Advanced Spray and Combustion Modelling

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Abstract
Advanced Spray and Combustion Modelling
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The first attempt at modelling a fully Eulerian model for poly-disperse nature of the spray flow without using droplet size classes was proposed by Beck and Watkins [2003a]. The parameters used to describe the distribution of droplet sizes are the moments of the droplet size distribution function. Transport equations for only some moments of the spray distribution function are derived and solved through classical Eulerian schemes. The velocities to be used in the two transport equations are obtained by defining moment-average quantities and constructing further transport equations for the relevant moment-average velocities. The continuous distribution of droplets is approximated using an analytically integrable function to use as a number distribution was sought such that the volume distribution it produced was a reasonable approximation to a Rosin-Rammler distribution. The new form of the continuous function was later revised by Yue and Watkins [2004], who implemented the Gamma distribution whose parameters were obtained from the transport equations for second, third and fourth moments. This permits the form of the two parameter number size distribution to be totally calculated and to all predictions of changes to the distribution in space and time. Hydrodynamics submodels were implemented in Jones [2009] with higher order of numerical tools. The model is implemented in a new code based on current numerical methods detailed in Ferziger and Perić [2002], so as to make use of high resolution differencing schemes for the transportation of the moments and enable improved resolution of the solution by using an unstructured grid topology.

The thesis presents work across three different subjects of investigations into the modelling of spray development and its interaction with non-reactive and reactive flow. The first part of this research is aimed to create a new and robust family of convective scheme to capture the interface between the dispersed and the carrier phases without the need to build up the interface boundary. The selection of Weighted Average Flux (WAF) scheme is due to this scheme being designed to deal with random flux scheme which is second-order accurate in space and time. The convective flux in each cell face utilizes the WAF scheme blended with Switching Technique for Advection and Capturing of Surfaces (STACS) scheme for high resolution flux limiters. However in the next step, the high resolution scheme is blended with the scheme to provide the sharpness and boundedness of the interface by using switching strategy. The proposed scheme is tested
on capturing the spray edges in modelling hollow cone type sprays without need to reconstruct two-phase interface. A test comparison between TVD scheme and WAF scheme using the same flux limiter on convective flow on hollow cone spray is presented. Results show that the WAF scheme gives better prediction than the TVD scheme. The only way to check the accuracy of the presented models are evaluations according to physical droplets behaviour and its interaction with air. In the second part, due to the effect of evaporation the temperature profile in the released fuel vapour has been proposed. The underlying equation utilizes transported vapour mass fraction. It can be used along with the solution of heat transfer inside a sphere. After applying boundary conditions, the equation can provide a solution of existing conditions at liquid-gas interface undergoing evaporation and it is put in a form similar to well-known one-third rule equation. The resulting equation is quadratic type that gives an accurate prediction for the thermo-physical properties due to the non-linear relation between measured properties and temperature. Comparisons are made with one-third rule where both equations are implemented in simulating hollow cone spray under evaporation conditions. The results show the presumed equation performs better than one-third rule in all comparisons.

The third part of this research is about a conceptual model for turbulent spray combustion for two combustion regimes that has been proposed and tested for n-heptane solid cone spray type injected into a high-pressure, high-temperature open reactor by comparing to the available experimental data and to results obtained using two well known combustion models named the Combined Combustion Model (CCM) and the unsteady two-dimensional conditional moment closure (CMC) model. A single-zone intermittent beta-two equation turbulent model is suggested to characterise the Lumped zone. This model can handle both unburned and burned zones. Intermittency theory is used to account for the spatially non-uniform distribution of viscous dissipation. The model suggests that the Lumped zone can be identified by using the concept of Tennekes and Kuo-Corssion of isotropic turbulence that suggests that dissipative eddies are most probably formed as vortex tubes with a diameter of the order of Kolmogorov length scale and a space of the order of Taylor length scale. Due to the complexity of mixture motion in the combustion chamber, there exist coherent turbulent small scale structures containing highly dissipative vortices. The small size eddies play an important role in extinguishing a diffusion spray flame and have an effect on the combustion reaction at molecular scale because small scales turbulence increase heat transfer due to the dissipation. A common hypothesis in constructing part of the model is if the Kolmogorov length scale is larger than the turbulent flame thickness. The Lumped strategy benefits from capturing small reactive scales information.
provided by numerics to improve the modelling and understand the exact implementation of the underlying chemical hypothesis. The Lumped rate is estimated from the ratio of the turbulent diffusion to reaction flame thickness. Three different initial gas temperature test cases are implemented in simulations. Lumped spray combustion model shows a very good agreement with available experimental data concerning auto-ignition delay points.
Declaration

No portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

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Firstly, Thanks to Allah Almighty

To the oppressed broken rib and stolen right, pure martyr and honourable lady Fatima Al-Zahra daughter of the Prophet Mohammad, prayers and blessings be upon them.

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To Safa, Ali and Bashar for their real brotherhood

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Chapter 1

Introduction

1.1 Motivation

Nowadays the burning of liquid fuel has multiple applications in everyday life or in industry. Gas turbines, internal combustion engines that are used in diesel powered cars or aircraft (jet engine or rocket cryogenic propellants) and the burners in thermal power plants all use liquid fuel as sprayed droplets via injection systems at different pressure. Pollution standards levels are increasing therefore engine operations must now be clean, efficient and effective. In recent years, significant effort has been made towards renewable energy sources or clean fuels to develop new sources for producing energy. Non-combustible renewable energy sources such as wind energy, water energy or solar energy are the main and common sources one can mention. Their special characteristics which are environmental cleanliness and virtual inexhaustibility are considered as advantages but they are not suitable for producing large amounts of energy nor suitable for transport applications as well as their relative costliness to build and maintain. Since ancient times combustion of fuels has provided for the majority of our energy needs and stays the cheapest and most direct way to generate energy. Therefore combustion remains a key energy technology for the foreseeable future. There is a need to improve the performance for any technical combustion devices for economy and efficiency. To improve these new concepts should be adopted for the engine design and simulation. Before that one must understand the physical phenomena in a way that all physical phenomena are involved and particularly those that are related to phase change. Using high level technology diagnostic methods, optical methods are now capable to have an access inside the combustion chamber but till now are unable to fully realise three dimensional flow. In addition, particularly in case of dense sprays the optics have
difficulty to enter the area near the nozzle where the primary breakup, collisions, coalescence and
the initial evaporation of droplets are taking place. These observation are true specially when
experimental analyses are investigated under engine operating conditions. Therefore there is
another way to do the analyses for both physical and chemical processes with their optimisation,
i.e. numerical simulation. The numerical simulation has the ability to describe the flow inside the
combustion chamber even with three dimensional flow analyses or the upstream flow. According
to the literature three kinds of solution procedures are listed below:

1. Direct Numerical Simulation (DNS). This solution procedure simulates Navier-Stokes
equations without using any modelling. Due to this the tool is considered a very ef-
ective method for understanding physical phenomena. The effectiveness comes from the
solution based on all length and time scales generated by the flow. However, the more im-
portant requirements in this method is the discretization of the space. At most it remains
restricted applicable only to academic studies.

2. Large Eddy Simulation (LES). This technique is used to model only the large scales of the
flow. However additional effort has to be done on the modelling of smaller scales. Partic-
ularly the difficulty is appearing in the simulation specially in two-phase flow. Generally
this method remains promising because its potential depends on capturing variations by
filtering scales.

