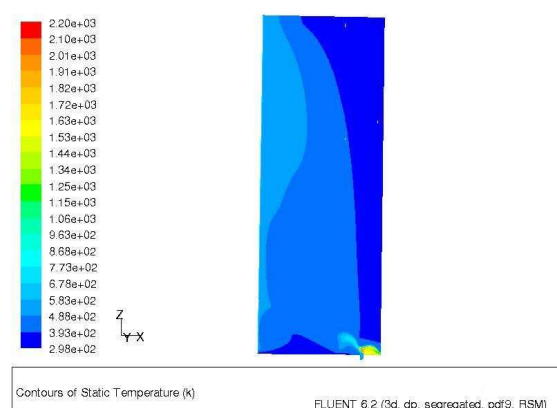


Figure 6.165 Temperature field at 10 atm

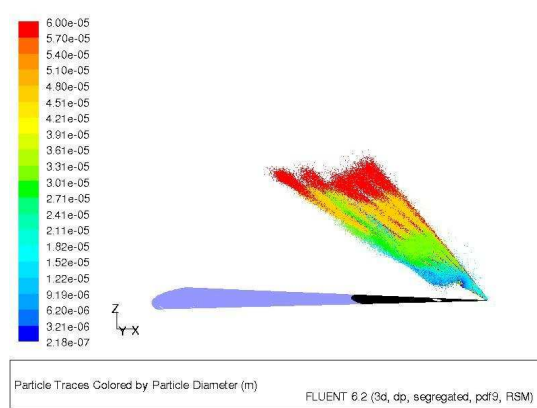


Figure 6.166 Spray trajectory at 3 atm

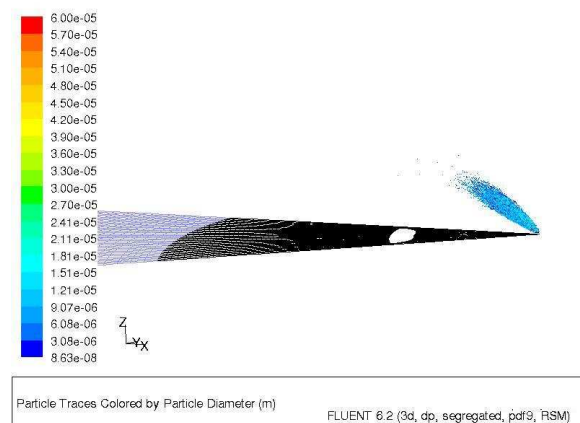


Figure 6.167 Spray trajectory at 10 atm

Normally, in industrial applications the air fuel ratio is maintained constant which implies that once pressure is increased, the fuel flow rate is normally increased at the same rate as the air flow rate. However in this study the fuel flow rate has been maintained constant to isolate the effects of pressure. Figure 6.167 shows that the spray penetration is substantially lower when the pressure is raised at 10 atm

compared to the penetration at 3 atm. Under 10 atm, the spray does not even reach the exit of the swirler (cf. figure 6.167) due to the high gas density.

Therefore a decrease in the droplet penetration is noticed as the pressure is raised, which leads to a substantial increase in spray density, which could result in spray collision and coalescence. The reduced droplet penetration is due not only to higher pressure but increased evaporation rates. Due to collision and coalescence, an increase in mean drop size might result as seen figure 6.166 where the maximum droplet diameter is at the tip of the spray. However, it could have been expected that due to higher pressure, resulting in an increase in air density, the aerodynamic shear forces would disintegrate the spray. Unfortunately, due to the extremely low penetration of the spray under higher pressures, it will not be possible to supply information on the evolution of the SMD.

The results show that as the air pressure is increased, the liquid penetration is decreased. Moreover the flame has considerably shortened due to the high air fuel ratio applied on the flame as illustrated figure 6.160 to 6.162 and enhanced rates of mixing. Further increase in pressure or primary air fuel flow rate might result in flame quenching, unless the fuel flow rate is increased alongside the air flow rate.

6.9 Discussion and Model evaluation

The turbulent spray flames have been modelled with varying degrees of success. The main failing of this model is its inability to predict local flame extinction and correctly predict the evaporation rate. However, the results have shown, that there are a number of issues involved in using the default FLUENT flamelet and evaporation models.

The model assessment will be based on the following questions:

- does the flamelet model offer a consistent calculation of the scalar dissipation rate and predict local flame extinction
- is the default FLUENT evaporation model accurately describing the evaporation process
- what would be the strategy and computational cost associated with the model improvement?

6.9.1 Evaporation model

The default FLUENT evaporation model is based on the infinite conductivity or rapid mixing model where it is assumed that rapid internal circulation occurs within the droplet and the droplet temperature is uniform but time varying. However, Sirignano (1978) mentioned that even in the limit of high vortex strength, the internal liquid circulation can reduce the length scale for diffusion only by one order of magnitude. Therefore the rapid mixing assumption is not valid.

The vortex model developed by Prakash and Sirignano (1978) (1980) and Tong and Sirignano (1982) is too complicated and computationally expensive to be implemented into any CFD model and moreover this model has not been validated.

Aggarwal et al. (1984) found that the infinite conductivity model was not suitable for practical applications, although no experimental validation was carried out and consequently, the vortex model was recommended for practical applications. But Chen et al. (1997) compared the performance of different models such as d^2 law, infinite conductivity, conduction limit and vortex model and concluded that the predictions of the different models were quite similar. Therefore, it is difficult to judge the quality of the infinite conductivity evaporation model based on conflicting conclusions.

The more sophisticated effective model Abramzon and Sirignano (1989) provided a relatively 'inexpensive' vaporization model of a moving fuel droplet, particularly suitable for the spray combustion calculation, which includes all the effect of variable thermophysical properties, non unity Lewis number (in the range 1-4) in the gas, the effect of transient liquid heating, droplet internal circulation and the effect of the Stefan flow on heat and mass transfer between the droplet and the gas. This model possess such advantages as simplicity, application to a wide range of parameters (Re, B, etc.) making it a more robust model, and necessitating low amount of computational time. However, to faithfully describe the model, temperature gradients inside the droplets need to be represented, which is not possible within FLUENT. Therefore the flexibility in using different evaporation models is at present extremely limited, and there is no other choice but to use the default model.

Accurate prediction of the thermo-transport properties is an essential part of modelling of droplet evaporation. In fact, Kneer et al. (1993) investigated the importance of variable liquid properties on droplet evaporation. The authors found that vaporization is highly affected by the dependence of liquid properties on temperature and composition. In particular, variable liquid diffusion coefficient controls the relative thermal and mass diffusion and in turn, the rate of evaporation.

FLUENT is quite flexible in determining the diffusion coefficient, viscosity and specific heat as a function of temperature, both for the liquid and the vapour phase. However, FLUENT assumes constant values for latent heat of vaporization, particle thermal conductivity and density. Particle thermal conductivity does not have any influence on the droplet evaporation, while particle density does affect the droplet motion, therefore droplet evaporation is not particularly involved with these properties.

However, FLUENT treats the Schmidt numbers ($Sc = \mu/\rho D$) and the Prandtl number ($Pr = \mu/C_p \lambda$) numbers as identical constants, resulting in unity Lewis number. But the assumption of unity Lewis number implies equal mass and heat diffusion in a flow field less dominated by convective effects. But, in most convective conditions, the mass diffusion is most likely two orders of magnitude slower than the thermal diffusion, and the unity Lewis number assumption may not be justified (Maru, 2005). In fact, the Lewis number is strongly dependent on the gas temperature, and its composition, which consists in several species whose molecular weight can vary broadly, such as CO₂, H₂O, hydrocarbons among others.

The convection effect is treated by an additional empirical Ranz and Marshall (1952) correlation. However, in real life situation, convection effects are quite important and the evaporation rate depends on the convection in the turbulent gas field. Convection will increase the gasification rate as well as heat transfer between the gas and liquid phase, the semi-empirical Ranz-Marshall correlation used in FLUENT has little justification for it, and the correlations are based on experiments conducted under quasi-steady conditions, justifying the overprediction in the simulations evaporation

rate. An alternative to the Ranz and Marshall correlation, Abramzon and Sirignano(1989) recommended the following correlation:

$$Nu = 1 + (1 + Re Pr)^{1/3} f_c(Re)$$

Where $f_c(Re) = 1$ at $Re \leq 1$ and $f_c(Re) = Re^{0.077}$ at $1 < Re \leq 400$. This equation approximated the numerical results by different authors in the range of $0.25 < Pr < 100$ with an error of less than 3 % (Abramzon and Sirignano, 1989) and could be tested in any future work.

The different shortcoming of the evaporation model has been highlighted. The lack of flexibility of FLUENT to support temperature gradient inside the droplet deters to use other evaporation models, especially the effective conductivity model and crucially, the unity Lewis number assumption is not justified. Moreover, the Ranz-Marshall correlation to account for convective effects is too simplistic and alternative correlations need to be looked at.

6.9.2 Flamelet model

In order for the flamelet equations to be consistent with the equations solved for the turbulent flow field, the temperature and species mass fraction distribution have to be calculated over mixture fraction space in such a manner that the values computed in the flow field can be retrieved in the flamelet libraries, eventually through interpolation between adjacent flamelets if the exact value is not available in the library. However, the extinguished flamelet exported into FLUENT are not accounted for, as they are excluded from the library.

Therefore the FLUENT flamelet model shows significant deficiencies in regions of high strain, where quenching of the flame may occur due to the aerodynamic straining of the flame. In fact, the results have shown evidence that while using partially extinguished flamelets, there is an increase of the local peak temperature while it would have been expected to obtain a better temperature prediction with a significant temperature decrease in that highly strain region. In fact, the behaviour observed immediately downstream of the swirler is not consistent with what is observed in the

experiments. The gross overprediction of the temperature in the highly strain region is a direct consequence of the failure of the FLUENT laminar flamelet to predict the quenching of the flame due to the strong turbulence level encountered in this region. It was then believed that instead of implementing extinguished flamelets, a better alternative would have been to describe partially extinguished flamelets. Yet again, no underprediction of temperature resulted.

Therefore, the laminar diffusion flamelets used in the calculation are inaccurate. Although the chemistry incorporated in the laminar flamelet calculation is to present knowledge accurate, other factors such as local strain rate in the flamelet is not properly considered, resulting in very poor predictions especially in highly strained regions. Such factors are especially important in the lower region of the flame where strain is greatest. Therefore, the fact that heat loss on the extinction limits is not taken into account is clearly a significant weakness of the model.

Moreover, the FLUENT flamelet model assumption that the species mass fraction is independent of heat loss is clearly wrong but it is difficult to quantify how it will affect the predictions. Experimental measurements would need to be taken in turbulent flames, but this does not affect this study since the species mass fractions are generated by CHEMKIN, a stand-alone package.

Eventually, one might have a closer look at the Beta function approximation to the PDF of mixture fraction. However, Chen et al. (1991), using simple models for chemical reaction and turbulent flow, explore the influence of the shape of the presumed pdf, $P(Z)$ in calculations of a diffusion flame in a boundary layer and concluded that profiles of mean velocity, enthalpy, mixture fraction and its variance are little affected by the pdf shape.

Eventually, the flamelet model could be replaced by the transport PDF which has the potential to predict weak extinction but PDF transport simulations are computationally expensive, when flamelet simulations already take a long time to compute. Therefore the laminar flamelet approach is still recommended.

The FLUENT laminar flamelet model is limited to flames with relatively fast chemistry and cannot capture deep non-equilibrium effects such as ignition, extinction

and slow chemistry, such as NO formation, which is not calculated in this study, but it is a matter of concern as to whether the flamelet model is capable of faithfully representing the transient effects such as local and partial extinction. As a result, the laminar flamelet model is believed to be a near equilibrium model, and this will have a significant impact on the numerical results obtained in this study. Because of the simplifying assumptions made in the derivation of the flamelet equations, the flamelet model fail in situation where local extinction and re-ignition are important. It is in fact only capable of predicting moderate non equilibrium effect in the flame due to aerodynamic straining by turbulence. In fact present day mixture fraction based model cannot predict local extinction. Also, the laminar flamelet approach, although frequently applied to model non premixed flames based on the assumption of adiabatic combustion, generally leads to a significant overprediction of temperature especially in the downstream region of the flames where radiation is important (Ma et al. 2002). Radiation heat transfer must therefore be taken into account when the laminar flamelet modelling is adopted to calculate turbulent flames. On the other hand, the laminar flamelet model modelling cost is far from being prohibitive compared to other combustion models, such as the joint PDF method or the Conditional Moment Closure model described in the earlier literature review.

6.9.3 Soot and radiation

The neglect of radiative heat loss for the biodiesel simulations results in overprediction by several hundred Kelvin of the flame temperature in the downstream regions. Indeed, it is believed that radiation can be neglected in ethanol flame since they are not very luminous but it could be significant in biodiesel flames which are much more luminous.

Since no experimental data is available for soot measurement in this study, results obtained with soot and radiation modelling would be rather speculative and uncertainties are likely to remain. However if the flame produces significant quantities of soot, then the impact of radiation on soot production needs to be carefully assessed. Therefore, methods for implementing radiation and soot modelling will be presented here.

For hydrocarbon flames, the minimum energy loss by radiation is approximately 20%. Syed (1990) suggested a method, further developed by Young (1993) and Young and Moss (1995), where a finite set of flamelets, each flamelet containing a different amount of radiative loss, may be generated creating a library of flamelets. The most appropriate model for local flame properties may be selected by comparing the radiative loss incorporated in each of the flamelets with the local radiative loss – determined from a balance equation for the enthalpy. If the strain rate reported in the flow field is different from the strain rate obtained in the flamelet library, the heat loss would linearly interpolated between two strain rates.

In order to defined different amount of heat loss, the flamelets can be manipulated by hand. One method could be to modify the temperature distribution according to the amount of heat loss without changing the species mass fraction. Although a relatively quick method, the relationship between the temperature and the species mass fraction might be inconsistent. Fairweather et al. (1992) suggested an adjustment to the flamelet temperature in the following manner:

$$T(Z) = T_{ad}(Z) \left(1 - \omega \left(\frac{T_{ad}(Z)}{T_{ad,max}} \right)^4 \right)$$

where $T_{ad}(Z)$ is the adiabatic flamelet temperature and where ω is an empirical constant with a value of 0.21 representing the heat loss fraction but the percentage of heat loss is not easily predictable since it is constantly changing according to the location in the pressure rig.

Alternatively, a fixed percentage heat loss could be applied to the flamelet calculation, and this allows changing not only the temperature distribution but the species mass fraction as well, although this procedure is more time consuming task since each individual flamelet must be generated. Finally, the optically thin radiation model could be used, with the soot concentration altered to change the amount of heat loss from the flame. This method also avoids inconsistencies between the temperature and species concentration and in addition it takes into account the impact of soot distribution on energy loss.

CHAPTER 7 – CONCLUSIONS

Validation of the numerical results has been a challenging task due to the numerous physical processes involved in spray combustion. A number of modelling difficulties are introduced, including flow turbulence, spray atomization, evaporation and combustion. Simulation is further complicated by the fact that all these models must work together since they are strongly coupled and consequently influence each other. A necessary step in this process is the creation of a detailed database of models and properties which can be used to benchmark the numerical simulations of burning sprays in turbulent environments. This thesis describes a benchmark spray combustion database which can inform future developments, particularly in relation to bio-fuels which are expected to assume an increasingly important role in the environmentally sensitive energy field.

The computational study began with the pilot study of an unconfined ethanol spray flame and was extended to confined ethanol and biodiesel flames. It has excluded rapeseed oil simulations, although these formed part of the linked experimental programme, since their behaviour when pre-heated must be expected to be close to the biodiesel simulations given the limited detail presently available on their chemistry.

A conventional laminar β -PDF flamelet model coupled with the Reynolds Stress turbulence model has been applied throughout this study. To represent the multiphase flow aspect of the spray in a gaseous environment, a Lagrangian model based on Discrete Random Walk was used to account for the effect of gas generated turbulence on the spray dispersion. The effects of soot production on the gaseous phase chemistry were assumed negligible – both oxygenated fuels are more weakly sooting than their hydrocarbon counterparts.

The flamelet computations used detailed gaseous ethanol and methylbutanoate reaction mechanisms to describe the ethanol and biodiesel spray flames respectively. The methylbutanoate mechanism was used as a surrogate reaction mechanism for biodiesel. Although methylbutanoate does not have the high molecular weight of a

biodiesel fuel, it has the essential (fatty acid) chemical structure, in the form $RC(=O)OCH_3$.

Comparisons of CFD prediction with experimental data for droplet velocity, diameter, gas phase velocity and temperature have been presented. Generally, good agreement was obtained for the droplet characteristics and the gas velocity. However, serious discrepancies were encountered for the gas temperature and therefore, by implication, the flame structure.

The ethanol simulations showed that the evaporation rate was overpredicted. The Ranz-Marshall correlation, which was used to account for the convective effects, is believed to be the main cause of the discrepancy and this issue was discussed in detail in the Discussion section. The validity of the correlation has been questioned and more sophisticated evaporation models advocated. In its present form FLUENT does not offer the additional flexibility needed. In particular, the user cannot implement either the vortex model or the effective conductivity model, which would better account for convective effects, since the temperature field inside the droplets is not addressed. The overpredicted evaporation rate led, in turn, to an underprediction of the flame temperature in the vicinity of the spray nozzle, where the fuel is too rich to burn – unlike the behaviour observed in the experiments. This also resulted in a cooled region due to the passage of the spray that was significantly wider than observed experimentally.

On the outer edges of the spray, a pronounced local peak temperature appears in the simulation that has not been observed in the experiments. The detailed flame structure is therefore far from being satisfactorily represented by the basic flamelet model. Changes in the flamelet extinction strain rate have been introduced to examine their effect on the flame structure but these seemed merely to have further exaggerated the local peak temperature. The steady flamelet technique would appear stretched beyond its limit of validity - resulting in significant errors in temperature prediction in such highly strained regions. The FLUENT strained flamelet model, which systematically excludes an extinguished flamelet from within its library, is therefore deficient in

predicting these strongly non equilibrium conditions. Profiles of artificially generated strained flames – close to extinction – did not remedy the poor agreement achieved.

Despite these two serious issues, a number of features of the ethanol flames have been predicted with some degree of success. The spray centreline temperature was accurately captured, although the quality of the CFD predictions is highly dependent on the specification of spray initial conditions. These are most difficult to measure, since the spray is not atomized immediately after exiting the spray injector, and an element of trial-and-error is introduced into their specification at locations further downstream.

A series of experimental simulations has been carried out to assess the effect of the initial conditions on the spray flame structure and judge the sensitivity of FLUENT models to changes in the initial spray conditions. This parametric study yielded some interesting results. For example, it was shown that increasing the Sauter mean diameter beyond a certain value did decrease the combustion efficiency, as might be expected, whilst burning very fine droplets might also decrease the heat release under fuel-rich conditions. This indicates that the simulations can identify an optimum Sauter mean diameter over which combustion efficiency is at its greatest. The fine droplets may evaporate rapidly without burning, and the region in the vicinity of the spray nozzle become too rich, decreasing the flame temperature. However, when the droplet size is further increased, the droplets will pass through this primary zone and travel further, without vaporizing, into a region where a large proportion of the droplets will evaporate in a comparatively cold environment, resulting in poor mixing. Burning will become less effective, reducing the combustion efficiency and the flame temperature. Such calculations emphasise the need for a good compromise to be found between large and small droplets, which should penetrate deep enough into the primary zone to ensure a sufficient high temperature residence time is achieved and burning is completed, but not so deep that a large proportion of unburnt fuel results. FLUENT does therefore show some useful sensitivity to the role of the SMD in the flame structure. On the other hand, it does not appear to be very sensitive to the number of size classes adopted, since the results obtained with 5 or 10 size classes are broadly similar.