3. Reynolds Averaged Navier-Stokes (RANS). This tool benefits from the statistical methods
to solve the Navier-Stokes equations. It allows prediction only of average quantities. The
method requires a greater modelling effort. Most industrial applications use this tool
because of the low cost in comparison with accuracy.

After describing the types of numerical simulation, the main frameworks that are implemented
to model sprays droplets must be presented. Sprays are usually described by a set of partial
differential equations. Three main approaches exist for this purpose. The first is PDF approach
in which the dispersed phase is described by the joint statistical properties in which behaviours
are presented by probability functions. The second is Eulerian approach that uses the continuum
mechanism to characterise the system of two-phase flow by using Navier-Stokes equations. The
third approach is known as Lagrangian approach where the dispersed phase is treated as discrete
entities. The Lagrangian equations provide a solution over a fixed domain in terms of droplet
parcels.
The spray combustion is a very complex phenomenon as it involves the motion and the inter-
action of the dispersed phase in a discrete form of droplets and ligaments with the gas phase,
turbulent gas, heat and mass transfer and combustion. The spray atomises into different liquid
droplets and ligament sizes where the primary breakup occurs near the injector orifice. These
droplets may or may not collide with each other or coalescence, but the situation becomes more
complex when phase change has taken place. Evaporation of droplets takes place to produce
vapour that mixes with oxidizer in the ambient gas to form a combustible mixture. In the
combustion zone, ignition is releasing hot combustible gases that modify the rate of physical
change from liquid to gas phase i.e., rate of droplets evaporation. Consequently the droplets
spatial distribution and combined hydrodynamics events will be influenced. Clearly the mixing
process is an important key parameter that affects the efficiency of the energy extraction
during combustion process. In case of incomplete burning of the mixture due to insufficient
oxygen, carbon monoxide ($CO$) will be produced instead of carbon dioxide ($CO_2$), contributing
to gaseous pollutants.

In the context of meeting the future needs of improved combustion processes, computational
methods have been developed significantly to the extent of an accurate prediction of analytical
models for the hydrodynamics, turbulence and thermal processes and from the other side that
eyear detailed information leads to reduced cost of build and test. At present computational fluid
dynamics (CFD) models are capable of tackling modern combustion technology requirements.
The complex multiphase flow phenomena in combustion chambers require detailed modelling
of fluid flow, heat transfer and combustion processes. CFD models have the ability to handle
complex geometries and comprehensive description for modelling features. In order to perform
a complete simulation of spray and combustion models involves modelling a number of complex
simultaneous interdependent processes implemented into numerical tools.

1.2 Classification of multiphase flows

Spray and combustion modelling are utilized in a large number of applications. The spray is
a complex phenomenon in which dispersion of drops and interaction with each other must be
accounted for. It is therefore essential to precisely predict the behaviour of the spray within
the equipment under design or operation. The starting step is to introduce the classification of
multiphase flows and then theory of spray modelling and how the underlying statistical theory
is used in describing the spray evolution.
In a few words the definition of a multiphase flow is whenever two or more phases simultaneously occur. In general, multiphase flow can be classified into transient flows, where the phase undergoes changes from its original state to another, and dispersed flows, in which one phase is present in dispersed form carried by the other phase. Dispersed two-phase flows are the majority of the current contribution Sommerfeld [2000]. In applications of gas-liquid flow, the volume fraction of the dispersed phase is the volume occupied by the particles per unit volume. The volume fraction can be estimated as

$$\Theta = \frac{\sum N_i V_i}{V}$$  \hspace{1cm} (1.1)

where $N_i$ is the number of particles of size $V_i$ and $V_i$ and $V$ are the particle volume and the total volume, respectively. The volume fraction of the continuous phase is commonly called void fraction. Hence the sum of the volume fraction of the dispersed and continuous phase is unity and then can be easily calculated from

$$\text{Void} = 1 - \Theta$$  \hspace{1cm} (1.2)

Considering phase interactions (coupling) is the basis to classify dispersed two-phase flows into different classes depending primarily on particle volume fraction where coupling necessitates correct modelling. When particle volume fraction is less than $10^{-6}$, the carrier phase is the dominating influence on the particles movement, this is known as one-way coupling. There is a mutual influence between the two phases when the particle volume fraction is in the range from $10^{-6}$ to $10^{-3}$, this regime is called diluted where the effect of turbulence created by particles on the fluid flow should be taken into account, which is often referred to as two-way coupling. A dense regime is characterised when particles are influenced by neighbouring particles behaviour, for example, drag, collision and breakup and has particle volume fraction higher than $10^{-3}$, this is known as four-way coupling.

1.3 Theory of spray

Sprays belong to an important constituent type of two-phase flows involving both natural and artificial dynamic interactions for liquid phase in a discrete form of ligaments and droplets with gas phase as the continuum. The aim of this paragraph is to cover the main concept of spray and how it is described by using statistical techniques. At first glance, the spray definition is a cloud of droplets forming from a liquid when the interface between a liquid and a gas becomes
deformed and droplets of liquid are created and migrated out into the body of the gas. As mentioned, the aim is to give an insight to the resulting droplets cloud which is spread over a wide range of droplet size. Several theoretical approaches for the distribution of droplet sizes in liquid sprays have been proposed based on statistical approaches and measuring probability density function over the droplet diameters. In spray applications droplets vary in diameter as a result of different processes such as atomisation, breakup, collision and evaporation processes taking place during the spray development. Due to this, it is important to estimate the droplet size distribution. Therefore, a presumed shape of a number of mathematical functions has been proposed. These use either probability or empirical considerations, which coincide with the mathematical representation of the measured droplet size distributions. A complete description for the supposed shape of the distribution function is presented and discussed in chapter two. The method of using moments of drop size distribution to model sprays was first introduced by Beck and Watkins [2002]. In this model, transport equations are written for two moments that represent the liquid volume and surface area. The velocities that are employed in order to convect these moments are obtained by solving separate momentum equations for each. The other two moments are representing total drop radii and droplets number, are approximated from a presumed drop number size distribution, which is allowed to vary in space and time, but which requires truncation at either the small drop size or large drop size end of the distribution, in order to match the local value of the Sauter mean radius calculated from dividing volume over surface area. The transport equations for both liquid and gaseous phases are written in Eulerian form, and coupled through source terms. These equations are solved using the finite volume approach.

1.4 Need for Closure

Yue and Watkins [2004] presented a method designed to remove, as much as is possible, the need to presume a particle distribution for drop sizes. This was done by developing transport equation for $Q_1$ and $Q_0$ and their respective momentum equations to obtain values of $U_{L1}$ and $U_{L0}$. Thus the liquid phase was represented by four moment transport equations and four sets of momentum equations. Although the need to prescribe a size of distribution was much reduced in this model over that of its predecessor, there were still three places in the model where such a distribution was required. These are:

1. The determination of inlet moments below the surface area averaged moment.
2. Truncated moments affected by primary or secondary breakup, droplet collisions and evaporation in case of reactive flow need to be prescribed.

3. The drag model requires moments which are two orders lower than the moment averaged momentum equation to which the drag term is associated. This means that lower order moments need to be evaluated.

Different distributions can be applied for these three effects. Yue and Watkins [2004] assumed a general gamma distribution. The form of the distribution changes due to convective and drop breakup, collision and evaporation effects. Although the full model was presented, the calculations did not include break-up or collision due to numerical instability. The gamma distribution is a two-parameter distribution. The method of Yue and Watkins over-prescribed the problem by evaluating three independent parameters, based on the ratios of $Q_3/Q_2$, $Q_2/Q_1$ and $Q_1/Q_0$. Watkins [2005] presented the outlines of a refined version of this model, which dispensed with the need to evaluate $Q_0$ from a transport equation. Instead it could be calculated from the derived gamma distribution. This had the added benefit that only moments down to $Q_{-1}$ were required. This enhanced the numerical stability of the method.

1.5 Project contributions

Higher-order techniques were implemented by Jones [2009] to develop the holistic continuous Eulerian spray model proposed by Beck and Watkins [2003a] and to minimize the occurrence of unphysical solutions. The general methodology is developed in Jones and Watkins [2008] to simulate injection and wall impaction, and the evaporation and heat transfer models in Beck and Watkins [2003b]. Although the above referenced works are successful, they did not handle certain important aspects of the model, leaving it in a state where further implementation into a standard CFD algorithm or theoretical perspective on work was required. The aim of this work is the continued research and development of higher-order methods and advanced models so as to be able to investigate both physical and chemical interacting spray droplets with the surrounding medium in different spray applications. The developed numerical techniques or models are implemented and validated with the available experimental data and existing tools. The problems that were either not addressed or inadequately dealt with previously are proposed and their solutions are the contributions of the present work. These can be summarized as follows:
1. A new higher order convection discretization scheme has been proposed to simulate non-reactive hollow cone type sprays. The latter can be considered a complex structure because the spray sheet is very thin consisting of inner and outer edges which need an accurate scheme to be modelled due to different interactions with the gas phase inside and outside the spray cone. A good candidate to construct a new convection scheme to be used as a platform for simulating the spray thin sheet thickness is developed here. The versatility of the scheme is demonstrated by the fact that it can be implemented for both moment and also momentum transport equations. This is considered a valuable benefit of the scheme. The new scheme does not need any treatment for grid interface which reduces the occurrence of unphysical solutions in contrast to the proposed work of Jones [2009] who constructed a two-phase interface convection scheme.

2. Predictions of all two-phase evaporation models depend on the thermodynamic properties at the liquid vapour interface. In addition the non-linear relationship between thermodynamic properties and temperature according to the unsteady heat equation needs to be taken into consideration. The existing one-third rule is a linear relation and this is replaced by a quadratic relation based on transported scalar variables proportional mainly to the local mass transfer rate. The relation works successfully again with hollow cone type spray. The proposed equation is derived from heat transfer principles which considers the case similar to the heat transfer from a sphere. This precisely matches the reduction in volume of a single droplet. The resulting Eulerian-Eulerian framework for evaporating turbulent spray has been extended and added to the code. It is set in terms of the theoretical methodology followed here of calculating the moments of drop size distribution proposed by Watkins [2007]. There are consistencies in both heat and mass transfer sub-models and the method is verified through validation the sub-models with experimental tests. Special attention is given to the hollow cone spray treatments.

3. The last contribution is the development of a combustion model to cover all spray combustion regimes. The mathematical relations and numerical treatments are consistent with definition of combustion regimes in the presence of droplets. The model is converted from a model used for LES approach to a model using RANS models. The previous combustion models were unable to combine between mixing and chemical reaction models. The main object of the model is to overcome the modelling error that occurs due to the incorrect prediction for the reaction rate which creates a strain regime. In order to eliminate such
as region, the model enhances the mixing process after capturing the regime. The mixing process is modelled by calculating transported mixture fraction and the turbulent reaction process through identifying two concepts for diffusion and reaction flame thickness. This is in addition to the main reason for using such a model which is the thickening of the region. The new model has been implemented in the code. The structure and features of the model are discussed in detail in chapter six.
Chapter 2

Modelling approach

2.1 Introduction

This chapter is organised as follows. Firstly, to account for the interaction between two-phase flow for both non-reactive and reactive cases, several numerical methods have to be implemented for solving the two-phase flow system. Firstly three methods are widely used to simulate the dispersed multiphase flow. In the Eulerian-Lagrangian approach the liquid phase is represented by numbers of physical droplets averaging their characteristics in terms of parcels of identical droplets, whereas in the Eulerian-Eulerian approach, the liquid and the gas phases are considered to be continuous functions in space and time and the flow variables at any point are obtained by taking the average over the computational domain. That means droplets can be represented by generalized functions (distribution) in which the effects on droplets of all sizes are considered. The probability density function is the third approach in which the liquid phase properties are joined with the gas phase properties statistically. Secondly, moment values are required at the inlet; the treatment of the spray injection is based on the injection cell treatment and boundary conditions are specified and techniques for numerical implementation are explained. Finally, the Eulerian-Eulerian approach to writing transport equations to model both phases is detailed with the poly-disperse liquid sprays undergoing droplet changes and through describing the fundamentals of moments equations in terms of the probability density function for liquid phase representing the sprays.
2.2 Theoretical perspective

2.2.1 Modelling approaches

Sprays enter in different applications in several fields according to its use in for example power generation and transportation. Concerning the physical model for liquid fuel sprays, modelling relating to the two-phase flow nature is believed to constitute an important field. Many researchers, years ago made their work and exhibited wide range of investigation for physical phenomena under the main field named as spray modelling. Approaches have been used to predict the flow properties in different situations where the liquid phase as considered as sprays is injected in a gas field. These fall into three general categories.

The first approach is Eulerian-Lagrangian (EL) where the sprays are represented by parcels of droplets (Lagrangian model) coupled with gas phase which is treated as a continuum (Eulerian model). Dukowicz [1980] employed (EL) for diesel engine spray due to computing the behaviour of atomised non-evaporating liquid spray injected into a gaseous environment. Mostafa and Mongia [1987] have reported that both Eulerian and Lagrangian approaches are capable of predicting the main features of turbulent evaporating spray. Moreover, the motion of individual fuel droplets in the steady two-phase turbulent combustion are treated as they vaporised within the combustor, for example Tolpadi [1995] adopted it to calculate the flow properties in an aircraft engine combustor and Zamuner et al. [2002] inside an industrial tubular burner. Schmehl and Wittig [1999] have tracked the same procedure to simulate complex two-phase flows in gas turbines. The gas phase and the wall film are described by Eulerian equations whereas sprays dispersion and evaporation are modelled by using Lagrangian models. The exchanging source terms in both phases are used for coupling to model the interaction in the flow simulations.

The second approach is known as the Eulerian-Eulerian approach where the analogy to the continuum approach of single phase flow is considered for both phases. Here, the spray is treated as an interacting and interpenetrating continuum. Therefore, each phase can be described by a set of transport equations for mass, momentum and energy where the interphase exchange source terms are included. From this point, the computational method used allows both phases to be discretized using the same method. Klose and Zarzalis [2001] solved two-phase equations by using Eulerian-Eulerian framework combined with combustion models and showed the solution is numerically stable for the behaviour of the aero engine combustor. A comprehensive numerical model for spray combustion has been reported by Guo et al. [2002] who applied an Eulerian model to extend the simulation to include most of sub-models inside an axisymmetric sudden expansion.
combustor. Furthermore due to interesting results obtained from testing spray combustion in gas turbine combustor Boileau et al. [2008] showed that the Euler-Euler model performed well when it was used for the liquid phase and coupled with LES (large eddy simulation) solver for the gas phase. In addition, several researchers made their work based on this approach, Beck and Watkins [2003b], Watkins [2007] and Moukalled and Darwish [2008] applied Eulerian models to different sprays whereas Jay et al. [2006] employed this model to simulate a jet flame formed by coaxial injection for cryogenic liquid.