Increasing the spread parameter in the size distribution led to higher flame temperatures since higher amounts of fuel vapour were then generated, leading to “less lean” conditions and consequently a higher combustion efficiency.

Modifying the spray azimuthal spread had a significant effect on the flame structure. Narrowing down the spray spread angle from 30 to 20 degrees leads to a higher flame temperature on the centreline in the vicinity of the spray nozzle. For an azimuthal spread of 30 degrees, the particle streams at 65 and 70 degrees are responsible for the lower temperature on the spray centreline due to the cooling effect of the spray. The PIV measurements showed positive velocities on the spray centreline which were interpreted as evidence for the presence of fuel droplets, rather than seed material from the air, although these are apparently very small since they are not detected by the PDPA. Adding droplets smaller than 5 microns to the initial spray conditions on the centreline produced simulations exhibiting flame lift off, with an extensive fuel rich region upstream.

The influence of droplet-droplet interaction was also investigated with simulations exhibiting a strong coupling between the number of particle streams, the evaporation rate and the temperature field. Increasing the number of particle streams lead to a reduction in the droplet evaporation rate.

In addition to the cases for which experimental data were available, a number of simulations were also performed to extend the range of operating conditions. Increasing the air fuel ratio by increasing the velocity (two-fold) substantially shortened the flame with a significantly lower peak temperature. Experimentally, the increased air velocity would be expected to lead to blow-out extinction but, as indicated earlier, flame extinction is not reproduced by a flamelet model. Increasing ambient pressure – whilst maintaining the flow velocities constant - similarly lead to a significant shortening of the flame length. The evaporation rate is also increased with a rise in pressure and there is evidence of droplet collision when the pressure is raised to 10 bar. At this pressure, due to the strong air flow rate, the droplets are

carried away by the swirling air flow towards the cooler wall, and consequently the combustion efficiency is reduced.

Biodiesel simulations were also carried out at the experimental conditions and although, at the lower heights in the flame, the calculations showed better agreement between predicted temperature and measured values, the comparison deteriorated at higher heights and the flame temperature was overpredicted in the downstream regions of the flame. The quality of the temperature prediction was generally unsatisfactory for biodiesel and including flame radiation in the simulations would appear to be imperative since the flames are more clearly luminous. Constraints on both time and model complexity ensured that soot and radiation modelling was not included in this study. This issue has been reviewed in the Discussion section and methods are suggested to incorporate radiative heat loss in the flamelets, recognising that the flamelet scalar dependence would then be three dimensional. Soot production should also be considered, even though there are no experimental data to validate the numerical predictions and many informative studies have been performed on methane diffusion flames in which soot/radiation modelling has been neglected. It is anticipated however that significant improvement can be obtained when soot and radiation modelling are included and it appears evident that the two processes should not be ignored in bio-diesel combustion simulations.

Specification of initial conditions is critical in estimating the structure of sprays. It has been judged preferable to set up the initial conditions rather than used an atomization model since they are valid only for particular ranges of conditions and not suitable for others. This study does illustrate some of the principal sensitivities when faced with modifying the droplet size initial distribution in the absence of measured data but also reveals that such decisions can significantly modify the structure of the flame.

Preheating the fuel and air appears to have a substantial effect on the flame structure since the droplet diameter has been reduced to values where it is possible to vaporize it in such a manner that it improves the combustion process while preheating the air tends to raise the gas temperature by as much as 150 K. Preheating ethanol is not possible since it is a much more volatile fuel than biodiesel, therefore it would

vaporize quickly and behave more like a premixed flame while preheating biodiesel will help in reducing the droplet diameter considerably.

The experimental data do critically test the capability of FLUENT to predict turbulent reacting spray behaviour and the difficulties encountered are not restricted to complex fuels like bio-diesel. Challenges such as modifying the evaporation model and coupling it to a more sophisticated combustion model that would account for local flame extinction need to be resolved to obtain significant improvement in the predictions. It is clear that the default model in FLUENT both overestimates the evaporation rate and fails to predict the effects of local flame extinction in steadily burning spray flames of a well-defined alcohol. It is clear that the success of the numerical prediction depends on the quality of several different submodels, most notably for evaporation and combustion. Unfortunately, in the absence of experiment it is tempting to focus principally on only one model. A compromise has also to be established between numerical accuracy and computational expense since the computations take generally more than a week to get convergence even on multi-processor clusters.

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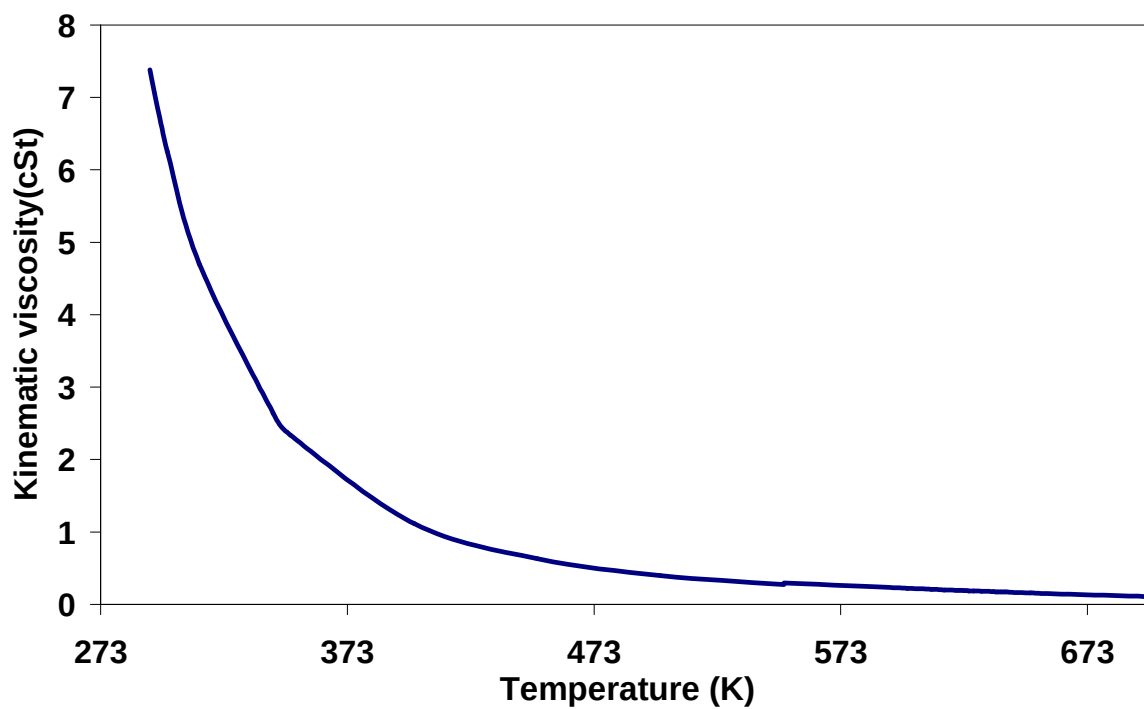
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APPENDIX A FUEL PROPERTIES

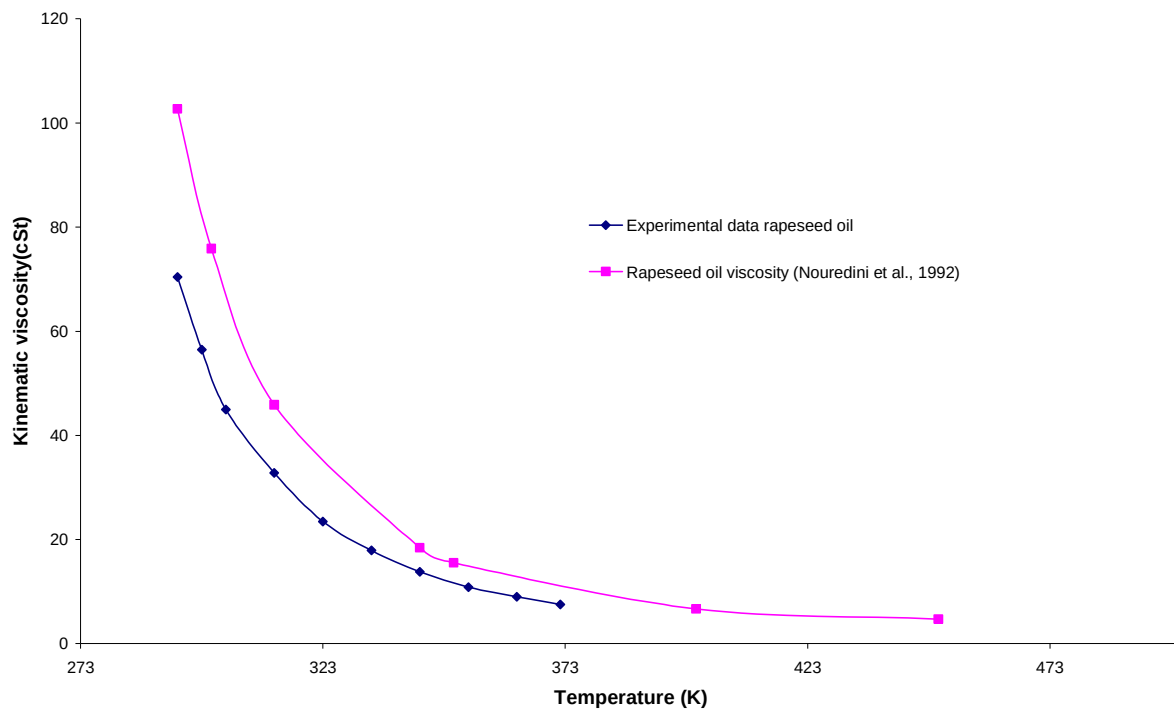
Viscosity

Rix biodiesel



Kinematic viscosity of rix biodiesel using Krisnangkura et al. , Tat and Van Gerpen and Reid et al. methods

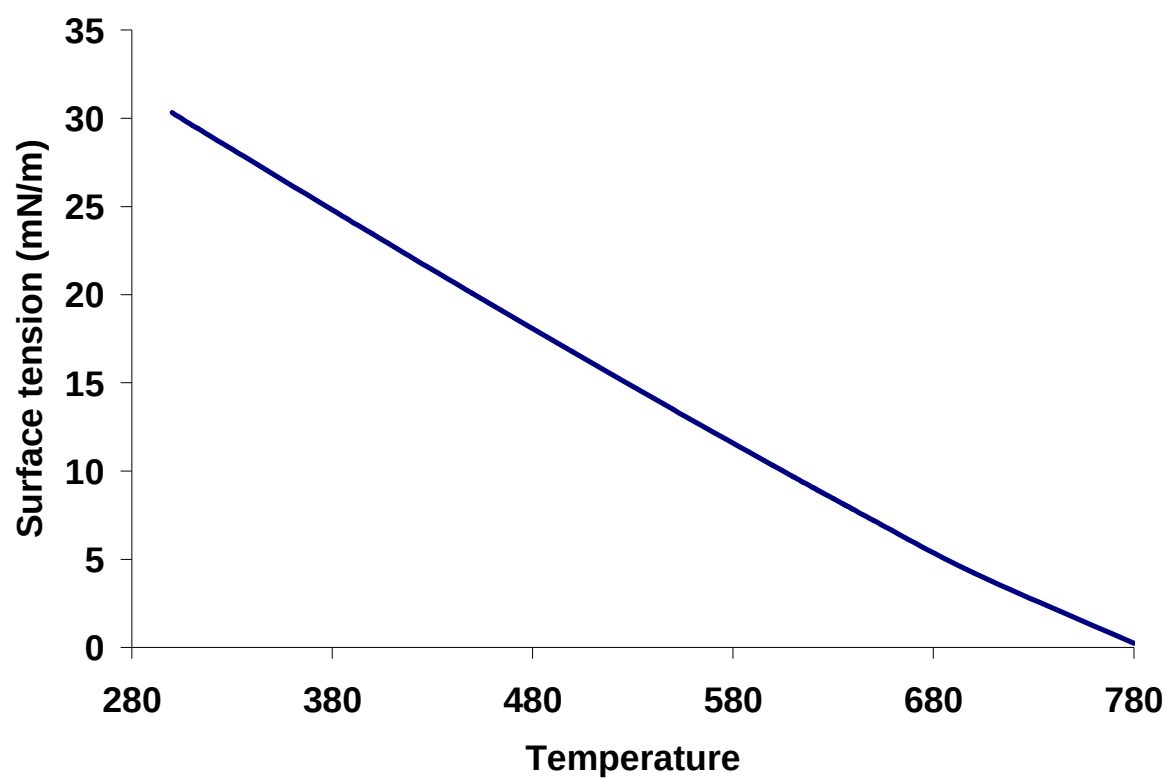
Rapeseed oil



Viscosity vs temperature for rapeseed oil

Surface tension

Rix biodiesel

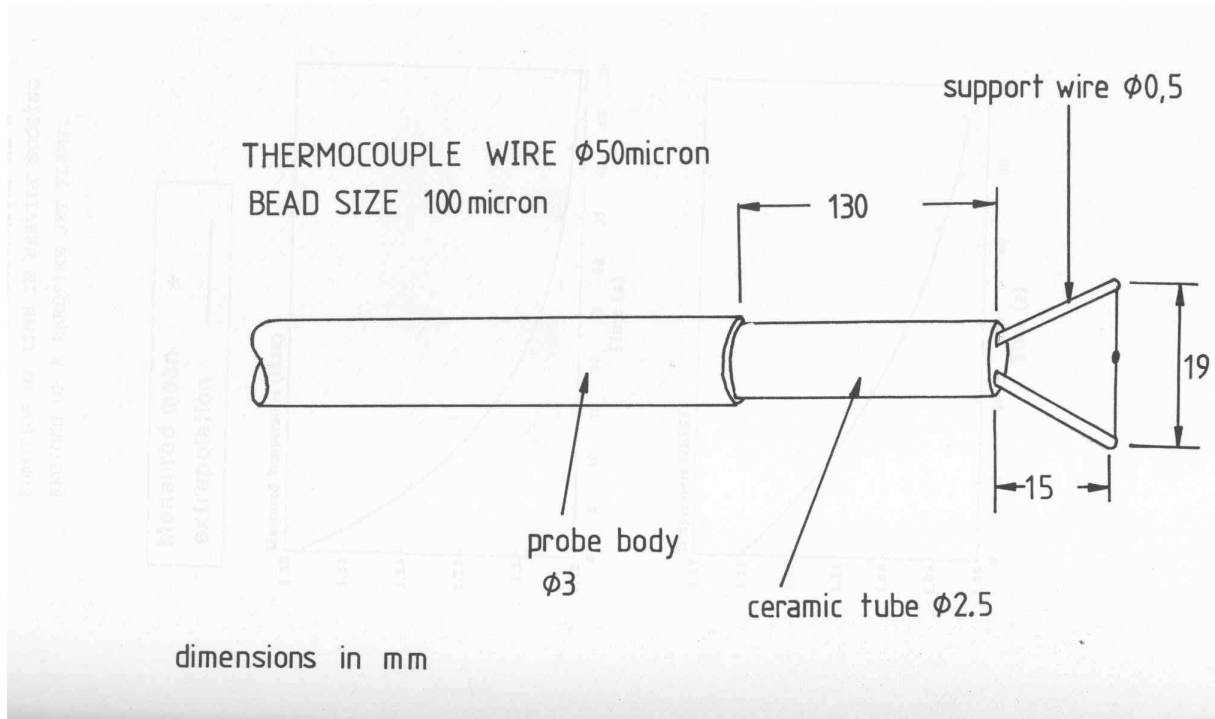


Predicted surface tension of rix biodiesel vs. temperature

APPENDIX B

EXPERIMENTAL DATA

THERMOCOUPLE



Schematic diagram of the bare fine wire thermocouple mounting arrangement (Brookes, 1996)

PDPA

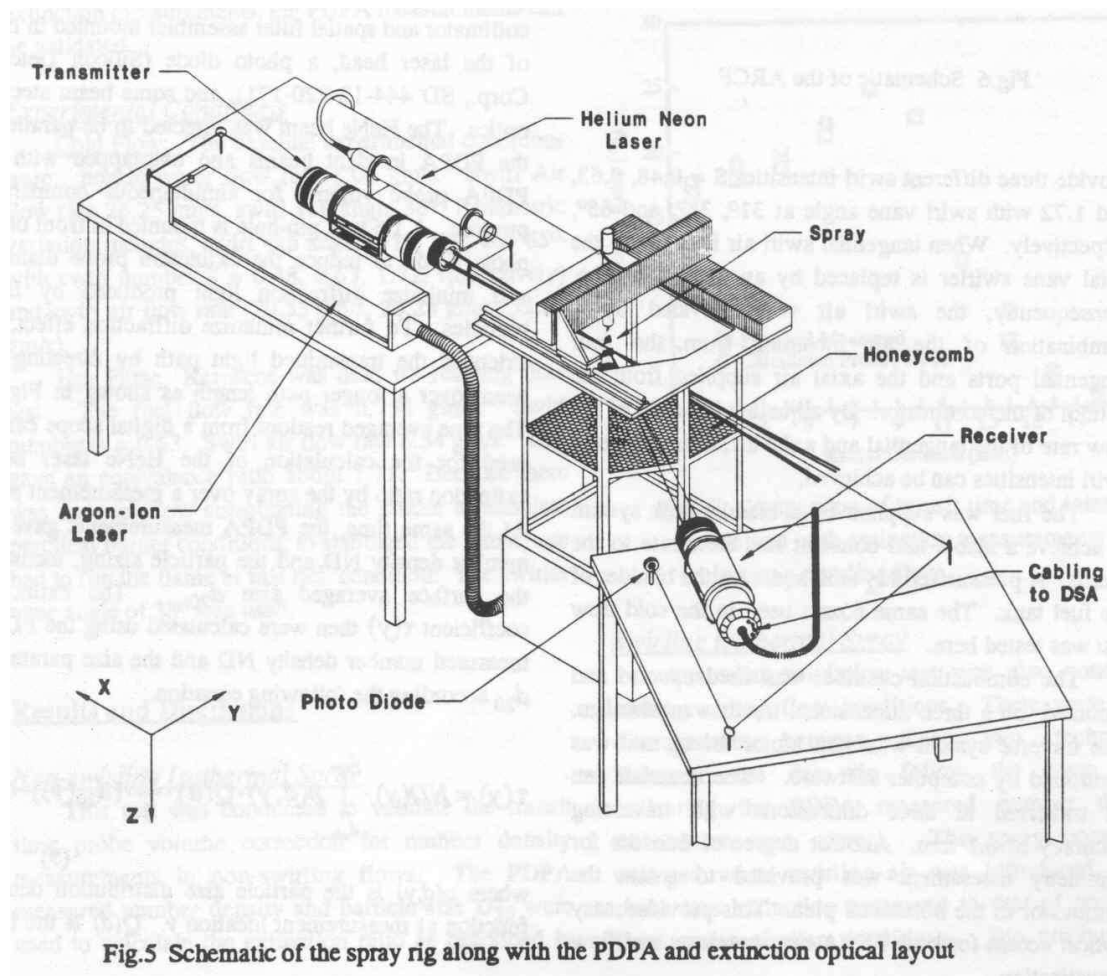


Fig.5 Schematic of the spray rig along with the PDPA and extinction optical layout

Schematic of the spray rig along with the PDPA (Zhu et al. 1993)

Pressure Rig Description

The burner, enclosed within a stainless chamber of 145 mm internal diameter to provide isolation from the environment, consists of a set of radial inflow swirlers surrounding a hollow liquid fuel injector with a cylindrical body placed coaxially in a cylindrical duct. The pressure rig is mounted on a movable platform, which allows the fixed measurement equipments located on either side of the rig to traverse the flame.