Lastly, the third method employs the probability density function, in which the spray is represented by the drop distribution function \( f(x, v, r, t) \), where \( f \) is the expected number of spray droplets in position-velocity-radius-time space. Jones and Sheen [1999] applied this approach to evaluate an equation for the joint PDF to describe the liquid fuel sprays properties in terms of droplet radius, number density velocity and temperature for modelling turbulent dispersion of liquid sprays.

### 2.2.2 Spray moment theory

This section is focused on the work of Beck and Watkins [2002] and Beck and Watkins [2003a] who proposed that statistical properties of sprays be used to describe the liquid and gas phases in an Eulerian-Eulerian approach. The main concept for this model is the possibility of describing a poly-disperse spray by using moments of a drop number size distribution function. The very large amount of calculations required due to the very large number of individual drop trajectories to be calculated or to divide the spray into a number of drop sizes, in order to solve a poly-disperse spray, is replaced by the statistical moments in terms of drop size distribution function which can be written in an Eulerian transport equation. They introduced \( n(r) \) as a multiple of the probability density function. When this function is integrated over all droplets, locally the total number of droplets per unit volume is obtained from

\[
Q_0 = \int_0^\infty n(r)dr \tag{2.1}
\]

The \( ith \) moment of the distribution is given as

\[
Q_i = \int_0^\infty r^i n(r)dr \tag{2.2}
\]
In their model they presented transport equations written in terms of $Q_3$, the liquid volume moment and $Q_2$, the liquid surface area moment only, along with their respective moment average momentum equations. Other required moments such as $Q_1$ and $Q_0$ can be estimated from the presumed size distribution function. The fourth moment is related to the liquid volume fraction via the following relation

$$\frac{V_{\text{liquid}}}{V_{\text{liquid}} + V_{\text{gas}}} = \frac{4\pi}{3} Q_3 = 1 - \text{Void}$$

where $\text{Void}$ is the gas volume fraction. In addition, they assumed all drops locally have the same liquid density, thus this parameter above evaluates the mass of liquid per unit volume. This means that the transport equation for the fourth moment is equivalent to a liquid phase continuity equation. Simply, the third moment defines the local value of the total drops surface area $4\pi Q_2$. Later Yue and Watkins [2004] extended the model to evaluate the first four moments from transport equations, so permitting the size distribution function to be determined from the value of the moments. An interesting model has here presented by Watkins [2005] who showed the outline of refined version of this model in which $Q_0$ can be calculated from the distribution function instead of the transport equation, with $Q_1$, $Q_2$ and $Q_3$ being calculated from the latter.

**Turbulence model**

In many applications, the relative motion due to the interaction of a spray with surrounding gas leads to deceleration, deformation and breakup. In addition to these dispersion or diffusion of drops occurs attributable to turbulent flow. In support of two-way coupling, this model is widely investigated and formulated in order to evaluate the source terms in both the average gas phase equation and the conservation laws for liquid phase. Predominantly, these source terms depend on the liquid state and the gas phase conditions. Launder and Spalding [1974] described a mathematical model for the turbulence model used for modelling the gas phase. Guo et al. [2002] implemented the model in the Eulerian-Eulerian models to simulate steady-state dilute spray combustion in a combustor. The transport equations of the gas phase of the turbulent kinetic energy and its dissipation rate contain source terms. The production term is expressed as

$$G_k = \mu_t \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \frac{\partial v_i}{\partial x_j}$$

(2.4)
where $\mu_t$ is the gas phase turbulence viscosity given by

$$\mu_t = C_{\mu} \rho k^2 \frac{k^2}{\epsilon} \quad (2.5)$$

and the gas phase effective viscosity equal to

$$\mu_c = \mu_t + \mu \quad (2.6)$$

The interaction of the gas phase with liquid phase are expressed by two source terms named as

$$G_p = \sum_k \frac{2\rho_k}{\tau_k} \left( C_p \sqrt{kk} - k \right) \quad (2.7)$$

where the subscript $k$ represents here the $k$-group of droplets phase. The above term caused a reduction in the gas phase turbulent kinetic energy when the latter is larger than the liquid phase turbulent kinetic energy. On the other hand, when the liquid phase is larger than that of the gas phase, the term gives increase in the production of gas phase turbulent kinetic energy. The change in spray droplets mass presented as the second term

$$G_R = -k \sum_k n_k \dot{m}_k \quad (2.8)$$

where $n$ is the droplet phase number density and $\dot{m}$ is the mass of spray droplets. When $\dot{m}$ is negative, $G_R$ is the production term for the gas phase turbulent kinetic energy. The work of Ma and Wang [1993] used the two-equation model with a modification through an assumption that turbulence kinetic energy is produced only by gas phase and the spray droplets share it. Thus, the dissipation energy equation remains invariant and the $k$-equation has been changed to cover the assumption. The turbulence kinetic energy is set in the diffusion term related to two parameters, the first parameter represents the flux flow and the second is related to the turbulent kinetic energy defined as the ratio in terms of droplet turbulent Schmidt number to its gas counterpart. The general form of the transport equation for a RANS model was implemented by Sadiki et al. [2005] to describe the turbulent gas phase tested on a configuration to study the effects of turbulence properties on droplets dispersion, vaporisation and mixing of non-reacting spray. The differential equation takes the general form of the transport equation. The right hand side of the equation are the source terms for phase exchange and phase transition, where they are referred to:
1. The turbulence source term due to monophasic flows.

2. The source term due to interphase transport without phase transition and represents the
two-way coupling when there is no evaporation and combustion processes.

3. The source term as a result of considering the transfer caused by the phase transition
processes.

Starting from the multiphase Navier-Stokes equations Beishuizen et al. [2007] derived a modified
Reynolds stress model for dispersed two-phase flows in which the pressure of strain due to the
presence of dispersed flow is taken into account. Two source terms were added to the model to
characterise the flow due to the two-way coupling.

2.3 Eulerian-Eulerian approach

The common treatments for modelling spray combustion fall under three kinds depending on
how the inter-phase transport rate is treated. The locally homogeneous flow model is the first
model which is based on the inter-transport rates assumed to be infinitely fast and the droplet
phase and gas phase assumed to be in kinetic and thermodynamic equilibrium at each point in
the flow, which means that there are no slip velocity and temperature differences between the
droplet and the gas phase, so can be considered as a single phase. The second procedure is the
deterministic separated flow model which solves the droplet temperature and velocity along the
droplet trajectory and the droplet trajectory is time dependent and the effect of droplet phase on
the turbulent gas phase is ignored. The third model is known as stochastic separated flow model
in which both the inter-phase transport rates and the effect of turbulence interaction between
the phases are taken into account. To capture these effects the Eulerian-Eulerian approach is
used, in which both gas phase and liquid phase are treated as a continuum in which the latter
phase, by analogy with single phase flow, is solved by a set of transport equations. This approach
allows both liquid and gas phase to be discretized by the same procedure. This leads to the
numerical solution being easier and efficient, since the computation effort is less because the
number of equations being solved is fewer than any other model.
2.4 Spray modelling

In this work the spray model is based on the work of Beck and Watkins [2003a] who used statistical properties of sprays to describe the liquid phase without segregation of droplets into parcels of equal radius as employed in other Eulerian methods. The main concept of this model is to use the moments of drop size distribution to describe a poly-disperse spray. It is worth noting at this point that only Eulerian transport equations for the moments and their momentum need to be solved instead of the massive amount of calculations due to dividing the spray into size classes and solving transport equations for each size class.

2.4.1 Constructing moments

In the previous section was illustrated the relationship between the assumed continuous distribution and droplet size. Before starting describing the proposed method in more details, it is worthwhile first to consider moments theory. The objective reason is to provide a useful summary. The correct presentation for the first four moments can assess the theory in which their direct relationship (i.e., moments) with the geometrical calculation for the sprays carrier. One convenient method is considered here which defines \( n(r) \) as a multiple of the probability density function of drop radius, such that the integral over all drops provides the total number of drops per unit total volume of gas and liquid. This is designated by \( Q_0 \). The \( ith \) moment of the distribution can be written as expressed in equation (2.1). With an assumption that the drops are approximately spherical. The moment \( Q_1 \) represents the total sum of drop radii per unit total volume, the surface area of the drops per unit total volume is \( 4\pi Q_2 \), and the liquid volume per unit total volume, i.e. the fractional volume of liquid \( \Theta \), is given in terms of \( Q_3 \) and the void fraction \( Void \), given by equation (2.3).

The first four moments contain a great deal of information about the spray. Beck and Watkins [2003a] use these parameters to build a fully polydisperse spray model without the need to separate the drops into size classes. Perhaps the most important of the first four moments is \( Q_3 \), as assuming all drops locally have the same liquid density, this parameter defines the mass of liquid present per unit volume. Thus the transport equation for \( Q_3 \) is equivalent to a liquid phase continuity or mass conservation equation. In the model presented here, the three moments \( Q_1, Q_2 \) and \( Q_3 \) are evaluated by means of transport equations.
2.4.2 Normalization and limits

For some closure methods, the moments require normalizing. There are several ways to normalize moments which prove useful in scaling the problem. Jones [2009] implemented this either to ensure the distribution is between certain limits such as the interval of 0 to 1, or more generally, to reduce the numerical difference between moments. In either case, a normalizing length scale is required. Using the ratio of any pair of successive moments a normalization radius \( r_n \) can be defined,

\[
r_n = \frac{Q_{i+1}}{Q_i}.
\]

(2.9)

Jones [2009] showed this radius can then be used to provide a sensible range in which the upper limit lies. From numerical tests, the upper limit can be assumed to lie in the range \( r_n < r_u < 3.5 r_n \) (for \( i = 2 \)) and the lower limit, \( r_l \), set to zero. In a couple of the methods presented where the limits are required John et al. [2007] and Talenti [1987], accuracy of the estimated interval significantly affects the accuracy of the resulting distribution. To obtain accurate limits (only the upper limit is corrected), an iterative procedure is required. Upon establishing a normalizing length scale, \( r_n \), and before the closure method is called, linear normalization of the moments is performed by substitution of \( x = \frac{r}{r_n} \) into equation (2.1), giving

\[
\frac{Q_i}{Q_0 r_n^{i+1}} = \int_{r_n x} \phi(r_n x) x^i \, dx
\]

(2.10)

2.4.3 Gamma distribution

The drop size distribution in a dispersed phase is different from the starting distribution due to many changes may occur. In general, concentration of drops having a certain volume is used to describe the presumed distribution. There are a number of continuous distributions which could be assumed to represent the underlying probability density function, such as the log-normal, gamma, beta and the Rayleigh distributions.

Considering the continuous variations in drop sizes, the method used for obtaining droplet size distribution is the general gamma number size distribution. The gamma distribution is defined as

\[
n(r) = \frac{r^{k-1} \exp \left( -\frac{r}{\theta} \right)}{\Gamma(k) \theta^k},
\]

(2.11)

where

\[
\Gamma(k) \theta^k = 1
\]

(2.12)
by definition. Combining equation (2.11) and equation (2.1) gives

$$\frac{\Gamma(k)\theta^kQ_j}{Q_0} = \int_0^\infty r^{k-1+j} \exp\left(-\frac{r}{\theta}\right) \, dr$$

$$= \left[ -\theta r^{k-1+j} \exp\left(-\frac{r}{\theta}\right) \right]_0^\infty + \theta(k-1+j) \int_0^\infty r^{k-2+j} \exp\left(-\frac{r}{\theta}\right) \, dr$$

$$= \frac{\theta(k-1+1)Q_{j-1}}{Q_0}, \quad (2.13)$$

which simplifies to

$$\frac{Q_{j+1}}{Q_j} = \theta(k+j). \quad (2.14)$$

From equation (2.14), the parameters can be related to three consecutive moments by

$$k = \frac{j \left(1 + \frac{Q_{j+2}}{Q_{j+1}} \frac{Q_j}{Q_{j+1}} - 1\right)}{\frac{Q_{j+2}}{Q_{j+1}} - 1} \quad (2.15)$$

$$\theta = \frac{Q_{j+1}}{Q_j(k+j)}. \quad (2.16)$$

To ensure the denominator of the above equation remains unconditionally positive, limits are set on parameter $k$ such that $1.5 < k < 20$. Truncated or partial moments of the gamma distribution can be calculated by

$$Q_\alpha|_{r_1} = Q_0 \theta^\alpha \frac{\Gamma(k+\alpha)}{\Gamma(k)} \left[ \gamma\left(k+\alpha, \frac{r_{\alpha}}{\theta}\right) - \gamma\left(k+\alpha, \frac{r_j}{\theta}\right) \right], \quad (2.17)$$

where $\gamma(k, x)$ is the lower incomplete gamma function.

### 2.4.4 Moment-average value

When transport equations for the droplet moments need to be written in the form of Eulerian framework, the velocity at which the moments are to be convected must be defined. In general, the drops are travelling at a variety of different velocities. Logically the net convection of volume would occur at the volume-average velocity, and the net convection of drop surface area (say) would occur at the surface-area-average velocity and these two values are expected to be different. Larger drops experience relatively less drag compared to their momentum than smaller ones and generally have higher velocities than the smaller drops and this is reflected by the volume-average velocity being higher than the surface-area-average velocity. Hence these moment-average velocities convect the moments such that they are not all convected at the
same rate. The result of this is that the moments provide a representation of the distribution of drop sizes at each point, and the moment-average velocities providing the means by which the distribution of drop sizes can change in time and space, even in the absence of effects such as drop break-up, collisions and evaporation. The two concepts together provide a picture of the behaviour of a poly-disperse spray. The moment-average, $\Psi_i$, of a quantity averaged over the $ith$ moment is defined as

$$\Psi_i = \frac{\int_0^\infty r^n n(r) r^i \psi(r) \, dr}{\int_0^\infty r^n n(r) r^i \, dr}$$

$$= \frac{Q_0}{Q_i} \int_0^\infty n(r) r^i \psi(r) \, dr$$

\hspace{1cm} (2.18)

\hspace{1cm} (2.19)

2.4.5 Stabilized closure

Woodbury [2004] makes use of the observation by Tagliani [2001] above, to aid the solution of the underlying distribution from the knowledge of the moments by defining the distribution, $n(r)$ to be the product of a known approximation to $n(r)$ and a second distribution, to be determined, i.e.

$$n(r) \approx p(r) n(r)^*$$

\hspace{1cm} (2.20)

where $p(r)$ is the known approximation. The role of $p(r)$ is very much analogous to the role of a preconditioning matrix in solving a system of linear equations: if $p(r) = 1$, the initial problem is recovered and so is of no benefit, but if $p(r)$ takes on a useful form, for example, a Gaussian distribution, the convergence of $n(r)^*$ is stabilized and accelerated.