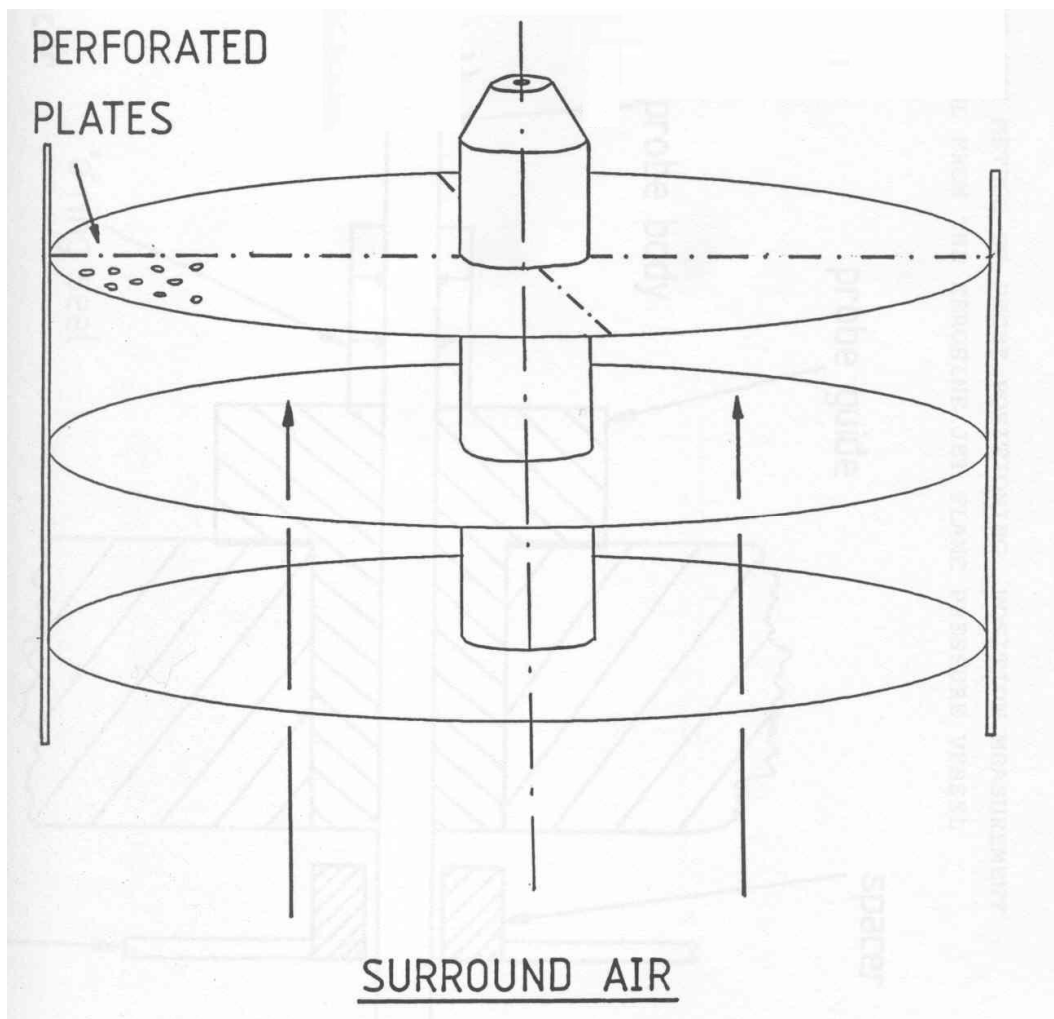
Air was delivered to the flame through an industrial blower. The air flows through an air heater before the air was passed around the central column which generated a significant perturbation to the flow such that the air velocity profile was far from uniform. A flow straightening system made of perforated stainless steel baffles was developed to correct this problem, thus giving a more homogeneous inlet velocity profile. The air was exiting through the swirler, entering the pressure rig. The swirler consists of eleven vanes at an angle of 43° , creating ten gaps with a total open area of approximately 95mm^2 . The air is swirled to enhance the mixing of fuel and air and create a recirculation zone to stabilise the flame and reaction zone.



Burner

The injector, a commercial Delavan pressure swirl atomizer injecting the liquid fuel into a swirling air flow, is designed to achieve proper atomization of the liquid fuels into fine droplets in order to increase the burning surface area and consequently the combustion efficiency. It is located at the

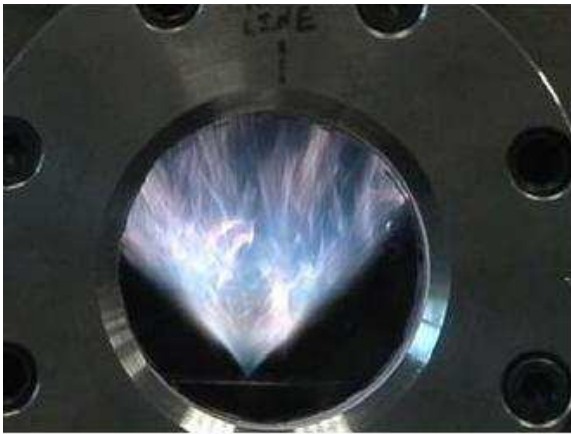
tip of the swirl generator. The fuel injector provides a solid cone when used in non burning and a hollow cone when used in burning conditions. In fact it is believed that the small droplets located on the inner edge of the spray disappear quickly as a result of evaporation, defining the conditions for a hollow cone spray. The nozzle diameter is 0.21 mm and the spray has a nominal half spray angle of around 45° . The fuel is delivered through a pipe which is not insulated and is exposed to the heated air so the fuel temperature is partly dependent on the air temperature, although they can be independently heated. Care has to be taken to ensure that no carbon deposit blocks the atomizer as it will significantly alter the drop size distribution and the velocity profiles, so the injector nozzle must be cleaned up regularly.



Air flow straightening system (Young, 1993)

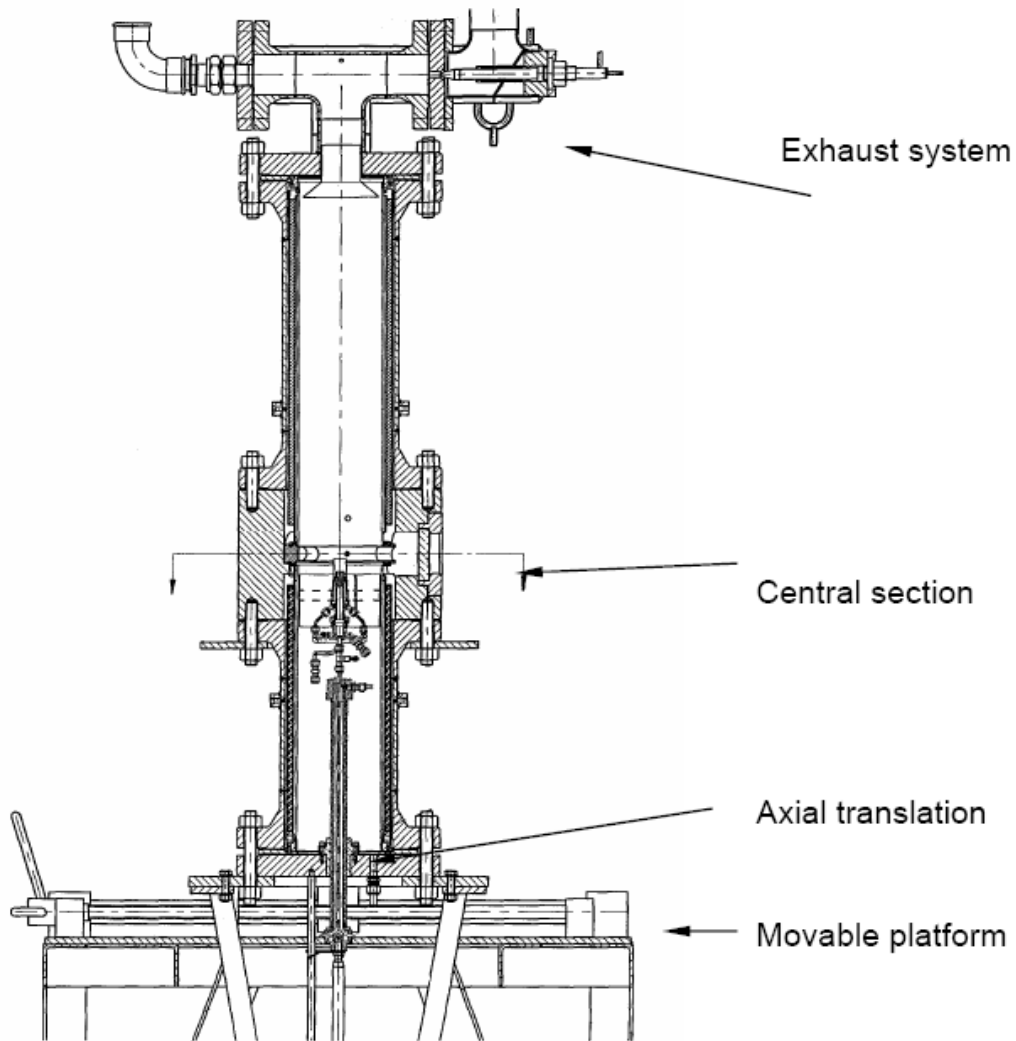
The pressure rig possesses a planar transparent circular quartz window of only 75 mm diameter illustrated figure 5.6, which allows optical access of the interior of the combustor up to height of 60 mm from the fuel nozzle, allowing to control the operating conditions and ensuring that an optimum flame stability is obtained, and also permits make a full optical traverse of the flame to

make the experimental measurements such as PIV and PDPA. A spark is generated to ignite the flame. The flame stability is crucial and will be a defining criterion for the experimental boundary conditions.



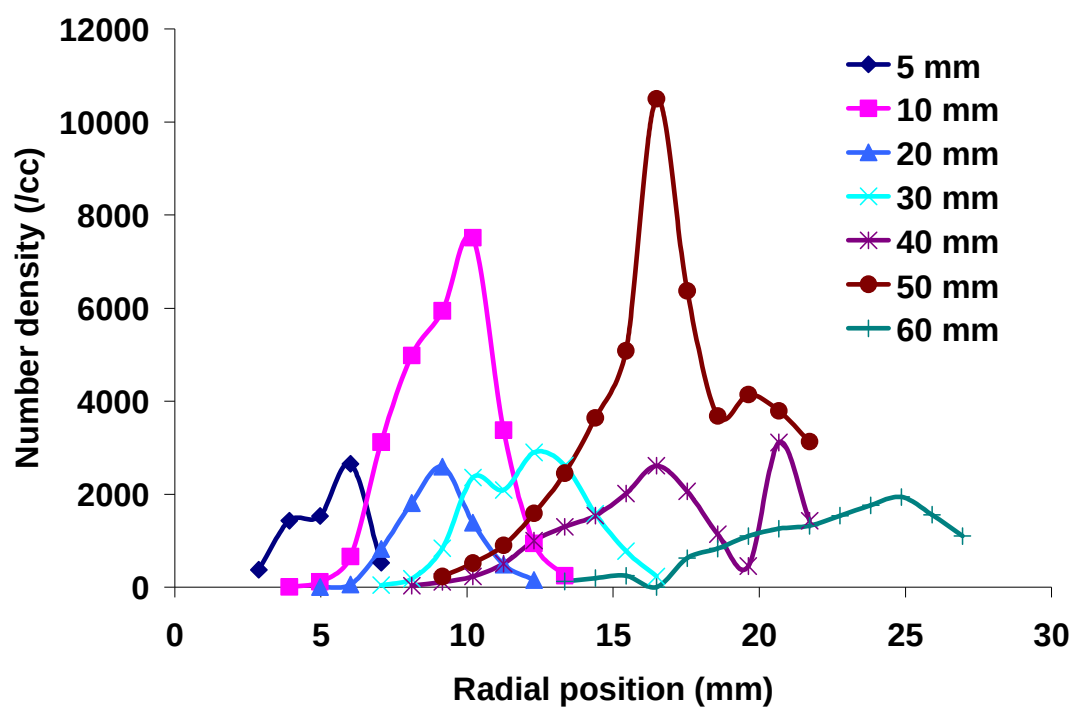
Quartz window for optical access to the flame

The flame at elevated pressure is expected to be of much lower size compared to flames encountered at atmospheric condition based on the operating conditions used in this study and should be also more stable, therefore the operating conditions at 1bar should be taking the most volumetric space. The combustion products were then exhausted into a hood situated on top of the combustion chamber through an exhaust pipe as shown in the detailed rig layout figure 5.7. Further details on the design of the high pressure experimental rig are given by Fischer (1996).

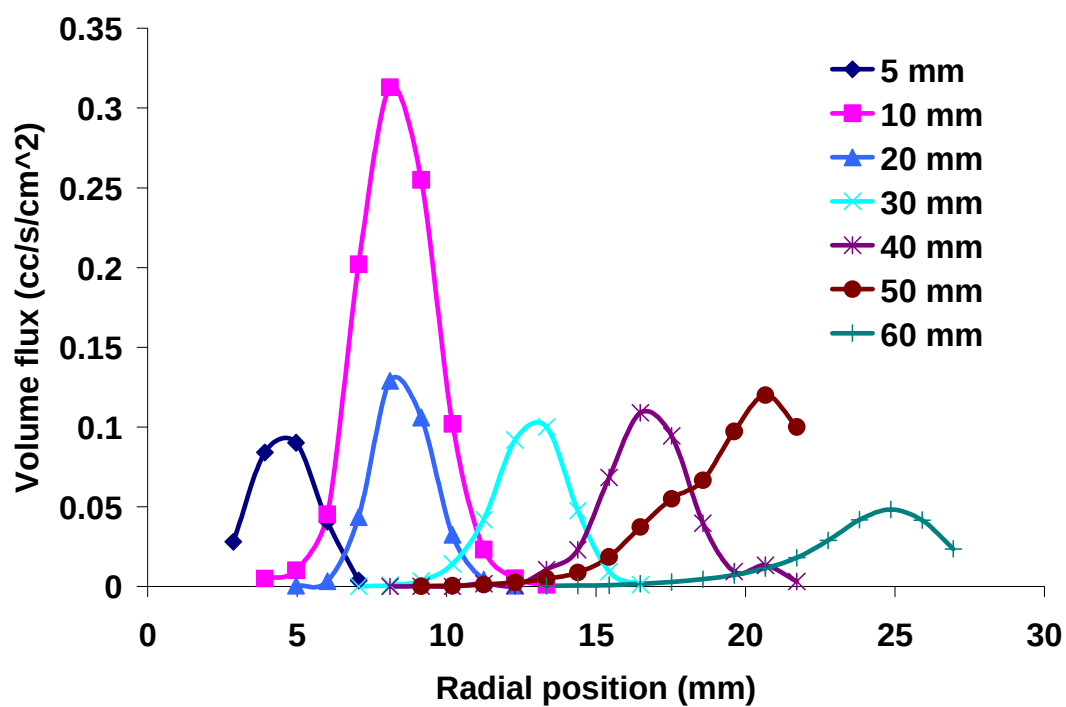


Rig assembly

Open ethanol droplet number density and volume flux

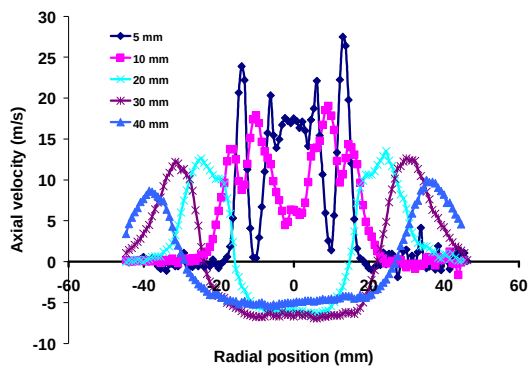


“Open” ethanol droplet number density at different axial locations

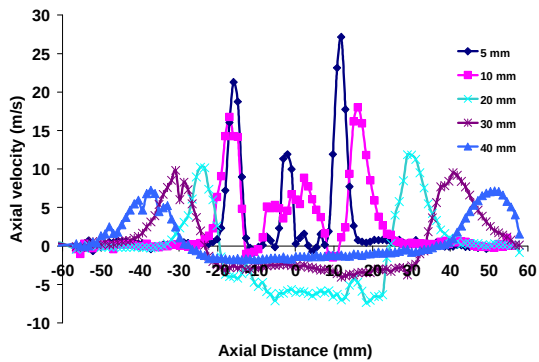


“Open” ethanol droplet volume flux at different axial locations

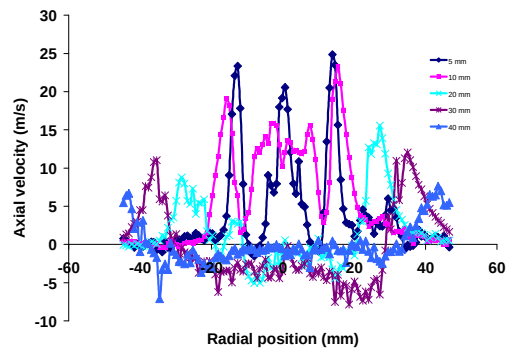
Biodiesel Gas velocity



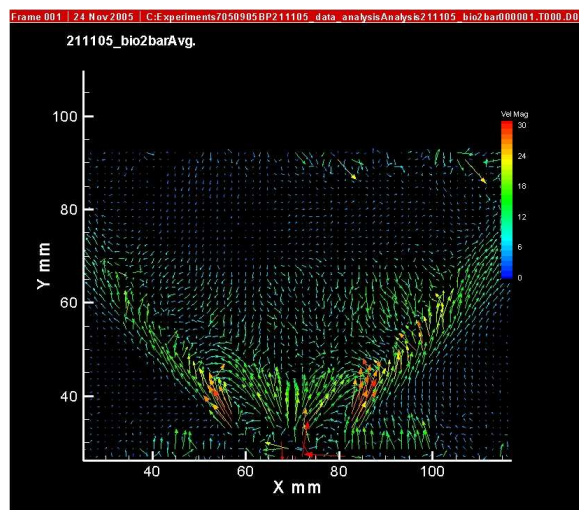
Axial velocity profile at 1 atm



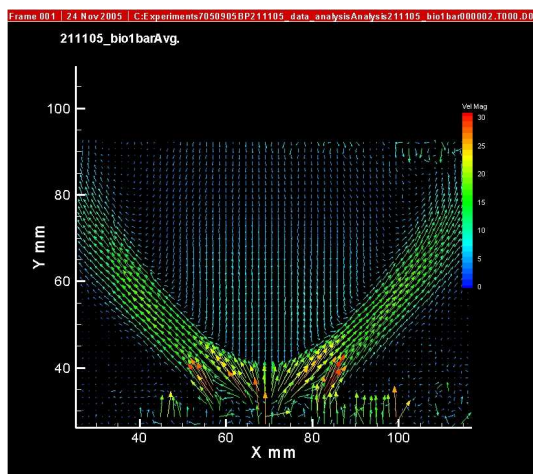
Axial velocity profile at 3 atm



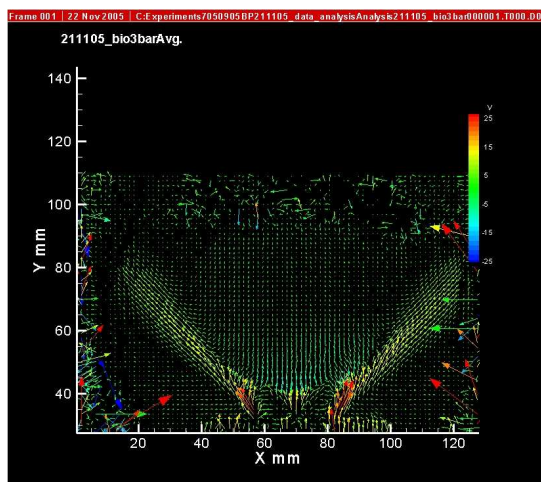
Axial velocity profile at 2 atm



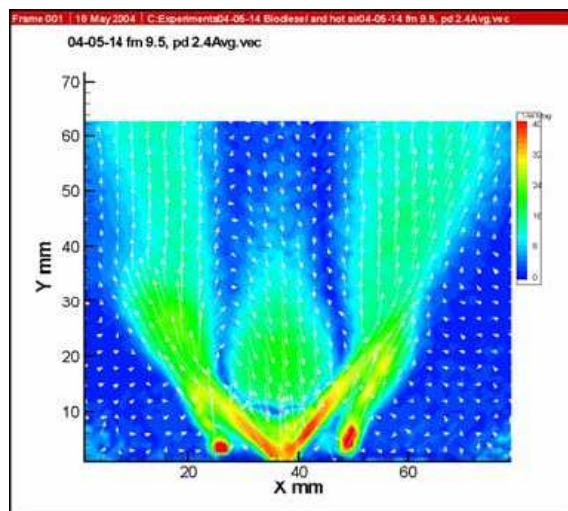
PIV image of the velocity magnitude at 2 atm



PIV image of the velocity magnitude at 1 atm



PIV image of the velocity magnitude at 3 atm



PIV image of the velocity magnitude at 1 atm

APPENDIX C TURBULENCE MODELS

Turbulent reacting flow

Turbulent reacting flows are often complicated by complex geometries, multiphase flow, spray evaporation and combustion, as well as radiation and soot modelling.