2.4.6 Droplet velocity profile

Two general forms for approximating the droplet velocity profile were proposed by Jones [2009]. The first profile (equation (2.21)) assumes that for small droplets, their velocity, $\vec{v}_d$, increases rapidly from the surrounding gas velocity, $\vec{v}$, with increasing droplet radius and for large droplets, velocity increases slowly (for $0 < b < 1$).

$$\vec{v}_d(r) = \vec{v} + a_1 r^b$$

\hspace{1cm} (2.21)
The coefficient, $\tilde{a}_1$, is determined by substituting equation (2.21) into equation (2.19), giving

$$\tilde{a}_1 = (\tilde{V}_{d,i} - \tilde{v}) \frac{Q_i}{Q_{i+b}}$$

(2.22)

where $\tilde{V}_{d,i}$ is the $i^{th}$ moment averaged velocity. The second method is to not take into account the surrounding gas velocity, but make use of all the available moment averaged velocities to obtain a functional form for the droplet velocity variation. The simplest form is to consider an $N^{th}$ degree polynomial, where there are $N + 1$ moment averaged velocities available. This is certainly not the best form (potentially forming an ill-conditioned problem for high order polynomials), but serves as a starting point for forming non-linear functions from a complete set of moment-averaged data.

$$\tilde{v}_d(r) = \sum_{j=0}^{N} \tilde{a}_j r^j$$

(2.23)

Substituting equation (2.23) into equation (2.19) results in a system of linear equations for solving the unknown coefficients, $\tilde{a}_j$. A variation on this method is to define the constant, $a_0$, as a function of the continuum phase velocity and the lowest available moment averaged velocity, such as

$$\tilde{a}_0 = \lambda \tilde{v} + (1 - \lambda) \tilde{V}_{d,0}$$

(2.24)

where $0 < \lambda < 1$ and change the summation in equation (2.23) to $j = 1, \ldots N + 1$. Coefficients of equation (2.24) are solved in a similar manner as above.

### 2.4.7 Transport equations

The moment averaged quantity that is the subject of a transport equation could be any related spray variable. Following Beck and Watkins [2003a] in their approach, they consider an equation for a droplet group $k$ with similar properties to be solved in a multi-size Eulerian treatment. After averaging across all group sizes (by integration) the moment equations ($i = 1, 2 \text{ and } 3$) can be compactly represented by the conservation of moments is analogous to the mass conservation (per unit volume) of the continuum phase.

The derivation of the moment and moment-averaged momentum conservation equations for the spray model begins from the Lagrangian definition of the total derivative of a droplet property with respect to time. The derivative of a fluid particle (droplet) property, $\phi$, per unit volume with respect to time which is travelling at velocity $u_d$ and has a density $\rho_d$ is defined as written
\[ \rho_d \frac{D}{Dt} (\phi) = \rho_d \left( \frac{\partial}{\partial t} (\phi) + \vec{v}_d \cdot \text{grad} \phi \right) \]  

(2.25)

This represents the change of the droplet property as it is being followed along its pathline. However, in the context of the spray model, the quantities being transported will be integral quantities, i.e. the moments are integrals of the droplet size distribution within a given region and are used to represent averaged quantities, such as the local SMR, which indicates that equation (2.26) would be better represented in an Eulerian manner. The relationship between equation (2.26) and the equivalent Eulerian description as stated in Versteeg and Malalasekera [2006] is

\[ \rho_d \left( \frac{\partial}{\partial t} (\phi) + \vec{v}_d \cdot \text{grad} \phi \right) = \frac{\partial}{\partial t} (\rho_d \phi) + \text{div} (\rho_d \vec{v}_d \phi) - \phi \left( \frac{\partial}{\partial t} (\rho_d) + \text{div} (\rho_d \vec{v}_d) \right) \]  

(2.26)

The important difference between the continuum phase transport equations and the discrete phase transport equation is that the last term in equation (2.26) is retained for the discrete phase when the Eulerian transport equation is cast, as in

\[ \frac{\partial}{\partial t} (\rho_d \phi) + \text{div} (\rho_d \vec{v}_d \phi) - \phi \left( \frac{\partial}{\partial t} (\rho_d) + \text{div} (\rho_d \vec{v}_d) \right) = \rho_d \frac{D}{Dt} (\phi) \]  

(2.27)

Casting the above equation into the generalised form for a transported property and applying Guass theorem, the template transport equation becomes (with the inclusion of source terms)

\[ \frac{\partial}{\partial t} \int_{\Omega} \rho_d \phi d\Omega + \int_S \rho_d [\vec{V}_{d,i} \cdot \vec{n}] \phi dS - \phi \left( \frac{\partial}{\partial t} \int_{\Omega} \rho_d d\Omega + \int_S \rho_d [\vec{V}_{d,i} \cdot \vec{n}] dS \right) = \int_{\Omega} q_\phi d\Omega \]  

(2.28)

where \( q_\phi \) represents any additional contributions to the rate of change of the transported property. In order to arrive at the governing equations of the spray modelling, the equations for the \( i \)th moment of the distribution (equation (2.2)) and a moment-averaged property (equation (2.19)) are introduced to equation (2.28), forming two conservation equations: when \( \phi \) represents a moment of the probability density function.
Moment

At this stage, the moment averaged properties can be brought in to the transport equation definition. The moments and their moment-averaged momentum must be conserved. These conservation equations are expressed in terms of moment-averaged quantities and are written in integral form by making use of Gauss’ divergence theorem. Substitution equation (2.19) the moment-averaged velocity instead of \( \vec{v}_d \) and \( \phi \) with the transported moment, \( Q_i \) in equation (2.28), the general moment equation becomes

\[
\frac{\partial}{\partial t} \int_{\Omega} \left\{ Q_0 \int_r n(r)r^i dr \right\} d\Omega + \int_S \left\{ \left( \frac{Q_0}{Q_i} \int_r n(r)r^i \vec{v}_d(r) dr \right) \cdot \vec{n} \right\} \left\{ Q_0 \int_r n(r)r^i dr \right\} dS = \int_{\Omega} \left\{ Q_0 \int_r n(r)r^i q_i(r) dr \right\} d\Omega \quad (2.29)
\]

The resulting transport equation, upon integration over all droplets, represents the conservation of moments. The moments represent quantity (per unit volume) and those moments are convected by their moment-averaged velocity.

\[
\frac{\partial}{\partial t} \int_{\Omega} Q_i d\Omega + \int_S [\vec{V}_{d,i} \cdot \vec{n}] Q_i dS = \int_{\Omega} q_{Q_i} d\Omega \quad (2.30)
\]

In above equation, the source terms represent the effects on the moments of drop drag, break-up, drop collisions and evaporation. Later, in order to evaluate the various source terms due to the sub-models knowledge of the underlying number size distribution \( n(r) \) is required. In this work the general gamma distributions are to be assumed to characterise the drop size distribution.

Momentum

The moment-averaged momentum transport equation (equation (2.31)) has its respective moments as coefficients in the temporal and convection terms. Since a given set of moments represent a single distribution, the entire set of moments must be present to represent droplets in a given region.

\[
\frac{\partial}{\partial t} \int_{\Omega} Q_i \vec{V}_{d,i} d\Omega + \int_S Q_i [\vec{V}_{d,i} \cdot \vec{n}] \vec{V}_{d,i} dS
\]

\[
- \vec{V}_{d,i} \left( \frac{\partial}{\partial t} \int_{\Omega} Q_i d\Omega + \int_S [\vec{V}_{d,i} \cdot \vec{n}] Q_i dS \right) = \int_{\Omega} q_{\vec{V}_{d,i}} d\Omega \quad (2.31)
\]
Energy

The liquid phase energy equation is more simply derived as the temperature of the droplets in a region of space that is, in the present version of the model, considered to be independent of the droplet radius. The equation is written as

\[
\frac{\partial}{\partial t} \int_{\Omega} Q_i E_{d,i} \, d\Omega + \int_{S} Q_i [\vec{V}_{d,i} \cdot \vec{n}] E_{d,i} \, dS + E_{d,i} q_{E_i} - \frac{\partial}{\partial x} \left( \int_{S} [\Gamma_{grad} E_{d,i} \cdot \vec{n}] Q_i \, dS \right) = \int_{\Omega} q_{E_{d,i}} \, d\Omega \tag{2.32}
\]

where \( q_{E_{d,i}} \) is the source term of energy transport. All the source terms relevant with the transport equations will be derived and discussed in separate sections in chapter four and five.

2.5 Injection conditions

2.5.1 Injector

The approach used in this methodology is to resolve the actual size of the nozzle orifice (Figure 2.1), rather than projecting a larger equivalent orifice in front of the injector Beck [2000]. The actual injector is represented computationally by the overall shape of the injector tip (Figure 2.2). The modelled nozzle orifice is protruded in order to clarify its size.

2.5.2 Injected moments

Moments of the injected droplet size distribution are based on the gamma distribution Yue and Watkins [2004]. Specifying three parameters: the liquid volume fraction, \( \Theta \), Sauter Mean Radius, \( r_{32} \) and the skewness parameter, \( k \), the first two moments \( Q_3 \) and \( Q_2 \) are found by

\[
Q_3 = \frac{\Theta}{\frac{4}{3}\pi} \tag{2.33}
\]

\[
Q_2 = \frac{Q_3}{r_{32}} \tag{2.34}
\]

and all other moments are determined recursively using the relation

\[
\frac{Q_{i+1}}{Q_i} = r_{32} \frac{k + i}{k + 2} \tag{2.35}
\]
The three parameters are related to the nozzle orifice radius, the injector operating conditions and how the nozzle orifice is modelled. Since the nozzle orifice is resolved, the exiting liquid volume fraction will be high (0.9 – 1). The exiting bulk liquid is assumed to have been broken up into droplets, so the Sauter Mean Radius is approximated to be in the range 0.05\( r_{orif} \) – 0.15\( r_{orif} \).

Finally, because only break-up of bulk liquid has taken place, the relative number of smaller droplets (than the mean) will be low, implying that the distribution will only have a weak positive skew, leading to a range of 3 – 7 for parameter \( k \) (Figure 2.3).

### 2.5.3 Injection velocity

From the ambient pressure and the operating pressure of the injector, the average speed of the exiting liquid and entrained gas can be approximated by

\[
U = C_d \sqrt{\frac{2(P_{inj} - P_{amb})}{\rho_d}}
\]  \hspace{1cm} (2.36)

where the discharge coefficient, \( C_d \), is approximately 0.7. The spray half-cone angle is then used to obtain the orifice outermost velocity. The variation of velocity towards the axis is controlled by the appropriate radial profile.

### 2.5.4 Radial profiles

To reasonably approximate the behaviour of the exiting spray, the nozzle orifice face is discretized into a number of faces (typically 2 - 5), allowing the injector conditions to be varied radially (Figure 2.4). Radial profiles are used for both the moments and the velocity (Figure 2.5). These profiles enable the representation of the higher concentration of the liquid towards the outer edge of the orifice (Figure 2.5(a)) due to swirl and the spread of the spray defined by the half-cone angle, applied to the velocity (Figure 2.5(b)). The functions are defined as

\[
p_1(r) = \left( \frac{1}{r_{orif}} \right)^{\beta_1} \hspace{1cm} (2.37)
\]

\[
p_2(r) = \left( \frac{1}{r_{orif}} \right)^{\beta_2} \hspace{1cm} (2.38)
\]

where \( \beta_2 < \beta_1 < 1 \). Currently \( \beta_1 \) is set as 0.7 and \( \beta_2 \) as 0.3.
2.5.5 Discharge profiles

Two profiles are used to govern the discharge of the liquid from the injector (Figure 2.6), where \( t_1 - t_0 \) is the injection duration. The first profile (Figure 2.6(a)) controls the quantity discharged, and the second profile (Figure 2.6(b)) controls the rate of discharge. The rate of discharge profile, \( p_2(t) \), extends beyond the liquid discharge profile, \( p_1(t) \), to represent the pressure potential remaining constant throughout the duration of the discharge.

2.6 Two-phase closure

2.6.1 Liquid phase

For computational efficiency, an entirely Eulerian framework proposed by Beck and Watkins [2003a] treats a two-phase medium as a single continuum. Therefore, to compute the properties of the liquid phase an Eulerian approach has been used. The crucial thing in using this model is to consider that the spray (the liquid phase) behaves as a fluid interacting with the gas phase. In this work and to cover the basic idea, the major features are represented by the fuel injected into any combustion chamber as fully atomised spray containing spherical droplets. The drop size distribution function is used to identify the spray shape. Each phase has its own velocity and temperature due to the interaction within the computational domain. The liquid phase has its own turbulent fluctuations that appear in turbulent transport of mass, momentum and energy which is determined by convection, diffusion and interaction with the gas phase. Under these assumptions each moment has a transport equation.

For the momentum equation or the mass-average velocity, following Beck and Watkins [2003a], it is started by deriving the Lagrangian form for a group of droplet with the same properties. The source terms describe the effects of change in the liquid phase momentums due to drag, breakup, collision and evaporation. This is discussed widely in previous publications by Watkins [2007] in terms of the drop size distribution. The diffusion terms are treated the same for all momentums. However, two different dispersion models are tested here. The first treatment applies an Eulerian approach by modelling the liquid phase turbulent viscosity according to the theory of Mostafa and Mongia [1987] so that it is evaluated in Elghobashi [1994] as a damped form of the gas phase turbulent viscosity. The damping is incorporated through the use of Melville and Bray [1979] coefficient, \( \sigma_v \). In these calculations a value of 0.7 is used throughout. The second dispersion model applies the Lagrangian approach used in many discrete droplet
models. This incorporates dispersion by adding a turbulent component to the gas phase velocity used in the drag equations. This is discussed in more detail later. To disable the first dispersion model, \( \sigma_v \) is set to zero. Thus, the governing equations in Eulerian coordinates can be written in the following generalised form

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho \phi \, d\Omega + \int_{S} \rho \phi \tilde{n} \cdot \tilde{n} \, dS = \int_{S} \Gamma_{\phi} \text{grad} \phi \cdot \tilde{n} \, dS + \int_{\Omega} q_{\phi} \, d\Omega
\] (2.39)

where the quantity \( \phi \) represents a conserved variable (velocity, temperature, moment, enthalpy), \( \Gamma_{\phi} = \rho_d \sigma_{v_d} \nu_d \) refers to the diffusivity coefficient, \( \Omega \) is the control volume for the computational cell, \( \nu_d \) is representing the component of the velocity vector of fluid, \( \rho \) is the fluid density and \( q_{\phi} \) is the sum of all source terms.