In flows involving turbulent combustion, all the processes are strongly linked, in such a manner that turbulence influences the mean rates of chemical reactions, while the heat release due to combustion alters the turbulence level (Libby & Williams, 1994). The simplifying assumption of constant gas densities exploited in most aerodynamic studies is not realistic for reacting flows since the heat release will generate large temperature gradients, even if the Mach number remains small.

For all flows, and in common with all RANS codes, FLUENT solves conservation equations for mass and momentum, and in the case of turbulent reacting flow, hence where heat transfer, combustion and turbulence are involved, the following additional equations are solved:

- energy conservation including balances at phase boundaries and walls
- transport equations for turbulence properties
- balance equations for scalar composition variables – notably mixture fraction mean and variance.

The mass and momentum conservation equations are briefly presented here while the turbulent transport equations and the species conservation equations for the non-premixed approach are described in a little more detail in subsequent sections.

The mass and momentum conservation equations are respectively written in the following manner:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_k} \rho u_k = 0$$

$$\frac{\partial}{\partial t} \rho u_i + \frac{\partial}{\partial x_k} \rho u_k u_i = -\frac{\partial p}{\partial x_k} + F_i + \frac{\partial}{\partial x_k} \tau_{ik} + \rho g$$

.

p is the static pressure, ρg and F_i respectively represent the gravitational body force and external body forces (e.g., that arise from interaction with the dispersed phase). τ_{ik} is the viscous stress tensor given by:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right)$$

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

Where δ_{ij} is the Kronecker delta, μ is the molecular viscosity. T

The following two equations of state link density, species mass fraction and enthalpy.

The equation of state for density assumes ideal gas behaviour:

$$\rho = \frac{p}{RT \sum_{k=1}^N \frac{Y_k}{MW_k}}$$

Where R is the universal gas constant, 82.06×10^6 kJ/kg.mol.K, where MW is the mixture molecular weight and MW_k is the molecular weight of species k .

It is estimated that for turbulent flows the following calorific equation of state can be written as follows with sufficient accuracy:

$$h_i = \int_{T_{ref}}^T C_{p_i} dT + \Delta H_{f_s}$$

With the total enthalpy defined as:

$$h = \sum_i Y_i h_i$$

The form of the energy equation is as follows:

$$\frac{\partial}{\partial t} \rho h + \frac{\partial}{\partial x_k} \rho u_k h = -\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_k} \left[\frac{\mu}{Pr} \frac{\partial h}{\partial x_k} \right] + S_h$$

h is the mixture enthalpy per unit mass and the mixture Prandtl number Pr is taken into consideration. Under the assumption that the Lewis number (Le) = 1, the energy equation takes the standard convective diffusive form.

Favre and Reynolds Averaging

In engineering applications, interest is mainly centred on the time mean value of any given variable and much less direct attention is paid to its fluctuating part. In Reynolds averaging, the solution variables in the instantaneous (exact) Navier-Stokes equations are decomposed into the mean (ensemble-averaged or time-averaged) and fluctuating components. For any variable components:

$$\phi = \bar{\phi} + \phi'$$

with $\bar{\phi}$ representing the mean value of the quantity and ϕ' its fluctuating part.

The Favre averaged scalar is written as

$$\tilde{\phi} = \frac{\overline{\rho\phi}}{\bar{\rho}}$$

Where $\bar{\rho}$ denotes the Reynolds averaged density, and the instantaneous values are found by summing average and fluctuations:

$$\phi = \tilde{\phi} + \phi''$$

Favre, or mass averaging is now considered to provide the most convenient way of obtaining equations in all turbulent flow with significant density fluctuations encountered in reacting flows. In combusting flows, the decomposition of density into mean and fluctuating component will lead to a considerable increase in the modelling complexity but Favre averaging, except for the density and pressure, will lead to a simplification of the physical interpretation of each term {Libby &

Williams 1994 #4360}. For situations in which the fluid has variable density such as in combustion or high Mach number flows, further correlations with the fluctuating component of density arise. In this case Favre averaging is more desirable since the inclusion of density in the mean form of the variable leads to a reduction in the number of correlation terms over conventional Reynolds averaging.

Turbulence models have been developed in order to close the system of equations. The equations can be written in two general forms, first and second order closure. The order determines at which stage modelling assumptions are introduced to make the equations mathematically determinant. Although higher closure order would be possible, they do not exist and are of little interest for engineering purposes. An increase of the closure order would mean an increase in the Reynolds stress terms and this would become rapidly impractical. The most widely used turbulence models are those which contain first order closure.

The k- ϵ model

The two-equation turbulence model is based on the k- ϵ model described by Launder (Launder, 1972). In this approach, the turbulent eddy viscosity is modelled using the equation

$$\nu_t = C_\mu l_k k^{1/2}$$

Where C_μ is a function of the local axial velocity gradient in axisymmetric flows, with a basic value of 0.09 and l_k being the length scale. A differential transport equation has been used for the dissipation rate:

$$\epsilon = \frac{C_\epsilon k^{3/2}}{l_k}$$

Using these two equations, one can write

$$\nu_t = \frac{C_\mu k^2}{\epsilon}$$

where the constant C_ε has been absorbed into C_μ .

For an axisymmetric jet flow, the k- ε turbulence model involves the equations:

$$\rho u \frac{\partial k}{\partial x} + \rho v \frac{\partial k}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \rho v_T}{Pr_k} \frac{\partial k}{\partial r} \right) + \rho v_T \left(\frac{\partial u}{\partial r} \right)^2 - \rho \varepsilon$$

$$\rho u \frac{\partial \varepsilon}{\partial x} + \rho v \frac{\partial \varepsilon}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \rho v_T}{Pr_\varepsilon} \frac{\partial \varepsilon}{\partial r} \right) + C_{\varepsilon 1} \frac{v_T \varepsilon}{k} \left(\frac{\partial u}{\partial r} \right)^2 - C_{\varepsilon 2} \frac{\rho \varepsilon^2}{k}$$

These equations form the foundation of the k- ε model. For results presented here, the five constant are given the following values:

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	Pr_k	Pr_ε
0.09	1.45	1.956	1.0	1.3

The model constants C_μ , $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ values were originally given by Jones and Launder (1972). A further correction to the “constant” C_μ has been developed by Rodi {Launder, Reece, et al. 1975 #5150 /d}for weak shear flows, i.e., flows in which the rate of turbulence energy production is appreciably less than the dissipation rate. In such circumstances, the value of C_μ increases, and Rodi has provided a correlation for the variation in C_μ with the average value of the ratio of turbulence energy production to dissipation at any cross section.

Different authors (Morse, 1977, McGuirk and Rodi 1977, Launder et al. 1972), however, have proposed simpler empirical modifications to the existing equations which, although restricting the generality of the model, have proven useful and accurate.

Liew (1983) and Syed (1990) found the correction proposed by Morse 1977 to be accurate in the case of free, round jets. This takes the form of a modification to the constant $C_{\varepsilon 1}$

$$C_{\varepsilon 1} = 1.4 - 3.4 \left[\frac{k}{\varepsilon} \frac{d\tilde{u}}{dx} \right]_{cl}^3$$

The subscript cl refers to centreline values and the effect of the expressions is to increase the value of $C_{\epsilon 1}$ and hence dissipation rate in regions of rapidly decaying centreline velocity. This expression was used in all calculations of the unconfined ethylene jet reported in this study where it proved to be the best. For all calculation of the confined kerosene jets, however, the correction by Rodi 1972 was used in preference:

$$C_{\epsilon 1} = 1.92 - 0.067 \left\{ \frac{\delta}{\tilde{u}} \frac{d\tilde{u}}{dx} \right\}_{cl}^{0.2}$$

$$C_{\mu} = 0.09 - 0.04 \left\{ \frac{\delta}{\tilde{u}} \frac{d\tilde{u}}{dx} \right\}_{cl}^{0.2}$$

Where δ is the half width of the jet – the radius at which the velocity has dropped to half its centreline value. The reason for this was due to instabilities in the confined jet calculation resulting from larger pressure correction with the geometry – due to the presence of the wall boundary. Although the corrections were small, so also was the initial step size. The resulting velocity gradient taken to the third power in the expression of Morse were sometimes large enough to perturb the calculation significantly. The modification proposed by Rodi (1972) was less sensitive to this initial instability since the exponent of the velocity was only 0.2

RSM model

The approach used for the RSM, is to solve transport equations for each of the terms in the Reynolds stress tensor. An additional scale-determining equation (normally for ϵ) is also required. This means that five additional transport equations are required in 2D flows and seven additional transport equations must be solved in 3D.

The governing equations for the reacting two-phase flow are presented.

$$\begin{aligned} \frac{\partial}{\partial t} (\overline{\rho u_i' u_j'}) + \frac{\partial}{\partial x_k} (\overline{\rho u_k' u_i' u_j'}) = & - \frac{\partial}{\partial x_k} [\overline{\rho u_i' u_j' u_k'} + \overline{p(\delta_{kj} u_i' + \delta_{ik} u_j')}] + \frac{\partial}{\partial x_k} \left[\mu \frac{\partial}{\partial x_k} (\overline{u_i' u_j'}) \right] \\ & - \rho \left(\overline{u_i' u_k'} \frac{\partial u_j'}{\partial x_k} + \overline{u_j' u_k'} \frac{\partial u_i'}{\partial x_k} \right) - \rho \beta (g_i \overline{u_j' \theta}) + \overline{p \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right)} - 2\mu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}} - 2\rho \Omega_k (\overline{u_j' u_m'} \epsilon_{ikm} + \overline{u_i' u_m'} \epsilon_{jkm}) \end{aligned}$$

The first, fourth, fifth and sixth term on the right hand side of the equation need to be modelled in order to close the equation while the others do not require any modelling.

APPENDIX D BOILING LAW

The CFD code Fluent follows the. In Fluent, the droplet boiling equation is called Law 3, applied as follow.

$$\frac{d(d)}{dt} = \frac{4k_g}{\rho_l c_{p,g} d} \left(1 + 0.23\sqrt{\text{Re}_d}\right) \ln \left[1 + \frac{c_{p,g}(T_g - T_l)}{h_{fg}}\right]$$

After integration the equation gives:

$$d^2 = d_0^2 - \left[\left(1 + 0.23\sqrt{\text{Re}_d}\right) \frac{8k_g}{\rho_l c_{p,g}} \ln \left(1 + \frac{c_{p,g}(T_g - T_l)}{h_{fg}}\right) \right] t$$

$$\text{with} \left[\left(1 + 0.23\sqrt{\text{Re}_d}\right) \frac{8k_g}{\rho_l c_{p,g}} \ln \left(1 + \frac{c_{p,g}(T_g - T_l)}{h_{fg}}\right) \right]$$

defining λ as the form of the d^2 -law which has been previously defined as: $d^2 = d_0^2 - \lambda t$.

The droplet lifetime in Fluent is therefore expressed as follows:

$$t_e = \frac{\rho_l d_0^2}{8(1 + 0.23\sqrt{\text{Re}_d})(k / c_p)_g \ln(1 + B)}$$

APPENDIX E ETHANOL THERMODYNAMIC DATA FOR SELECTED SPECIES

Species	$\Delta H_f(298\text{ K})$	$S(298\text{ K})$	$C_p(300\text{ K})$	$C_p(400\text{ K})$	$C_p(500\text{ K})$	$C_p(600\text{ K})$	$C_p(800\text{ K})$	$C_p(1000\text{ K})$	$C_p(2500\text{ K})$
HO ₂	3.50	54.77 ^(b)	8.40 ^(b)	8.92	9.42	9.90	10.72	11.34	12.09
CH ₂ ^(a)	93.50	46.71	8.19	8.57	8.93	9.28	9.93	10.52	11.75
CH ₂ (s) ^(a)	102.50	45.10	7.91	8.33	8.72	9.11	9.83	10.49	11.86
CH ₂ OH	-2.10 ^(c)	58.87 ^(b)	11.32 ^(b)	12.94	14.38	15.62	17.54	18.79	20.95
C ₂ H ^(d)	135.0	49.55	8.90	9.63	10.22	10.72	11.54	12.18	13.31
C ₂ H ₃ ^(a)	70.40	55.50	9.88	11.37	12.82	14.20	16.70	18.74	21.83
C ₂ H ₅ ^(a)	28.73	59.02	11.85	14.44	16.81	18.98	22.70	25.64	30.20
HCOH ^(a)	23.33	55.42	9.83	12.88	15.17	16.85	18.89	19.84	20.65
HCOOH ^(e)	-90.47	59.47	10.95	13.04	14.96	16.68	19.44	21.37	23.47
CH ₂ HCO ^(d)	6.00	64.00	13.18	15.15	16.96	18.60	21.30	23.34	26.35
CHOCHO ^(a)	-50.60	68.16	14.90	17.51	19.69	21.48	24.15	25.89	28.10
HOC ₂ H ₄ O ₂ ^(f)	-38.60	84.71	21.34	24.77	27.71	30.25	34.42	37.74	43.67
IC ₃ H ₇ ^(a)	21.51	68.88	16.90	20.76	24.51	27.81	33.39	37.73	44.35
NC ₃ H ₇ ^(a)	24.05	69.16	17.18	21.71	25.54	28.81	34.00	37.91	44.36
AC ₃ H ₅ ^{†(a)}	38.64	64.73	16.07	19.55	22.72	25.53	29.99	32.89	37.43
PC ₃ H ₅ ^(a)	64.75	68.74	15.54	18.56	21.44	24.12	28.65	31.68	36.13
SC ₃ H ₅ ^(a)	61.09	69.24	15.45	18.38	21.21	23.89	28.50	31.61	36.09
CH ₂ CHCH ₂ O ^(a)	22.40	69.59	17.12	21.25	24.75	27.73	32.39	36.44	41.11
CH ₂ CHCHO ^(f)	-16.05	67.40	16.37	20.06	23.20	25.86	29.99	32.94	37.18
CH ₂ CHCO ^(a)	14.85	68.08	15.24	18.46	21.15	23.38	26.79	29.15	32.51
CH ₂ CHCO ^(a)	-20.06	67.75	17.63	20.72	23.39	25.71	29.42	32.19	36.43
PC ₃ H ₄ ^(d)	45.77	58.89	14.52	17.06	19.40	21.54	25.16	27.90	31.79
AC ₃ H ₄ ^(d)	47.63	57.94	14.25	16.97	19.46	21.71	25.45	28.20	32.06
H ₂ CCCH ^(d)	83.04	61.48	15.84	17.74	19.48	21.01	23.43	25.01	27.55
C ₃ H ₂ ^(d)	129.6	64.81	14.93	16.10	16.91	17.55	18.72	19.74	21.22
C ₂ H ₅ OH ^(e)	-56.15	67.05	15.67	19.31	22.84	25.96	30.59	34.15	39.53
C ₂ H ₄ OH ^(f)	-8.20	68.19	15.48	18.84	21.70	24.11	27.87	30.58	34.73
CH ₃ CHOH ^(f)	-10.30	62.69	14.64	17.64	20.37	22.84	26.98	30.13	34.72
CH ₃ CH ₂ O ^(f)	-4.10	62.21	14.08	17.72	20.85	23.53	27.75	30.80	35.32

Thermodynamic properties for selected species {Marinov 1999 #1700}

Units: kcal/mol for ΔH_f , cal/mol/K for S and Cp

APPENDIX F ETHANOL TRANSPORT DATA

!Marinov, N. M, "A Detailed Chemical Kinetic Model for High Temperature Ethanol Oxidation"

!Int. J. Chem. Kinet. 31:183-220 (1999);

!Lawrence Livermore National Laboratory, Livermore, CA,

!UCRL-JC-131657

!UCRL-WEB-204236

!Review and release date: May 19, 2004.

!Date: Mon, 26 Apr 1999 15:25:31 -0700 (PDT)

!From: "Nick M. Marinov" <marinov@west.llnl.gov>

!

ar	0	136.500	3.330	0.000	0.000	0.000	
as	0	1045.500	4.580	0.000	0.000	0.000	! mec
ash	1	199.300	4.215	0.000	0.000	1.000	! mec
ash2	2	229.600	4.180	0.000	0.000	1.000	! mec
c	0	71.400	3.298	0.000	0.000	0.000	! *
c2	1	97.530	3.621	0.000	1.760	4.000	
c2o	1	232.400	3.828	0.000	0.000	1.000	! *
cn2	1	232.400	3.828	0.000	0.000	1.000	! ois
c2h	1	265.300	3.721	0.000	0.000	2.500	! nmm
c2h2	1	265.300	3.721	0.000	0.000	2.500	! nmm
c2h2oh	2	224.700	4.162	0.000	0.000	1.000	! *
c2h3	2	265.300	3.721	0.000	0.000	1.000	! nmm
c2h4	2	238.400	3.496	0.000	0.000	1.500	! nmm
c2h5	2	247.500	4.350	0.000	0.000	1.500	! nmm
c2h5oh	2	470.600	4.410	0.000	0.000	1.500	! nmm
ch3ch2o	2	470.600	4.410	0.000	0.000	1.500	! nmm
c2h4oh	2	470.600	4.410	0.000	0.000	1.500	
hoc2h4o2	2	470.600	4.410	0.000	0.000	1.500	!7/01 same
as c2h5oh, wjp							
ch3choh	2	470.600	4.410	0.000	0.000	1.500	
c2h6	2	247.500	4.350	0.000	0.000	1.500	! nmm
c2n	1	232.400	3.828	0.000	0.000	1.000	! ois
c2n2	1	349.000	4.361	0.000	0.000	1.000	! ois
c3	1	232.400	3.828	0.000	0.000	1.000	!
c3h	1	232.400	3.828	0.000	0.000	1.000	!
c3h2	2	209.000	4.100	0.000	0.000	1.000	! *
c3h2(s)	2	209.000	4.100	0.000	0.000	1.000	! *
c3h3	1	324.800	4.290	0.000	0.000	1.000	! nmm
c4h3	1	357.000	4.720	0.000	0.000	1.000	! nmm
ch2chcho	2	443.200	4.120	0.000	0.000	1.000	! nmm
chchcho	2	443.200	4.120	0.000	0.000	1.000	! nmm
hcccho	2	443.200	4.120	0.000	0.000	1.000	! nmm
hccco	2	443.200	4.120	0.000	0.000	1.000	! nmm
h2cchco	2	443.200	4.120	0.000	0.000	1.000	! nmm
ch3chco	2	443.200	4.120	0.000	0.000	1.000	! nmm
ch2chco	2	443.200	4.120	0.000	0.000	1.000	! nmm
c2h3co	2	443.200	4.120	0.000	0.000	1.000	! nmm
c2h5cho	2	424.600	4.820	0.000	0.000	1.000	! nmm
ch2ch2cho	2	424.600	4.820	0.000	0.000	1.000	! nmm
ch2chch2o	2	424.600	4.820	0.000	0.000	1.000	
c2h5co	2	424.600	4.820	0.000	0.000	1.000	! nmm
ch3coch3	2	435.500	4.860	0.000	0.000	1.000	! nmm
ch3coch2	2	435.500	4.860	0.000	0.000	1.000	! nmm
ac3h4	1	324.800	4.290	0.000	0.000	1.000	! nmm
pc3h4	1	324.800	4.290	0.000	0.000	1.000	! nmm
c3h4c	2	324.800	4.290	0.000	0.000	1.000	! nmm
c3h6	2	307.800	4.140	0.000	0.000	1.000	! nmm

c3h6oh	2	487.900	4.820	0.000	0.000	1.000	!	nmm
hoc3h6o2	2	487.900	4.820	0.000	0.000	1.000	!	nmm
c3h6o	2	411.000	4.820	0.000	0.000	1.000	!	nmm
c3h5o	2	411.000	4.820	0.000	0.000	1.000	!	nmm
c3h7	2	303.400	4.810	0.000	0.000	1.000	!	nmm
c4h6	2	357.000	4.720	0.000	0.000	1.000	!	nmm
cyc4h6	2	357.000	4.720	0.000	0.000	1.000		
cyc3h3ch3	2	357.000	4.720	0.000	0.000	1.000		
ic3h7	2	303.400	4.810	0.000	0.000	1.000	!	nmm
nc3h7	2	303.400	4.810	0.000	0.000	1.000	!	nmm
ic3h7o	2	468.300	4.760	0.000	0.000	1.000	!	nmm
nc3h7o	2	487.900	4.820	0.000	0.000	1.000	!	nmm
c3h8	2	303.400	4.810	0.000	0.000	1.000	!	nmm
c4h	1	357.000	4.720	0.000	0.000	1.000	!	nmm
c4h2	1	357.000	4.720	0.000	0.000	1.000	!	nmm
c4h2oh	2	224.700	4.162	0.000	0.000	1.000	!	*
ch3chcch	2	355.000	4.650	0.000	0.000	1.000	!	nmm
ic4h7	2	355.000	4.650	0.000	0.000	1.000	!	nmm
c4h7	2	355.000	4.650	0.000	0.000	1.000	!	nmm
c4h8	2	355.000	4.650	0.000	0.000	1.000	!	nmm
c4h8-1	2	355.000	4.650	0.000	0.000	1.000	!	nmm
c4h8-2	2	355.000	4.650	0.000	0.000	1.000	!	nmm
ic4h8	2	355.000	4.650	0.000	0.000	1.000	!	nmm
pc4h9	2	352.000	5.240	0.000	0.000	1.000	!	nmm
c4h9	2	352.000	5.240	0.000	0.000	1.000	!	nmm
sc4h9	2	352.000	5.240	0.000	0.000	1.000	!	nmm
tc4h9	2	352.000	5.240	0.000	0.000	1.000	!	nmm
ic4h9	2	352.000	5.240	0.000	0.000	1.000	!	nmm
ch2chcoch3	2	427.400	4.940	0.0000	0.000	1.000	!	nmm
ch2chcoch2	2	427.400	4.940	0.000	0.000	1.000		
pc4h9o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
tc4h9o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
c4h8oh-1	2	496.000	5.200	0.000	0.000	1.000	!	nmm
sc4h9o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
ic4h9o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
c4h8oh-2	2	496.000	5.200	0.000	0.000	1.000	!	nmm
ic4h8oh	2	496.000	5.200	0.000	0.000	1.000	!	nmm
ic4h7oh	2	496.000	5.200	0.000	0.000	1.000	!	nmm
o2c4h8oh-1	2	496.000	5.200	0.000	0.000	1.000	!	*
o2c4h8oh-2	2	496.000	5.200	0.000	0.000	1.000	!	*
io2c4h8oh	2	496.000	5.200	0.000	0.000	1.000	!	*
c4h7o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
ic4h7o	2	496.000	5.200	0.000	0.000	1.000	!	nmm
c4h10	2	352.000	5.240	0.000	0.000	1.000	!	nmm
ic4h10	2	352.000	5.240	0.000	0.000	1.000	!	nmm
c5h2	1	408.000	5.200	0.000	0.000	1.000	!	nmm
c5h3	1	408.000	5.200	0.000	0.000	1.000	!	nmm
h2ccchcch	2	408.000	5.200	0.000	0.000	1.000		
hccch2cch	2	408.00	5.200	0.000	0.000	1.000		
hccchcch	2	408.00	5.200	0.000	0.000	1.000		
c-c5h5	2	408.000	5.200	0.000	0.000	1.000	!	nmm
c-c5h4	2	408.000	5.200	0.000	0.000	1.000		
c-c5h4(s)	2	408.000	5.200	0.000	0.000	1.000		
dhfuran	2	408.000	5.200	0.000	0.000	1.000		
furan	2	408.000	5.200	0.000	0.000	1.000		
c-c5h6	2	408.000	5.200	0.000	0.000	1.000	!	nmm
l-c5h5	2	408.000	5.200	0.000	0.000	1.000		
l-c5h6	2	408.000	5.200	0.000	0.000	1.000		
l-c5h7	2	408.000	5.200	0.000	0.000	1.000	!	nmm
c-c5h7	2	408.000	5.200	0.000	0.000	1.000	!	
l-c5h8	2	408.000	5.200	0.000	0.000	1.000	!	nmm

c6h2	1	408.000	5.200	0.000	0.000	1.000	! nmm
c6h4	2	412.300	5.349	0.000	0.000	1.000	! jam
c6h5	2	412.300	5.349	0.000	0.000	1.000	! jam
fulvenyl	2	412.300	5.349	0.000	0.000	1.000	
c6h5(l)	2	412.300	5.349	0.000	0.000	1.000	! jam
c2h3c4h3	2	412.300	5.349	0.000	0.000	1.000	
c6h5oh	2	450.000	5.500	0.000	0.000	1.000	! nmm
c6h5o	2	450.000	5.500	0.000	0.000	1.000	! jam
c-2*4c6h6o	2	450.000	5.500	0.000	0.000	1.000	!
oc6h4o	2	450.000	5.500	0.000	0.000	1.000	
c6h4o	2	450.000	5.500	0.000	0.000	1.000	
c-c5h4o	2	450.000	5.500	0.000	0.000	1.000	! nmm
c-c5h4oh	2	450.000	5.500	0.000	0.000	1.000	! nmm
c-c5h5o	2	450.000	5.500	0.000	0.000	1.000	! nmm
ch3cy24pd1	2	450.000	5.500	0.000	0.000	1.000	!
ch3cy24pd	2	450.000	5.500	0.000	0.000	1.000	
ch3dcy24pd	2	450.000	5.500	0.000	0.000	1.000	
c5h5oh	2	450.000	5.500	0.000	0.000	1.000	! nmm
c6h5c2h	2	468.500	5.230	0.000	0.000	1.000	! nmm
lc6h5	2	426.300	5.510	0.000	0.000	1.000	
hx13d5yn	2	426.300	5.510	0.000	0.000	1.000	
lc6h7	2	426.300	5.510	0.000	0.000	1.000	
l-c6h8	2	426.300	5.510	0.000	0.000	1.000	
c4h3cch2	2	426.300	5.510	0.000	0.000	1.000	
hx15d3yn	2	426.300	5.510	0.000	0.000	1.000	
h2c4hch2	2	426.300	5.510	0.000	0.000	1.000	
c4h3c2h3	2	426.300	5.510	0.000	0.000	1.000	
c6h6	2	468.500	5.230	0.000	10.30	1.000	! nmm
c6h7	2	468.500	5.230	0.000	0.000	1.000	! nmm
cyc6h7	2	468.500	5.230	0.000	0.000	1.000	! nmm
cyc6h8	2	468.500	5.230	0.000	0.000	1.000	! nmm
fulvene	2	468.500	5.230	0.000	0.000	1.000	
ch2c6h6	2	495.300	5.680	0.000	0.000	1.000	
c6h5ch2	2	495.300	5.680	0.000	0.000	1.000	! nmm
c6h5ch3	2	495.300	5.680	0.430	12.30	1.000	! nmm
c6h5co	2	622.400	5.530	0.000	0.000	1.000	! nmm
c6h5cho	2	622.400	5.530	0.000	0.000	1.000	! nmm
c6h5ch2oh	2	622.400	5.530	0.000	0.000	1.000	! nmm
oc6h4ch3	2	621.100	5.640	0.000	0.000	1.000	! nmm
hoc6h4ch3	2	621.100	5.640	0.000	0.000	1.000	! nmm
xylylene	2	523.600	6.182	0.000	0.000	1.000	
xylylrad	2	523.600	6.182	0.000	0.000	1.000	
c6h5c2h5	2	523.600	5.960	0.000	0.000	1.000	! nmm
ch3c6h4ch3	2	523.600	5.960	0.000	0.000	1.000	!
ch3c6h4ch2	2	523.600	5.960	0.000	0.000	1.000	
ch3c6h4c2h5	2	523.600	5.960	0.000	0.000	1.000	
ch3c6h4c2h3	2	523.600	5.960	0.000	0.000	1.000	
oc6h4c2h	2	523.600	5.960	0.000	0.000	1.000	
hoc6h4c2h	2	523.600	5.960	0.000	0.000	1.000	
ach2cch	2	523.600	5.960	0.000	0.000	1.000	
achcch	2	523.600	5.960	0.000	0.000	1.000	
accch2	2	523.600	5.960	0.000	0.000	1.000	
achcch2	2	523.600	5.960	0.000	0.000	1.000	
c6h9	2	426.300	5.510	0.000	0.000	1.000	! nmm
c6h10	2	426.300	5.510	0.000	0.000	1.000	! nmm
c8h14	2	494.000	6.170	0.000	0.000	1.000	! nmm
ic8h14	2	494.000	6.170	0.000	0.000	1.000	! nmm
c6h5chch3	2	523.600	5.960	0.000	0.000	1.000	
c6h5c2h3	2	546.200	6.000	0.130	15.00	1.000	! nmm
c6h5chch	2	546.200	6.000	0.000	0.000	1.000	! nmm
c6h5cch2	2	546.200	6.000	0.000	0.000	1.000	

c6h5c2h	2	534.300	5.710	0.770	0.000	1.000	! nmm
c6h5c2	2	534.300	5.710	0.000	0.000	1.000	! nmm
c6h4c2h3	2	546.200	6.000	0.000	0.000	1.000	! nmm
c6h4c2h	2	534.300	5.710	0.000	0.000	1.000	! nmm
c10h7c2h5	2	695.000	6.530	0.000	0.000	1.000	
c10h7c2h3	2	689.800	6.500	0.000	0.000	1.000	
c10h7cch2	2	689.800	6.500	0.000	0.000	1.000	
c10h7cch	2	689.800	6.500	0.000	0.000	1.000	
c10h6cch	2	689.800	6.500	0.000	0.000	1.000	
c10h6c2h3	2	687.200	6.490	0.000	0.000	1.000	
c6h5cco	2	588.200	5.940	0.000	0.000	1.000	
c2hc6h4c2h	2	630.400	6.180	0.000	0.000	1.000	
c10h7	2	630.400	6.180	0.000	0.000	1.000	! nmm
c10h7o	2	630.400	6.180	0.000	0.000	1.000	! nmm
c10h8	2	630.400	6.180	0.000	16.50	1.000	! nmm
c10h9	2	630.400	6.180	0.000	0.000	1.000	! nmm
c10h10	2	630.400	6.180	0.000	0.000	1.000	! nmm
adhfulv	2	630.40	6.180	0.000	0.000	1.000	
adhflvyl	2	630.40	6.180	0.000	0.000	1.000	
bnzofulv	2	630.40	6.18	0.000	0.000	1.000	
cpcp	2	630.400	6.180	0.000	0.000	1.000	
cpcpd	2	630.400	6.180	0.000	0.000	1.000	
bcp11	2	630.4	6.18	0.0	0.0	1.0	
bcp12	2	630.4	6.18	0.0	0.0	1.0	
bcp22	2	630.4	6.18	0.0	0.0	1.0	
cpcpyl11	2	630.4	6.18	0.0	0.0	1.0	
cpcpyl12	2	630.4	6.18	0.0	0.0	1.0	
difulvene	2	630.4	6.18	0.0	0.0	1.0	
c10h7ch2	2	660.00	6.350	0.000	0.000	1.000	! nmm
c10h7oh	2	663.45	6.362	0.000	0.000	1.000	
c10h7ch3	2	660.0	6.350	0.000	0.000	1.000	! nmm
c11h8	2	660.0	6.350	0.000	0.000	1.000	
c11h7	2	660.0	6.350	0.000	0.000	1.000	
flrnthn	2	812.3	7.170	0.000	0.000	1.000	! nmm
naphbenz	2	812.3	7.170	0.000	0.000	1.000	
anthracn	2	772.0	6.960	0.000	25.40	1.000	
ch3indene	2	625.0	6.150	0.000	0.000	1.000	
ch3indenyl	2	625.0	6.150	0.000	0.000	1.000	
c9h7ch3	2	625.0	6.150	0.000	0.000	1.000	
c9h6ch3	2	625.0	6.150	0.000	0.000	1.000	
c9h6o	2	625.0	6.150	0.000	0.000	1.000	
indench3	2	625.0	6.150	0.000	0.000	1.000	
indench2	2	625.0	6.150	0.000	0.000	1.000	
ch3phnthrn	2	783.9	6.995	0.000	0.000	1.000	
phnthrol-1	2	783.9	6.995	0.000	0.000	1.000	
phnthrol-9	2	783.9	6.995	0.000	0.000	1.000	
phnthroxy-1	2	783.9	6.995	0.000	0.000	1.000	
phnthroxy-9	2	783.9	6.995	0.000	0.000	1.000	
phnthrn	2	772.0	6.960	0.000	38.80	1.000	
bz(a)ndene	2	772.0	6.960	0.000	0.000	1.000	
bz(a)ndnyl	2	772.0	6.960	0.000	0.000	1.000	
bnzofulv	2	772.0	6.960	0.000	0.000	1.000	
bzondcrb	2	772.0	6.960	0.000	0.000	1.000	
c14h10	2	772.0	6.960	0.000	0.000	1.000	
naphfulv	2	772.0	6.960	0.000	0.000	1.000	
phnthryl-1	2	772.0	6.960	0.000	38.80	1.000	! nmm
phnthryl-9	2	772.0	6.960	0.000	38.80	1.000	
pyrene	2	834.9	7.240	0.000	0.000	1.000	! nmm
dindnyl	2	834.9	7.240	0.000	0.000	1.000	
chrysene	2	834.9	7.240	0.000	0.000	1.000	
cyp(cd)pyrene	2	862.0	7.382	0.000	0.000	1.000	

hc4-p(def)pthn	2	834.9	7.240	0.000	0.000	1.000	
hc4-p(def)pthyl	2	834.9	7.240	0.000	0.000	1.000	
ch3-4hc15h9	2	834.9	7.240	0.000	0.000	1.000	
pyrenyl	2	834.9	7.240	0.000	0.000	1.000	! nmm
dhpyprene	2	834.9	7.240	0.000	0.000	1.000	
benzoap	2	832.5	7.550	1.400	0.000	1.000	! nmm
bz(a)phnthrn	2	832.5	7.550	0.000	0.000	1.000	
bz(ghi)fln	2	832.5	7.550	0.000	0.000	1.000	
biphenyl	2	676.5	6.310	0.000	0.000	1.000	
cypdrbenz	2	676.5	6.310	0.000	0.000	1.000	
obphnlyl	2	676.5	6.310	0.000	0.000	1.000	
phoph	2	676.5	6.310	0.000	0.000	1.000	
phohph	2	676.5	6.310	0.000	0.000	1.000	
cpentacd	2	832.5	7.550	0.000	0.000	1.000	
acenphthln	2	695.4	6.760	0.000	0.000	1.000	! nmm
acenphthyl	2	695.4	6.760	0.000	0.000	1.000	
indene	2	588.6	5.960	0.650	0.000	1.000	! nmm
indenyl	2	588.6	5.960	0.000	0.000	1.000	! nmm
indylin	2	588.6	5.960	0.000	0.000	1.000	
ch3ndene	2	588.6	5.960	0.000	0.000	1.000	! nmm
ch3ndnyl	2	588.6	5.960	0.000	0.000	1.000	! nmm
ch3flrne	2	712.6	6.890	0.000	0.000	1.000	
ch3flrnl	2	712.6	6.890	0.000	0.000	1.000	
fluorene	2	712.6	6.890	0.000	0.000	1.000	
fluoryl	2	712.6	6.890	0.000	0.000	1.000	
ch2flrne	2	712.6	6.890	0.000	0.000	1.000	
bnzcpd	2	783.800	6.640	0.000	0.000	1.000	
bnzcpdyl	2	783.800	6.640	0.000	0.000	1.000	
bibenzylyl	2	783.800	6.640	0.000	0.000	1.000	! nmm
stilbene	2	772.0	6.960	0.000	0.000	1.000	! nmm
stilbnrd	2	772.0	6.960	0.000	0.000	1.000	! nmm
anthracn	2	772.0	6.960	0.000	0.000	1.000	! nmm
dhanthrn	2	772.0	6.960	0.000	0.000	1.000	
obzyltol	2	772.0	6.960	0.000	0.000	1.000	
obzyltlr	2	772.0	6.960	0.000	0.000	1.000	
dmdp	2	712.6	6.890	0.000	0.000	1.000	
dmdprd	2	712.6	6.890	0.000	0.000	1.000	
ch	1	80.000	2.750	0.000	0.000	0.000	
ch2	1	144.000	3.800	0.000	0.000	0.000	
sch2	1	144.000	3.800	0.000	0.000	0.000	
ch2(s)	1	144.000	3.800	0.000	0.000	0.000	
ch2cychch	2	373.700	4.790	0.000	0.000	1.000	
ch2chcch	2	373.700	4.790	0.000	0.000	1.000	! nmm
ch2chcch2	2	373.700	4.790	0.000	0.000	1.000	! nmm
ch3ccch2	2	357.100	4.720	0.000	0.000	1.000	
ch3chcch2	2	357.100	4.720	0.000	0.000	1.000	
ch2ch2cch	2	373.700	4.790	0.000	0.000	1.000	! nmm
ch2chch2	2	316.000	4.220	0.000	0.000	1.000	! nmm
ac3h5	2	316.000	4.220	0.000	0.000	1.000	
ch2chchch	2	357.100	4.720	0.000	0.000	1.000	! nmm
chchchch	2	357.100	4.720	0.000	0.000	1.000	! nmm
cyc4h6	2	357.100	4.720	0.000	0.000	1.000	
cyc3h3ch3	2	357.100	4.720	0.000	0.000	1.000	
ch2chchch2	2	357.100	4.720	0.000	0.000	1.000	! nmm
ch2co	2	436.000	3.970	0.000	0.000	2.000	
hcooh	2	436.000	3.970	0.000	0.000	2.000	
ch2o	2	498.000	3.590	0.000	0.000	2.000	
hcoh	2	498.000	3.590	0.000	0.000	1.000	
h2co	2	498.000	3.590	0.000	0.000	2.000	
ch2oh	2	417.000	3.690	1.700	0.000	2.000	
ch2hco	2	436.000	3.970	0.000	0.000	2.000	

chocho	2	440.200	4.010	0.000	0.000	2.000	! nmm
choco	2	440.200	4.010	0.000	0.000	2.000	! nmm
ch3	1	144.000	3.800	0.000	0.000	0.000	
ch3cc	2	252.000	4.760	0.000	0.000	1.000	! jam
ch3chcch	2	373.700	4.790	0.000	0.000	1.000	! nmm
ch3ccch2	2	357.100	4.720	0.000	0.000	1.000	! nmm
ch3ccch3	2	357.100	4.720	0.000	0.000	1.000	! nmm
ch3cch2	2	316.000	4.220	0.000	0.000	1.000	! nmm
sc3h5	2	316.000	4.220	0.000	0.000	1.000	
ch3chch	2	316.000	4.220	0.000	0.000	1.000	! nmm
pc3h5	2	316.000	4.220	0.000	0.000	1.000	
ch3ch2cch	2	357.100	4.720	0.000	0.000	1.000	! nmm
ch3hco	2	436.000	3.970	0.000	0.000	2.000	
ch3co	2	436.000	3.970	0.000	0.000	2.000	
ch3o	2	417.000	3.690	1.700	0.000	2.000	
ch3oh	2	481.800	3.626	0.000	0.000	1.000	! sve
ch4	2	141.400	3.746	0.000	2.600	13.000	
ch4o	2	417.000	3.690	1.700	0.000	2.000	
cn	1	75.000	3.856	0.000	0.000	1.000	! ois
cnc	1	232.400	3.828	0.000	0.000	1.000	! ois
cnn	1	232.400	3.828	0.000	0.000	1.000	! ois
co	1	98.100	3.650	0.000	1.950	1.800	
co2	1	244.000	3.763	0.000	2.650	2.100	
f	0	80.000	2.750	0.000	0.000	0.000	
f2	1	125.700	3.301	0.000	1.600	3.800	
h	0	145.000	2.050	0.000	0.000	0.000	
gah	1	335.500	4.240	0.000	0.000	1.000	! mec
h2c4o	2	357.000	5.180	0.000	0.000	1.000	! jam
h2	1	38.000	2.920	0.000	0.790	280.000	
h2ccc	2	265.300	3.721	0.000	0.000	1.000	! *
h2ccc(s)	2	265.300	3.721	0.000	0.000	1.000	! *
h2ccch	2	252.000	4.760	0.000	0.000	1.000	! jam
h2cccch	2	357.100	4.720	0.000	0.000	1.000	! nmm
h2cccch2	2	357.100	4.720	0.000	0.000	1.000	! nmm
h2ccccch	1	408.000	5.200	0.000	0.000	1.000	! nmm
h2cn	1	569.000	3.630	0.000	0.000	1.000	! os/jm
h2no	2	116.700	3.492	0.000	0.000	1.000	! jam
h2o	2	572.400	2.605	1.844	0.000	4.000	
h2o2	2	107.400	3.458	0.000	0.000	3.800	
h2s	2	301.000	3.600	0.000	0.000	1.000	! ois
hc2n2	1	349.000	4.361	0.000	0.000	1.000	! ois
hcchcch	2	357.100	4.720	0.000	0.000	1.000	! nmm
hcco	2	150.000	2.500	0.000	0.000	1.000	! *
hccoh	2	436.000	3.970	0.000	0.000	2.000	
hccchcch	2	408.000	5.200	0.000	0.000	1.000	! nmm
hcn	1	569.000	3.630	0.000	0.000	1.000	! ois
hco	2	498.000	3.590	0.000	0.000	0.000	
hco+	1	498.000	3.590	0.000	0.000	0.000	
he	0	10.200	2.576	0.000	0.000	0.000	! *
hf	1	330.000	3.148	1.920	2.460	1.000	! sv/mec
hf0	1	352.000	2.490	1.730	0.000	5.000	
hf1	1	352.000	2.490	1.730	0.000	5.000	
hf2	1	352.000	2.490	1.730	0.000	5.000	
hf3	1	352.000	2.490	1.730	0.000	5.000	
hf4	1	352.000	2.490	1.730	0.000	5.000	
hf5	1	352.000	2.490	1.730	0.000	5.000	
hf6	1	352.000	2.490	1.730	0.000	5.000	
hf7	1	352.000	2.490	1.730	0.000	5.000	
hf8	1	352.000	2.490	1.730	0.000	5.000	
hcno	2	232.400	3.828	0.000	0.000	1.000	! jam
hocn	2	232.400	3.828	0.000	0.000	1.000	! jam

hnco	2	232.400	3.828	0.000	0.000	1.000	! ois
hnno	2	232.400	3.828	0.000	0.000	1.000	! *
hno	2	116.700	3.492	0.000	0.000	1.000	! *
hnoh	2	116.700	3.492	0.000	0.000	1.000	! jam
ho2	2	107.400	3.458	0.000	0.000	1.000	! *
hso2	2	252.000	4.290	0.000	0.000	1.000	! ois
n	0	71.400	3.298	0.000	0.000	0.000	! *
n2	1	97.530	3.621	0.000	1.760	4.000	
n2h2	2	71.400	3.798	0.000	0.000	1.000	! *
n2h3	2	200.000	3.900	0.000	0.000	1.000	! *
n2h4	2	205.000	4.230	0.000	4.260	1.500	
n2o	1	232.400	3.828	0.000	0.000	1.000	! *
ncn	1	232.400	3.828	0.000	0.000	1.000	! ois
nco	1	232.400	3.828	0.000	0.000	1.000	! ois
nh	1	80.000	2.650	0.000	0.000	4.000	
nh2	2	80.000	2.650	0.000	2.260	4.000	
nh3	2	481.000	2.920	1.470	0.000	10.000	
nnh	2	71.400	3.798	0.000	0.000	1.000	! *
no	1	97.530	3.621	0.000	1.760	4.000	
ncno	2	232.400	3.828	0.000	0.000	1.000	! ois
no2	2	200.000	3.500	0.000	0.000	1.000	! *
o	0	80.000	2.750	0.000	0.000	0.000	
o2	1	107.400	3.458	0.000	1.600	3.800	
o3	2	180.000	4.100	0.000	0.000	2.000	
oh	1	80.000	2.750	0.000	0.000	0.000	
s	0	847.000	3.839	0.000	0.000	0.000	! ois
s2	1	847.000	3.900	0.000	0.000	1.000	! ois
sh	1	847.000	3.900	0.000	0.000	1.000	! ois
so	1	301.000	3.993	0.000	0.000	1.000	! ois
so2	2	252.000	4.290	0.000	0.000	1.000	! ois
so3	2	378.400	4.175	0.000	0.000	1.000	! ois
sih4	2	207.6	4.084	0.000	0.000	1.000	! mec
sih3	2	170.3	3.943	0.000	0.000	1.000	! mec
sih2	2	133.1	3.803	0.000	0.000	1.000	! mec
sih	1	95.8	3.662	0.000	0.000	1.000	! mec
si	0	3036.	2.910	0.000	0.000	0.000	! mec
si2h6	2	301.3	4.828	0.000	0.000	1.000	! mec
si2h5	2	306.9	4.717	0.000	0.000	1.000	! mec
si2h4	2	312.6	4.601	0.000	0.000	1.000	! mec
si2h3	2	318.2	4.494	0.000	0.000	1.000	! mec
si2h2	2	323.8	4.383	0.000	0.000	1.000	! mec
si2	1	3036.	3.280	0.000	0.000	1.000	! mec
si3	2	3036.	3.550	0.000	0.000	1.000	! mec
sif3	2	309.6	4.359	0.000	0.000	1.000	! mec
sif3nh2	2	231.0	4.975	0.000	0.000	1.000	! mec
sif4	2	171.9	4.880	0.000	0.000	1.000	! sve
sihf3	2	180.8	4.681	0.000	0.000	1.000	! mec
h2sisih2	2	312.6	4.601	0.000	0.000	1.000	! mec
h3sisih	2	312.6	4.601	0.000	0.000	1.000	! mec
si3h8	2	331.2	5.562	0.000	0.000	1.000	! mec
ash3	2	259.8	4.145	0.000	0.000	1.000	! mec
as2	1	1045.5	5.510	0.000	0.000	1.000	! mec
game3	2	378.2	5.52	0.000	0.000	1.000	! mec
game2	2	675.8	5.22	0.000	0.000	1.000	! mec
game	2	972.7	4.92	0.000	0.000	1.000	! mec
ga	0	2961.8	4.62	0.000	0.000	0.000	! mec
k	0	850.	4.25	0.000	0.000	1.000	! singh
koh	2	1213.	4.52	0.000	0.000	1.000	! singh
ko2	2	1213.	4.69	0.000	0.000	1.000	! singh
kh	1	93.3	3.542	0.000	0.000	1.000	! singh
k+	0	850.	4.25	0.000	0.000	1.000	! singh

e	0	850.	425.	0.000	0.000	1.000 ! singh
kcl	1	1989.	4.186	0.000	0.000	1.000 ! singh
cl	0	130.8	3.613	0.000	0.000	1.000 ! singh
cl-	0	130.8	3.613	0.000	0.000	1.000 ! singh
hcl	1	344.7	3.339	1.084	0.000	1.000 ! singh
ko	1	383.0	3.812	0.000	0.000	1.000 ! singh

APPENDIX G

METHYLBUTANOATE TRANSPORT DATA

tc3h6oh	2	487.900	4.820	0.000	0.000	1.000 !nmm
ac3h4coc2h5	2	527.994	5.587	0.000	0.000	0.000!FLAMEMASTER
c3h4coch3	2	482.331	5.306	0.000	0.000	0.000!FLAMEMASTER
ac3h5chcho	2	435.2	4.662	2.7	0.0	1.000 !wjp
ac3h5chcoch3	2	527.994	5.587	0.000	0.000	0.000!FLAMEMASTER
ac3h5cho	2	464.2	5.009	2.6	0.0	0.000 !WJP
ac3h5co	2	464.2	5.009	2.6	0.0	1.000 !WJP
baoj	2	357.0	5.176	0.0	0.0	1.0 !MIE 2005
baoj2*o	2	357.0	5.176	0.0	0.0	1.0 !MIE 2005
baoj2d	2	357.0	5.176	0.0	0.0	1.0 !MIE 2005
c2h	1	265.300	3.721	0.000	0.000	2.500 !nmm
c2h2	1	265.300	3.721	0.000	0.000	2.500 !nmm
c2h3	2	265.300	3.721	0.000	0.000	1.000 !nmm
c2h3chcho	2	464.2	5.009	2.6	0.0	1.0 !WJP
c2h3cho	2	428.8	4.958	2.9	0.0	1.0 !wjp
c2h3co	2	443.200	4.120	0.000	0.000	1.000 !nmm
c2h3coch3	2	454.0	5.413	3.3	0.000	1.000 !c2h5coch3
c2h3o1,2	2	436.000	3.970	0.000	0.000	2.000 !WJP
c2h4	2	238.400	3.496	0.000	0.000	1.500 !nmm
c2h4o1,2	2	387.3	4.349	1.9	0.0	1.0 !wjp
c2h4o2h	2	470.600	4.410	0.000	0.000	1.500 !c2h5oh
c2h4oh	2	470.600	4.410	0.000	0.000	1.500 !c2h5oh
c2h5	2	247.500	4.350	0.000	0.000	1.500 !nmm
c2h5chco	2	436.950	5.016	0.000	0.000	
0.000!FLAMEMASTER						
c2h5cho	2	435.2	4.662	2.7	0.0	1.0 !wjp
c2h5co	2	424.600	4.820	0.000	0.000	1.000 !nmm
c2h5coc2h3	2	476.7	5.714	2.7	0.0	1.0 !WJP
c2h5coc2h4p	2	489.084	5.348	0.000	0.000	0.000
!FLAMEMASTER						
c2h5coc2h4s	2	489.084	5.348	0.000	0.000	0.000
!FLAMEMASTER						
c2h5coc2h5	2	476.7	5.714	2.7	0.0	1.0 !TCPC
c2h5coch2	2	454.0	5.413	3.3	0.000	1.000
!c2h5coch3						
c2h5coch3	2	454.0	5.413	3.3	0.000	1.000 !wjp, rp
c2h5coco	2	395.0	4.037	1.3	0.0	1.0 !ch3och3
c2h5o	2	470.600	4.410	0.000	0.000	1.500 !nmm
c2h5o2	2	470.600	4.410	0.000	0.000	1.500 !c2h5o
c2h5o2h	2	470.600	4.410	0.000	0.000	1.500 !c2h5oh
c2h5oh	2	470.600	4.410	0.000	0.000	1.500 !nmm
c2h6	2	247.500	4.350	0.000	0.000	1.500 !nmm
c3h2	2	209.000	4.100	0.000	0.000	1.000 ! *
c3h3	1	324.800	4.290	0.000	0.000	1.000 !nmm
c3h4-a	1	324.800	4.290	0.000	0.000	1.000 !nmm
c3h4-p	1	324.800	4.290	0.000	0.000	1.000 !nmm
c3h5-a	2	316.000	4.220	0.000	0.000	1.000
c3h5o	2	411.000	4.820	0.000	0.000	1.000 !nmm
c3h5oh	2	481.5	4.997	1.7	0.0	1.0 !wjp
c3h5-s	2	316.000	4.220	0.000	0.000	1.000
c3h5-t	2	316.000	4.220	0.000	0.000	1.000
c3h6	2	307.800	4.140	0.000	0.000	1.000 !nmm
c3h6cho-1	2	464.2	5.009	2.6	0.0	1.0 !WJP
c3h6cho-2	2	464.2	5.009	2.6	0.0	1.0 !WJP
c3h6cho-3	2	464.2	5.009	2.6	0.0	1.0 !WJP

c3h6coc2h5-1	2	534.323	5.625	0.000	0.000	0.000	
FLAMEMASTER							
c3h6coc2h5-2	2	534.323	5.625	0.000	0.000	0.000	
!FLAMEMASTER							
c3h6coc2h5-3	2	534.323	5.625	0.000	0.000	0.000	
!FLAMEMASTER							
c3h6coch3-1	2	489.084	5.348	0.000	0.000	0.000	
!FLAMEMASTER							
c3h6coch3-2	2	489.084	5.348	0.000	0.000	0.000	
!FLAMEMASTER							
c3h6coch3-3	2	489.084	5.348	0.000	0.000	0.000	
!FLAMEMASTER							
c3h6o1-2	2	403.6	4.968	2.0	0.0	1.0	!WJP
c3h6o1-3	2	403.6	4.968	2.0	0.0	1.0	!WJP
c3h6oh	2	487.900	4.820	0.000	0.000	1.000	!nmm
c3h6ooh1-2	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h6ooh1-2o2	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h6ooh1-3	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h6ooh1-3o2	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h6ooh2-1	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h6ooh2-1o2	2	435.2	4.662	2.7	0.0	1.0	!WJP
c3h8	2	303.400	4.810	0.000	0.000	1.000	!nmm
c3ket12	2	464.2	5.009	2.6	0.0	1.0	!WJP
c3ket13	2	464.2	5.009	2.6	0.0	1.0	!WJP
c3ket21	2	464.2	5.009	2.6	0.0	1.0	!WJP
c5h7o2	2	266.800	4.982	0.000	0.000	1.000	!=C3H7
ch	1	80.000	2.750	0.000	0.000	0.000	
ch2	1	144.000	3.800	0.000	0.000	0.000	
ch2(s)	1	144.000	3.800	0.000	0.000	0.000	
ch2cch2oh	2	481.5	4.997	1.7	0.0	1.0	!wjp
ch2ch2cho	2	424.600	4.820	0.000	0.000	1.000	!nmm
ch2ch2coch3	2	435.500	4.860	2.9	0.000	1.000	!ch3coch3
ch2ch2coch3	2	454.0	5.413	3.3	0.000	1.000	
!c2h5coch3							
ch2chchco	2	435.2	4.662	2.7	0.0	1.0	!wjp
ch2cho	2	436.000	3.970	0.000	0.000	2.000	
ch2choohcoch3	2	454.0	5.413	3.3	0.000	1.000	
!c2h5coch3							
ch2co	2	436.000	3.970	0.000	0.000	2.000	
ch2o	2	498.000	3.590	0.000	0.000	2.000	
ch2o2hcho	2	435.2	4.662	2.7	0.0	1.0	!wjp
ch2oh	2	417.000	3.690	1.700	0.000	2.000	
ch3	1	144.000	3.800	0.000	0.000	0.000	
ch3chcho	2	435.2	4.662	2.7	0.0	1.0	!wjp
ch3chco	2	443.200	4.120	0.000	0.000	1.000	!nmm
ch3chcoch3	2	454.0	5.413	3.3	0.000	1.000	
!c2h5coch3							
ch3cho	2	436.000	3.970	2.5	0.000	2.000	!rpd
ch3chocho	1	440.200	4.010	0.000	0.000	2.000	!nmm
ch3choococh3	2	454.0	5.413	3.3	0.000	1.000	
!c2h5coch3							
ch3choohcoch3	2	454.0	5.413	3.3	0.000	1.000	
!c2h5coch3							
ch3co	2	436.000	3.970	2.5	0.000	2.000	!ch3cho
ch3co2	2	514.0	5.007	1.3	0.0	1.0	!ch3co2h
ch3co3	2	514.0	5.007	1.3	0.0	1.0	!ch3co2h
ch3co3h	2	514.0	5.007	1.3	0.0	1.0	!ch3co2h
ch3coch2	2	477.0	5.735	2.5	0.0	1.0	!wjp
ch3coch2o	2	435.500	4.860	2.9	0.000	1.000	!ch3coch
ch3coch2o2	2	435.500	4.860	2.9	0.000	1.000	!ch3coch3
ch3coch2o2h	2	435.500	4.860	2.9	0.000	1.000	!ch3coch3

ch3coch3	2	435.500	4.860	2.9	0.000	1.000	!nmm,wjp
ch3cocho	1	440.200	4.010	0.000	0.000	2.000	!nmm
ch3coco	2	395.0	4.037	1.3	0.0	1.0	!ch3och3
ch3o	2	417.000	3.690	1.700	0.000	2.000	
ch3o2	2	481.800	3.626	1.7	0.000	1.000	!ch3oh
ch3o2h	2	481.800	3.626	1.7	0.000	1.000	!ch3oh
ch3oco	2	395.0	4.037	1.3	0.0	1.0	!ch3och3
ch3oh	2	481.800	3.626	1.7	0.000	1.000	!sve,rpd
ch4	2	141.400	3.746	0.000	2.600	13.000	
chocho	1	440.200	4.010	0.000	0.000	2.000	!nmm
chooco	2	395.0	4.037	1.3	0.0	1.0	!ch3och3
cjhchchco	2	443.200	4.120	0.000	0.000	1.000	!nmm
co	1	98.100	3.650	0.000	1.950	1.800	
co2	1	244.000	3.763	0.000	2.650	2.100	
cochoo	1	440.200	4.010	0.000	0.000	2.000	!nmm
h	0	145.000	2.050	0.000	0.000	0.000	
h2	1	38.000	2.920	0.000	0.790	280.000	
h2o	2	572.400	2.605	1.844	0.000	4.000	
h2o2	2	107.400	3.458	0.000	0.000	3.800	
hcco	2	150.000	2.500	0.000	0.000	1.000	!*
hco	2	498.000	3.590	0.000	0.000	0.000	
ho2	2	107.400	3.458	0.000	0.000	1.000	!*
ho2cho	1	440.200	4.010	0.000	0.000	2.000	!nmm
hoc3h6o2	2	487.900	4.820	0.000	0.000	1.000	!nmm
hoch2o	2	481.800	3.626	1.7	0.000	1.000	!ch3oh
hocho	1	440.200	4.010	0.000	0.000	2.000	!nmm
ic3h5cho	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h5co	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h5coc2h4p	2	527.994	5.587	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h5coc2h4s	2	527.994	5.587	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h5coc2h5	2	531.165	5.606	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h5coch2	2	482.331	5.306	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h5coch3	2	485.716	5.327	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h5o2hcho	2	436.4	5.352	0.0	0.0	1.0	!WJP
ic3h5oh	2	459.5	5.036	1.7	0.0	1.0	!WJP
ic3h6chcho	2	435.2	4.662	2.7	0.0	1.0	!wjp
ic3h6chco	2	443.200	4.120	0.000	0.000	1.000	!nmm
ic3h6chcoch2	2	527.994	5.587	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h6chcoch3	2	531.165	5.606	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h6cho	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h6co	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h6coc2h3	2	527.994	5.587	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h6coc2h5	2	534.323	5.625	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h6coch3	2	489.084	5.348	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h7	2	303.400	4.810	0.000	0.000	1.000	!nmm
ic3h7cho	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h7co	2	436.4	5.352	0.0	0.0	1.0	!wjp
ic3h7coc2h3	2	531.165	5.606	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h7coc2h4p	2	534.323	5.625	0.000	0.000	0.000	
!FLAMEMASTER							

ic3h7coc2h4s	2	534.323	5.625	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h7coc2h5	2	537.467	5.643	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h7coch2	2	489.084	5.348	0.000	0.000	0.000	
!FLAMEMASTER							
ic3h7coch3	2	469.0	5.632	2.8	0.0	1.0	!WJP
ic3h7o	2	459.5	5.036	1.7	0.0	1.0	!wjp
ic3h7o2	2	459.5	5.036	1.7	0.0	1.0	!WJP
ic3h7o2h	2	459.5	5.036	1.7	0.0	1.0	!WJP
mb	2	386.2	5.489	0.4	0.0	1.0	!WJP
mb2d	2	386.2	5.489	0.4	0.0	1.0	!WJP
mb2j	2	386.2	5.489	0.4	0.0	1.0	!WJP
mb2o	2	396.8	5.458	0.0	0.0	1.0	!WJP
mb2oh3j	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2oh3oo	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2oo-3	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh4	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh3*o	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh3j	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh3oo	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh4*o	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh4j	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2ooh4oo	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2oohm*o	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2oohmj	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb2oohmoo	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb3d	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb3j	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb3o	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb3oh4j	2	523.2	5.664	1.7	0.0	1.0	!WJP
mb3oh4oo	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3oo	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh2*o	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh2j	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh2oo	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh4*o	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh4j	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb3ooh4oo	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4*o	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4j	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4j*o	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4o	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4oo	2	523.2	5.664	1.7	0.0	1.0	! WJP
mb4ooh	2	498.6	6.009	2.0	0.0	1.0	
!C2H5COC3H7-N WJP							
mb4ooh2*o	2	498.6	6.009	2.0	0.0	1.0	
!C2H5COC3H7-N WJP							
mb4ooh2d	2	498.6	6.009	2.0	0.0	1.0	
!C2H5COC3H7-N WJP							
mb4ooh2j	2	498.6	6.009	2.0	0.0	1.0	
!C2H5COC3H7-N WJP							
mb4ooh2oo	2	498.6	6.009	2.0	0.0	1.0	
!C2H5COC3H7-N WJP							
mb4ooh3*o	2	494.8	6.174	1.8	0.0	1.0	!TCPC
mb4ooh3j	2	494.8	6.174	1.8	0.0	1.0	!TCPC
mb4ooh3oo	2	494.8	6.174	1.8	0.0	1.0	!TCPC
mbcy2om	2	494.8	6.174	1.8	0.0	1.0	!TCPC
mbcy3o2	2	494.8	6.174	1.8	0.0	1.0	!TCPC
mbcy4o2	2	494.8	6.174	1.8	0.0	1.0	!TCPC

mbcy4o3	2	494.8	6.174	1.8	0.0	1.0 !TCPC
mbm*o	2	494.8	6.174	1.8	0.0	1.0 !TCPC
mbmj	2	494.8	6.174	1.8	0.0	1.0 !TCPC
mbmj*o	2	494.8	6.174	1.8	0.0	1.0 !TCPC
mbmo0	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmoo	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmooh	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmooh2*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmooh2d	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmooh2j	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmooh2oo	2	523.2	5.664	1.7	0.0	1.0 !WJP
me2*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
me2*om*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
me2*o	2	357.8	5.550	0.0	0.0	1.0 !WJP
me2j	2	523.2	5.664	1.7	0.0	1.0 !WJP
me2j*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
me2j*om*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp2d	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp2d3j	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp2oh3j	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp2oh3oo	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3*o2*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3j	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3j*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3j*o2*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
mp3j2*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
n2	1	97.530	3.621	0.000	1.760	4.0
nc3h7	2	303.400	4.810	0.000	0.000	1.0 !nmm
nc3h7cho	2	464.2	5.009	2.6	0.0	1.0 !wjp
nc3h7co	2	464.2	5.009	2.6	0.0	1.0 !wjp
nc3h7coc2h4p	2	477.0	5.735	2.5	0.0	1.0 !wjp
nc3h7coc2h4s	2	477.0	5.735	2.5	0.0	1.0 !wjp
nc3h7coc2h5	2	477.0	5.735	2.5	0.0	1.0 !wjp
nc3h7coch2	2	477.0	5.735	2.5	0.0	1.0 !wjp
nc3h7coch3	2	477.0	5.735	2.5	0.0	1.0 !wjp
nc3h7o	2	481.5	4.997	1.7	0.0	1.0 !wjp
nc3h7o2	2	266.800	4.982	0.000	0.000	1.0 !=C3H7
nc3h7o2h	2	266.800	4.982	0.000	0.000	1.0 !=C3H7
o	0	80.000	2.750	0.000	0.000	0.000
o2	1	107.400	3.458	0.000	1.600	3.800
o2c2h4o2h	2	510.5	4.762	2.2	0.0	1.5 !hoc2h4oh
o2c2h4oh	2	510.5	4.762	2.2	0.0	1.5 !hoc2h4oh
o2cho	2	436.000	3.970	0.000	0.000	2.0 !WJP
ocho	2	498.000	3.590	0.000	0.000	2.0 ! WJP
oh	1	80.000	2.750	0.000	0.000	0.000
pc2h4coc2h3	2	476.7	5.714	2.7	0.0	1.0 !WJP
pc2h4oh	2	470.600	4.410	0.000	0.000	1.5 !NMM
sc2h4coc2h3	2	476.7	5.714	2.7 0.	0	1.0 !WJP
sc2h4oh	2	470.600	4.410	0.000	0.000	1.5 !nmm
sc3h5cho	2	464.2	5.009	2.6	0.0	1.0 !TCPC
sc3h5co	2	464.2	5.009	2.6	0.0	1.0 !TCPC
sc3h5coch2	2	482.331	5.306	0.000	0.000	0.0 !FLAMEMASTER
sc3h5och2	1	440.200	4.010	0.000	0.000	2.0 !nmm
tc3h6cho	2	436.4	5.352	0.0	0.0	1.0 !wjp
tc3h6coc2h3	2	527.994	5.587	0.000	0.000	0.0 !FLAMEMASTER
tc3h6coc2h5	2	534.323	5.625	0.000	0.000	0.0 !FLAMEMASTER
tc3h6coch3	2	489.084	5.348	0.000	0.000	0.0 !FLAMEMASTER
tc3h6o2cho	2	436.4	5.352	0.0	0.0	1.0 !WJP
tc3h6o2hco	2	436.4	5.352	0.0	0.0	1.0 !wjp
tc3h6ocho	2	440.200	4.010	0.000	0.000	2.0 !nmm

tc3h6ohcho	2	436.4	5.352	0.0	0.0	1.0 !WJP
cocho	1	440.200	4.010	0.000	0.000	2.0 !nmm
mb2oo	2	523.2	5.664	1.7	0.0	1.0 !WJP
mb2ooh	2	523.2	5.664	1.7	0.0	1.0 !WJP
mbmo	2	494.8	6.174	1.8	0.0	1.0 !TCPC
me2*omj*o	2	523.2	5.664	1.7	0.0	1.0 !WJP
ar	0	136.500	3.330	0.000	0.000	0.0

APPENDIX H TYPICAL ETHANOL FLAMELET DATA

HEADER

STRAINRATE 52.83
NUMOFSPECIES 9
GRIDPOINTS 90
PRESSURE 0.101000E+06
BODY

Z
0.000000E+00 8.088502E-03 8.441835E-03 1.005965E-02 1.303230E-02
1.558491E-02 1.841679E-02 2.195917E-02 2.600105E-02 3.086584E-02
3.564887E-02 4.056280E-02 4.939774E-02 5.907797E-02 6.472071E-02
7.059261E-02 8.168707E-02 9.054016E-02 9.594596E-02 1.017103E-01
1.049652E-01 1.077597E-01 1.091460E-01 1.105258E-01 1.125145E-01
1.140059E-01 1.152272E-01 1.166839E-01 1.180991E-01 1.194775E-01
1.208640E-01 1.222618E-01 1.244100E-01 1.267180E-01 1.284214E-01
1.302517E-01 1.322157E-01 1.343949E-01 1.368037E-01 1.394168E-01
1.422469E-01 1.454094E-01 1.489291E-01 1.507372E-01 1.529240E-01
2.019825E-01 2.088364E-01 2.181386E-01 2.279542E-01 2.382978E-01
2.499367E-01 2.630042E-01 2.782777E-01 2.959771E-01 3.171518E-01
3.294161E-01 3.420721E-01 3.550875E-01 3.686956E-01 3.826123E-01
3.968075E-01 4.112528E-01 4.249545E-01 4.388317E-01 4.670377E-01
4.958650E-01 5.556700E-01 6.020774E-01 6.333677E-01 6.631965E-01
6.844335E-01 6.984117E-01 7.181060E-01 7.431281E-01 7.775481E-01
7.989092E-01 8.181851E-01 8.365688E-01 8.534783E-01 8.694150E-01
8.857446E-01 9.007875E-01 9.133355E-01 9.247574E-01 9.441578E-01
9.602314E-01 9.739370E-01 9.961343E-01 9.993735E-01 1.000000E+00

MASSFRACTION-H2
0.000000E+00 2.180279E-05 2.210670E-05 2.341171E-05 2.555805E-05
2.729651E-05 2.928687E-05 3.222078E-05 3.682677E-05 4.517496E-05
5.725686E-05 7.411988E-05 1.160502E-04 1.800324E-04 2.271224E-04
2.849861E-04 2.484524E-04 5.767164E-04 6.962902E-04 8.577303E-04
9.711092E-04 1.085023E-03 1.148006E-03 1.215135E-03 1.319490E-03
1.402909E-03 1.473728E-03 1.560060E-03 1.644585E-03 1.726281E-03
1.806815E-03 1.885581E-03 2.000901E-03 2.116354E-03 2.195975E-03
2.276511E-03 2.357522E-03 2.441363E-03 2.527268E-03 2.613172E-03
2.698504E-03 2.785426E-03 2.873016E-03 2.914706E-03 2.962454E-03
3.621404E-03 3.672309E-03 3.727263E-03 3.768844E-03 3.796696E-03
3.811732E-03 3.812252E-03 3.796236E-03 3.761548E-03 3.704650E-03
3.666463E-03 3.624246E-03 3.578615E-03 3.529155E-03 3.477263E-03
3.423394E-03 3.367933E-03 3.314949E-03 3.261060E-03 3.151224E-03
3.038919E-03 2.806310E-03 2.625786E-03 2.503619E-03 2.386487E-03
2.302493E-03 2.246847E-03 2.167850E-03 2.066230E-03 1.923409E-03
1.832362E-03 1.748108E-03 1.665408E-03 1.586781E-03 1.509831E-03
1.427301E-03 1.347046E-03 1.276032E-03 1.207134E-03 1.077241E-03
9.502811E-04 8.160606E-04 4.323400E-04 2.795675E-04 1.213140E-06

MASSFRACTION-CO
0.000000E+00 1.356797E-04 1.421514E-04 1.722906E-04 2.305409E-04
2.849036E-04 3.510528E-04 4.445547E-04 5.710109E-04 7.636335E-04
1.016142E-03 1.366525E-03 2.312004E-03 4.003878E-03 5.414945E-03
7.290861E-03 1.222388E-02 1.788329E-02 2.236097E-02 2.822686E-02
3.214163E-02 3.588980E-02 3.788109E-02 3.994204E-02 4.302289E-02
4.537891E-02 4.730508E-02 4.956153E-02 5.167240E-02 5.361939E-02
5.544854E-02 5.715101E-02 5.949048E-02 6.165727E-02 6.305511E-02
6.439395E-02 6.567087E-02 6.692661E-02 6.815378E-02 6.933223E-02
7.046725E-02 7.160113E-02 7.273673E-02 7.327959E-02 7.390616E-02
8.377255E-02 8.458772E-02 8.542992E-02 8.599486E-02 8.626154E-02
8.621541E-02 8.580826E-02 8.496538E-02 8.362895E-02 8.168471E-02
8.044092E-02 7.909386E-02 7.765808E-02 7.611642E-02 7.450868E-02
7.284555E-02 7.113604E-02 6.950343E-02 6.784211E-02 6.445032E-02
6.097275E-02 5.747171E-02 4.814253E-02 4.436736E-02 4.077211E-02
3.821481E-02 3.653274E-02 3.416438E-02 3.115804E-02 2.702736E-02
2.446638E-02 2.215678E-02 1.995493E-02 1.792996E-02 1.602126E-02
1.406455E-02 1.226036E-02 1.075340E-02 9.379262E-03 7.037381E-03
5.085228E-03 3.405383E-03 6.072926E-04 1.639308E-04 0.000000E+00

MASSFRACTION-OH
8.019451E-23 1.493127E-05 1.731739E-05 3.023522E-05 5.839108E-05
8.406108E-05 1.184408E-04 1.816402E-04 2.931305E-04 4.908098E-04
7.517577E-04 1.078879E-03 1.772243E-03 2.595131E-03 3.058359E-03
3.496312E-03 4.110600E-03 4.291816E-03 4.211282E-03 3.921014E-03
3.646224E-03 3.340831E-03 3.165845E-03 2.977483E-03 2.685332E-03
2.455948E-03 2.266105E-03 2.042547E-03 1.833684E-03 1.642440E-03
1.464929E-03 1.302333E-03 1.084302E-03 8.894874E-04 7.683470E-04
6.564181E-04 5.541937E-04 4.589710E-04 3.722150E-04 2.961111E-04
2.308077E-04 1.745650E-04 1.280069E-04 1.092568E-04 9.036821E-05
6.860457E-06 6.204464E-06 5.536008E-06 4.951553E-06 4.399700E-06
3.828478E-06 3.239368E-06 2.619694E-06 1.998994E-06 1.397600E-06
1.117162E-06 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
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0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

MASSFRACTION-C2H2
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

TEMPERATURE
3.000000E+02 5.792767E+02 5.901377E+02 6.387706E+02 7.236103E+02
7.918752E+02 8.628767E+02 9.453768E+02 1.032170E+03 1.127971E+03
1.214299E+03 1.295854E+03 1.426625E+03 1.549374E+03 1.611966E+03
1.670629E+03 1.764981E+03 1.826109E+03 1.857753E+03 1.887139E+03
1.901888E+03 1.913478E+03 1.918812E+03 1.923795E+03 1.930264E+03
1.934399E+03 1.937209E+03 1.939768E+03 1.941328E+03 1.941918E+03
1.941583E+03 1.940342E+03 1.936830E+03 1.931215E+03 1.926070E+03
1.919765E+03 1.912263E+03 1.903219E+03 1.892524E+03 1.880285E+03
1.866474E+03 1.850559E+03 1.832461E+03 1.823069E+03 1.811661E+03
1.575976E+03 1.549248E+03 1.516065E+03 1.484677E+03 1.455119E+03
1.425421E+03 1.395621E+03 1.364380E+03 1.331685E+03 1.296005E+03
1.276553E+03 1.257168E+03 1.237806E+03 1.218047E+03 1.198239E+03
1.178355E+03 1.158376E+03 1.139608E+03 1.120742E+03 1.082705E+03
1.044098E+03 9.642957E+02 9.021679E+02 8.599764E+02 8.194233E+02
7.903085E+02 7.710190E+02 7.436530E+02 7.085372E+02 6.595292E+02
6.286713E+02 6.005209E+02 5.734069E+02 5.482536E+02 5.243921E+02
4.998451E+02 4.772339E+02 4.584540E+02 4.415310E+02 4.135306E+02
3.915534E+02 3.744664E+02 3.531674E+02 3.513004E+02 3.510000E+02

MASSFRACTION-CO2
0.000000E+00 7.685812E-03 8.102896E-03 1.006233E-02 1.384512E-02
1.725104E-02 2.117326E-02 2.625684E-02 3.226309E-02 3.974243E-02
4.731589E-02 5.526684E-02 6.980132E-02 8.569280E-02 9.474792E-02
1.038819E-01 1.199038E-01 1.308439E-01 1.363031E-01 1.407702E-01
1.425380E-01 1.435619E-01 1.438915E-01 1.441004E-01 1.441973E-01
1.441229E-01 1.439791E-01 1.437254E-01 1.434121E-01 1.430625E-01
1.426833E-01 1.422871E-01 1.416738E-01 1.410334E-01 1.405817E-01
1.401186E-01 1.396471E-01 1.391528E-01 1.386378E-01 1.381107E-01
1.375702E-01 1.369952E-01 1.363820E-01 1.360752E-01 1.357100E-01
1.279497E-01 1.268735E-01 1.254084E-01 1.238546E-01 1.222072E-01
1.203405E-01 1.182289E-01 1.157412E-01 1.128352E-01 1.093308E-01
1.072892E-01 1.051747E-01 1.029926E-01 1.007038E-01 9.835616E-02
9.595500E-02 9.350539E-02 9.117674E-02 8.881364E-02 8.399819E-02
7.906297E-02 6.879736E-02 6.082875E-02 5.546682E-02 5.037136E-02
4.675755E-02 4.438715E-02 4.106063E-02 3.686132E-02 3.114778E-02
2.764953E-02 2.453230E-02 2.160152E-02 1.894936E-02 1.649551E-02
1.403629E-02 1.182886E-02 1.003766E-02 8.454832E-03 5.889166E-03
3.907795E-03 2.360142E-03 2.815244E-04 5.311080E-05 0.000000E+00

MASSFRACTION-O2
2.329175E-01 2.144118E-01 2.135976E-01 2.098686E-01 2.030115E-01
1.971102E-01 1.905376E-01 1.822746E-01 1.728114E-01 1.614199E-01
1.502632E-01 1.388818E-01 1.187149E-01 9.724162E-02 8.512969E-02
7.291630E-02 5.117204E-02 3.545230E-02 2.680731E-02 1.860889E-02
1.455495E-02 1.146576E-02 1.008292E-02 8.812702E-03 7.178146E-03
6.110662E-03 5.339059E-03 4.537226E-03 3.875311E-03 3.332149E-03
2.875166E-03 2.492412E-03 2.029087E-03 1.658894E-03 1.447786E-03
1.265348E-03 1.108665E-03 9.704363E-04 8.498743E-04 7.469099E-04
6.588841E-04 5.810777E-04 5.124139E-04 4.825755E-04 4.503581E-04
1.185471E-04 9.570697E-05 7.025335E-05 4.963634E-05 3.376054E-05
2.149791E-05 1.276823E-05 6.889265E-06 3.378003E-06 1.471421E-06
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
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0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

MASSFRACTION-H2O
3.409915E-16 1.803657E-02 1.868166E-02 2.155650E-02 2.655932E-02
3.061976E-02 3.490727E-02 3.999258E-02 4.546838E-02 5.165915E-02
5.737213E-02 6.290238E-02 7.211521E-02 8.131637E-02 8.631040E-02
9.124689E-02 9.990597E-02 1.061989E-01 1.097369E-01 1.131788E-01
1.149153E-01 1.162481E-01 1.168438E-01 1.173880E-01 1.180803E-01
1.185246E-01 1.188407E-01 1.191645E-01 1.194294E-01 1.196477E-01
1.198358E-01 1.200017E-01 1.202251E-01 1.204422E-01 1.205961E-01
1.207597E-01 1.209358E-01 1.211336E-01 1.213559E-01 1.216010E-01
1.218706E-01 1.221756E-01 1.225182E-01 1.226949E-01 1.229092E-01
1.272874E-01 1.276612E-01 1.279822E-01 1.280733E-01 1.279022E-01
1.274144E-01 1.265496E-01 1.251956E-01 1.232717E-01 1.206078E-01
1.189334E-01 1.171304E-01 1.152138E-01 1.131572E-01 1.110113E-01
1.087888E-01 1.065006E-01 1.043114E-01 1.020797E-01 9.750997E-02
9.280471E-02 8.295150E-02 7.521689E-02 6.994920E-02 6.488097E-02
6.124078E-02 5.882863E-02 5.540625E-02 5.101366E-02 4.487845E-02
4.100803E-02 3.746779E-02 3.404415E-02 3.084949E-02 2.779405E-02
2.461321E-02 2.163365E-02 1.910842E-02 1.677475E-02 1.272708E-02
9.283246E-03 6.267087E-03 1.135296E-03 3.087532E-04 6.270037E-11

MASSFRACTION-C2H5OH
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
1.854437E-06 7.788193E-06 1.542550E-05 2.919830E-05 6.811759E-05
1.223180E-04 1.906134E-04 3.089321E-04 4.709661E-04 6.796605E-04
9.432904E-04 1.263473E-03 1.854947E-03 2.604499E-03 3.217242E-03
3.917890E-03 4.704026E-03 5.601450E-03 6.605659E-03 7.690441E-03
8.841319E-03 1.008072E-02 1.138780E-02 1.202673E-02 1.276919E-02
2.247816E-02 2.305657E-02 2.362379E-02 2.399561E-02 2.419088E-02
2.423198E-02 2.411969E-02 2.384763E-02 2.341468E-02 2.280170E-02
2.241913E-02 2.201150E-02 2.158316E-02 2.112873E-02 2.065946E-02
2.017776E-02 1.968553E-02 1.921740E-02 1.874242E-02 1.777529E-02
1.678525E-02 1.472787E-02 1.312931E-02 1.205108E-02 1.102334E-02
1.029199E-02 9.810893E-03 9.133598E-03 8.274328E-03 7.095624E-03
6.366916E-03 5.711878E-03 5.090050E-03 4.521267E-03 3.988746E-03
3.447617E-03 2.954161E-03 2.547161E-03 2.181307E-03 1.572583E-03
1.084355E-03 6.852554E-04 9.663349E-05 2.117014E-05 0.000000E+00

MASSFRACTION-N2

7.670825E-01 7.596665E-01 7.594084E-01 7.582536E-01 7.562179E-01
7.545334E-01 7.527185E-01 7.505097E-01 7.480397E-01 7.450864E-01
7.421611E-01 7.391048E-01 7.334313E-01 7.268949E-01 7.229062E-01
7.186023E-01 7.100243E-01 7.027518E-01 6.981173E-01 6.929932E-01
6.899989E-01 6.873587E-01 6.860228E-01 6.846761E-01 6.827071E-01
6.812139E-01 6.799852E-01 6.785188E-01 6.770997E-01 6.757289E-01
6.743654E-01 6.730090E-01 6.709615E-01 6.688102E-01 6.672513E-01
6.656004E-01 6.638531E-01 6.619400E-01 6.598525E-01 6.576156E-01
6.552212E-01 6.525754E-01 6.496622E-01 6.481767E-01 6.463890E-01
6.075947E-01 6.022883E-01 5.951101E-01 5.875563E-01 5.796111E-01
5.706816E-01 5.606640E-01 5.489613E-01 5.354059E-01 5.191977E-01
5.098149E-01 5.001368E-01 4.901887E-01 4.797934E-01 4.691685E-01
4.583377E-01 4.473231E-01 4.368822E-01 4.263140E-01 4.048536E-01
3.829476E-01 3.375856E-01 3.024598E-01 2.788108E-01 2.562914E-01
2.402727E-01 2.297354E-01 2.148969E-01 1.960569E-01 1.701606E-01
1.540977E-01 1.396057E-01 1.257843E-01 1.130678E-01 1.010763E-01
8.877755E-02 7.743186E-02 6.795078E-02 5.930106E-02 4.454879E-02
3.223775E-02 2.162832E-02 3.888677E-03 1.057435E-03 0.000000E+00

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
1.652659E-03 2.965358E-03 5.658199E-03 9.729419E-03 1.536571E-02
2.321798E-02 3.368166E-02 4.772891E-02 6.592638E-02 8.970728E-02
1.042269E-01 1.196454E-01 1.358688E-01 1.531435E-01 1.710653E-01
1.895481E-01 2.085142E-01 2.266133E-01 2.450252E-01 2.826188E-01
3.211838E-01 4.014096E-01 4.637415E-01 5.057829E-01 5.458649E-01
5.744022E-01 5.931851E-01 6.196481E-01 6.532672E-01 6.995056E-01
7.281952E-01 7.540786E-01 7.787582E-01 8.014527E-01 8.228352E-01
8.447378E-01 8.649079E-01 8.817281E-01 8.970352E-01 9.230319E-01
9.445821E-01 9.629942E-01 9.932714E-01 9.980453E-01 9.999988E-01

APPENDIX I TYPICAL METHYLBUTANOATE FLAMELET DATA

HEADER

STRAINRATE 400.00
NUMOFSPECIES 9
GRIDPOINTS 54
PRESSURE 0.101000E+06
BODY

Z

0.000000E+00 3.802244E-03 5.530401E-03 7.866319E-03 1.087925E-02
1.460635E-02 1.906129E-02 2.424821E-02 3.016486E-02 3.679454E-02
4.410244E-02 5.204149E-02 6.055879E-02 7.915682E-02 9.923376E-02
1.095314E-01 1.147986E-01 1.202352E-01 1.259473E-01 1.320301E-01
1.385540E-01 1.455811E-01 1.531903E-01 1.614972E-01 1.706599E-01
1.808767E-01 2.052732E-01 2.203100E-01 2.378283E-01 2.581997E-01
2.815452E-01 3.077261E-01 3.364227E-01 4.000437E-01 4.688707E-01
5.400307E-01 5.754780E-01 6.445784E-01 7.093234E-01 7.245981E-01
7.394675E-01 7.679277E-01 7.814939E-01 8.072530E-01 8.194287E-01
8.423617E-01 8.633925E-01 8.825489E-01 8.998538E-01 9.290137E-01
9.409601E-01 9.512470E-01 9.672823E-01 1.000000E+00

MASSFRACTION-H₂

0.000000E+00 4.133399E-05 4.728632E-05 5.357934E-05 6.014879E-05
6.701279E-05 7.439415E-05 8.294637E-05 9.403646E-05 1.099513E-04
1.338553E-04 1.695367E-04 2.213474E-04 3.894383E-04 7.147637E-04
9.934974E-04 1.165294E-03 1.355308E-03 1.556884E-03 1.762053E-03
1.963232E-03 2.153973E-03 2.329058E-03 2.484471E-03 2.617439E-03
2.726470E-03 2.870798E-03 2.906946E-03 2.917319E-03 2.901183E-03
2.859453E-03 2.795049E-03 2.712188E-03 2.505173E-03 2.269268E-03
2.021748E-03 1.898219E-03 1.657543E-03 1.432385E-03 1.379262E-03
1.327514E-03 1.228285E-03 1.180847E-03 1.090370E-03 1.047342E-03
9.656422E-04 8.896427E-04 8.191191E-04 7.538437E-04 6.382143E-04
5.874213E-04 5.409901E-04 4.601034E-04 0.000000E+00

MASSFRACTION-H₂O

0.000000E+00 7.171646E-03 9.894222E-03 1.330643E-02 1.738051E-02
2.203698E-02 2.716906E-02 3.266531E-02 3.841374E-02 4.429697E-02
5.019620E-02 5.600494E-02 6.163843E-02 7.221125E-02 8.119440E-02
8.432637E-02 8.536671E-02 8.601385E-02 8.627238E-02 8.619122E-02
8.584391E-02 8.530434E-02 8.463022E-02 8.385538E-02 8.298943E-02
8.202255E-02 7.971131E-02 7.827419E-02 7.658955E-02 7.461988E-02
7.235400E-02 6.980763E-02 6.701452E-02 6.082262E-02 5.412837E-02
4.720708E-02 4.375570E-02 3.701427E-02 3.066729E-02 2.916293E-02
2.769515E-02 2.487488E-02 2.352459E-02 2.094766E-02 1.972251E-02
1.739982E-02 1.524855E-02 1.326713E-02 1.145495E-02 8.338439E-03
7.032109E-03 5.889550E-03 4.067026E-03 0.000000E+00

MASSFRACTION-OH

0.000000E+00 7.008973E-06 1.438971E-05 3.139648E-05 6.752005E-05
1.315312E-04 2.279700E-04 3.655316E-04 5.638719E-04 8.443068E-04
1.214922E-03 1.661686E-03 2.145475E-03 3.012804E-03 3.151310E-03
2.663082E-03 2.284336E-03 1.858084E-03 1.439774E-03 1.074861E-03
7.831091E-04 5.613451E-04 3.957258E-04 2.720222E-04 1.800726E-04
1.134984E-04 4.084121E-05 2.284964E-05 1.238094E-05 6.430530E-06
3.184815E-06 1.512939E-06 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00

MASSFRACTION-C₂H₂

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 1.745894E-05
1.618540E-04 4.360727E-04 9.660694E-04 1.842667E-03 3.066477E-03
4.536917E-03 6.103212E-03 7.620593E-03 8.978349E-03 1.010587E-02
1.096954E-02 1.188858E-02 1.202335E-02 1.197109E-02 1.176916E-02
1.145349E-02 1.105496E-02 1.059736E-02 9.557930E-03 8.431704E-03
7.269007E-03 6.690310E-03 5.563575E-03 4.510517E-03 4.262685E-03
4.021723E-03 3.561502E-03 3.342670E-03 2.928331E-03 2.733107E-03
2.366688E-03 2.032438E-03 1.729783E-03 1.458239E-03 1.006294E-03
8.240946E-04 6.692457E-04 4.334255E-04 0.000000E+00

MASSFRACTION-N₂

7.670825E-01 7.638846E-01 7.626654E-01 7.610945E-01 7.591435E-01
7.567906E-01 7.540145E-01 7.507924E-01 7.470929E-01 7.428652E-01
7.380409E-01 7.325501E-01 7.263379E-01 7.116443E-01 6.942328E-01
6.845664E-01 6.794666E-01 6.741749E-01 6.686725E-01 6.629296E-01
6.569086E-01 6.505644E-01 6.438367E-01 6.366374E-01 6.288427E-01
6.202921E-01 6.002869E-01 5.881750E-01 5.742455E-01 5.582559E-01
5.401474E-01 5.200427E-01 4.981852E-01 4.501874E-01 3.987098E-01
3.458209E-01 3.195632E-01 2.684924E-01 2.206975E-01 2.094178E-01
1.984330E-01 1.773907E-01 1.673499E-01 1.482585E-01 1.392193E-01
1.221591E-01 1.064629E-01 9.211019E-02 7.908546E-02 5.695637E-02
4.779691E-02 3.984793E-02 2.729618E-02 0.000000E+00

TEMPERATURE

4.200000E+02 4.367608E+02 4.867377E+02 5.616846E+02 5.974005E+02
6.705740E+02 7.055687E+02 7.385630E+02 7.971093E+02 8.223677E+02
8.449750E+02 8.648997E+02 8.734583E+02 8.805500E+02 8.854467E+02
8.874623E+02 8.872757E+02 8.862963E+02 8.820587E+02 8.752113E+02
8.661807E+02 8.553257E+02 8.429333E+02 8.292487E+02 8.145340E+02
7.991447E+02 7.835103E+02 7.679863E+02 7.527343E+02 7.377230E+02
7.228130E+02 7.078500E+02 6.927197E+02 6.617310E+02 6.297737E+02
6.135537E+02 5.972041E+02 5.890088E+02 5.808063E+02 5.644024E+02
5.562444E+02 5.481270E+02 5.400650E+02 5.320741E+02 5.087024E+02
4.938201E+02 4.866551E+02 4.797065E+02 4.665612E+02 4.545901E+02
4.392160E+02 4.239823E+02 4.146417E+02 3.759000E+02

MASSFRACTION-O₂

2.329175E-01 2.248997E-01 2.211473E-01 2.160578E-01 2.094799E-01
2.013299E-01 1.915659E-01 1.801609E-01 1.671248E-01 1.525621E-01
1.366930E-01 1.198272E-01 1.023372E-01 6.677575E-02 3.447868E-02
2.185299E-02 1.686016E-02 1.283300E-02 9.743839E-03 7.464125E-03
5.817722E-03 4.636345E-03 3.785947E-03 3.168705E-03 2.715399E-03
2.377115E-03 1.942920E-03 1.785346E-03 1.655685E-03 1.544815E-03
1.446072E-03 1.354731E-03 1.267662E-03 1.100858E-03 9.383469E-04
7.809864E-04 7.053629E-04 5.623203E-04 4.326525E-04 4.026117E-04
3.735790E-04 3.190359E-04 2.939528E-04 2.489300E-04 2.289699E-04
1.937815E-04 1.641479E-04 1.390508E-04 1.174503E-04 8.258882E-05
6.867057E-05 5.678572E-05 3.835076E-05 0.000000E+00

MASSFRACTION-CO₂

0.000000E+00 3.432534E-03 5.398827E-03 8.255612E-03 1.218928E-02
1.735309E-02 2.386197E-02 3.179377E-02 4.118590E-02 5.201863E-02
6.418678E-02 7.746825E-02 9.149710E-02 1.202675E-01 1.442783E-01
1.521768E-01 1.549856E-01 1.570991E-01 1.586609E-01 1.598342E-01
1.607539E-01 1.615028E-01 1.621149E-01 1.625899E-01 1.629071E-01
1.630297E-01 1.624740E-01 1.614536E-01 1.596693E-01 1.569327E-01
1.531688E-01 1.484215E-01 1.428141E-01 1.295013E-01 1.144734E-01
9.856701E-02 9.055646E-02 7.483236E-02 6.004827E-02 5.656495E-02
5.317869E-02 4.671692E-02 4.364932E-02 3.785528E-02 3.513417E-02
3.004770E-02 2.543998E-02 2.130399E-02 1.763317E-02 1.164934E-02
9.302609E-03 7.351688E-03 4.491217E-03 0.000000E+00

MASSFRACTION-CO

0.000000E+00 5.353366E-04 7.829179E-04 1.119200E-03 1.557968E-03
2.113747E-03 2.806043E-03 3.664371E-03 4.735013E-03 6.091616E-03
7.849092E-03 1.017791E-02 1.331575E-02 2.291542E-02 3.975404E-02
5.157348E-02 5.785104E-02 6.401649E-02 6.973824E-02 7.484268E-02
7.932764E-02 8.327976E-02 8.678595E-02 8.988353E-02 9.254838E-02
9.471121E-02 9.725273E-02 9.743864E-02 9.681619E-02 9.537424E-02
9.316629E-02 9.029655E-02 8.688958E-02 7.883912E-02 6.985565E-02
6.046061E-02 5.576923E-02 4.662573E-02 3.808206E-02 3.607178E-02
3.411719E-02 3.038327E-02 2.860708E-02 2.524155E-02 2.365408E-02
2.066992E-02 1.793983E-02 1.545792E-02 1.321894E-02 9.447800E-03
7.900471E-03 6.564827E-03 4.470911E-03 0.000000E+00

MASSFRACTION-MB

0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 9.985204E-06
8.192755E-05 1.207049E-03 4.298768E-03 1.095198E-02 2.286066E-02
4.112033E-02 6.595789E-02 9.684853E-02 1.738286E-01 2.635995E-01
3.602018E-01 4.091927E-01 5.058607E-01 5.972330E-01 6.188310E-01
6.398588E-01 6.800920E-01 6.992529E-01 7.355793E-01 7.527128E-01
7.848969E-01 8.142814E-01 8.409117E-01 8.648329E-01 9.047703E-01
9.209660E-01 9.348194E-01 9.562215E-01 1.000000E+00