### 2.6.2 Gas phase

The unsteady, turbulent conservations for mass, momentum, species concentration and energy are to be solved conjugated with the liquid phase conservation equations. All transport equations for the gas phase can be written in terms of the void fraction \( (1 - \Theta) \) in the general form as

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho (1 - \Theta) \phi \, d\Omega + \int_{S} \rho (1 - \Theta) \phi \tilde{n} \cdot \tilde{n} \, dS = \int_{S} \Gamma_{\phi} (1 - \Theta) \text{grad} \phi \cdot \tilde{n} \, dS + \int_{\Omega} q_{g\phi} \, d\Omega
\] (2.40)

where \( q_{g\phi} \) is the gas phase source term representing the mass transferred from the liquid phase to the gas phase per unit time within a control volume. Similar to the liquid phase, the source term in gas phase represents the effects of turbulence, chemical reaction due to combustion. In this section the effect of turbulence is included and the remaining effects are to be expanded separately as sub-models due to the interaction with the liquid phase in the following sections.

For modelling turbulence motion, the standard two-equation \((k - \varepsilon)\)turbulence model is applied here which calculates a turbulent viscosity by using two scalars. The equations being solved for are the turbulence kinetic energy \( k \) and its dissipation rate \( \varepsilon \). The equations are

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho (1 - \Theta) k \, d\Omega + \int_{S} \rho (1 - \Theta) k \tilde{n} \cdot \tilde{n} \, dS - k Q_i = \int_{S} \Gamma_{\phi} (1 - \Theta) \text{grad} k \cdot \tilde{n} \, dS + (1 - \Theta) P_k - (1 - \Theta) \rho g \varepsilon
\] (2.41)
The turbulence kinetic energy production rate is given by

\[ P_k = \rho_g C_\mu \frac{k^2}{\varepsilon} (\text{grad(\bar{u}))}^2 \]  

(2.43)

The constants take the values \( C_{\varepsilon,1} = 1.44, \) \( C_{\varepsilon,2} = 1.92, \) \( C_{\varepsilon,3} = -0.373 \) and \( C_\mu = 0.09. \) The term involving \( C_{\varepsilon,3} = -0.373 \) is an additional term represents the effect of the liquid phase on the gas phase turbulence. From the interaction of liquid-gas, it is possible to calculate source terms by considering the effect of the gas phase on the liquid phase in terms of the droplet size distribution function moments through integration over the presumed shape of the droplet number size distribution. The gas phase energy transport equation including the mass transfer term can be written as

\[ \frac{\partial}{\partial t} \int \rho(1 - \Theta)E_g d\Omega + \int_S \rho(1 - \Theta)E_g \bar{u} \cdot \bar{n} dS - E_g q_i = \int_S \Gamma \phi (1 - \Theta) \text{grad}E_g \cdot \bar{n} dS + \int \Omega q_E d\Omega \]  

(2.44)

The source term in the conservation equation of energy is representing the energy exchange between the liquid and gas phases due to mass change of droplet spray and the interphase energy transfer. Adding to that the evaporation of fuel will introduce a mass transfer term when the fuel droplets change phase from liquid to gas and will be transported together with the rest of the surrounding gas. Hence to account for the phase change there is a requirement to construct a separate transport equation for the fuel vapour mass fraction present. This reads as follows,

\[ \frac{\partial}{\partial t} \int \rho(1 - \Theta)f d\Omega + \int_S \rho(1 - \Theta)f \bar{u} \cdot \bar{n} dS = \int_S \Gamma \phi (1 - \Theta) \text{grad}f \cdot \bar{n} dS + \int \Omega q_f d\Omega \]  

(2.45)
This effectively changes the properties of the carrier gas. The state equation becomes,

\[ P = \rho_g R_{mix} T_g \] (2.46)

where

\[ R_{mix} = R_0 \left( \frac{1 - f}{m_a} + \frac{f}{m_f} \right) \] (2.47)

The specific heat capacity of the mixture is given by,

\[ c_{p,mix} = \frac{(1 - pr) m_a c_{pa} + pr m_f c_{pv}}{(1 - pr) m_a + pr m_f} \] (2.48)

where \( pr \) is the ratio of the average partial pressure of the fuel vapour to the total pressure is given by,

\[ pr = \frac{P_{vs}}{2P} \] (2.49)

Figure 2.1: Schematic of a typical injector tip

(a) Represented injector tip

Figure 2.2: Represented injector tip
Figure 2.3: Inlet PDFs with $r_{32} = 1$ and $k = 1.5, 2.25, 3, 7$ and 14.

Figure 2.4: Modelling of the nozzle orifice
Figure 2.5: Nozzle radial profiles

Figure 2.6: Nozzle discharge profiles
Chapter 3

Numerical method

3.1 Introduction

As stated in chapter two, the only way to get usable results is by transforming the theoretical model into a practical mathematical model; this is the main subject of this chapter. The equations modelling two-phase flows are primarily partial differential equations which cannot be solved by classical mathematical methods i.e. analytically. Therefore, the use of discretization methods for a system consisting of a set of partial differential equations is required and then implantation of the solution scheme into respective algorithms. In this chapter the finite volume method is adopted as in the work presented by Jones [2009] for solving the conservation equations. The method is based on higher order accurate spatial discretization methods which are implemented with unstructured grids with an arbitrary shape for the computational cells. In addition a fully implicit three time level scheme is used for the solution of the unsteady terms. The collocated variable arrangement is used where computational points are located in the cell centre. The discretized equation systems are solved using a conjugate gradients type solver with incomplete Cholesky preconditioning. The PISO algorithm is used to establish the pressure-velocity coupling for the gas phase and calculate pressure. Lastly the numerical integration has been performed to approximate the probability density function, that is constructed from the moments. It should be pointed out that the convection schemes mentioned in this chapter are applied in chapters five and six only while different schemes are used in chapter four.
3.2 Finite volume method

The finite volume method is considered as a numerical tool which can provide solution for average values of flow variables and properties over a given control volume. In the frame of this work the finite volume of discretization is adopted to describe the two phase flows. The reason to use such a method is because it utilises the conservation laws of mass, momentum and energy. The governing equations in the integral form are discretized using the three steps as follows:

1. Grid generation:

   the computational domain in space is divided into a finite number of discrete elements with computational points at their faces or centres. The space discretization gives a definition for numerical grids is a that the solution of dependent variables is computed at these points.

2. Time intervals

   The entire time is also divided into a finite number of sub-intervals called time steps.

3. Equation transformation

   The individual terms in the equation to be solved are replaced by algebraic expressions referring to the variables values at computational points in the domain.

3.3 Discretization procedure

In the finite volume method the transport equation which characterise fluid dynamic or heat transfer phenomena (continuity, momentum, energy and scalar quantity, etc.) is underpinned by the concept of discretization. The integrated form of the transport equation uses the divergence theorem for the fluxes integrated over each control volume that covers the computational domain. Finally, using the Gauss-Green theorem, the volume integral of the transport terms can be transformed into a surface integral to allow the balance equation for the generic scalar in the computational cell

$$\frac{\partial}{\partial t} \int_{\Omega} \Theta \rho \phi \, d\Omega + \int_{S} \Theta \rho \vec{\nu}_{\phi} \cdot \vec{n} \, \phi \, dS = \int_{S} \Theta \Gamma_{\phi} \text{grad} \phi \cdot \vec{n} \, dS + \int_{\Omega} q_{\phi} \, d\Omega \quad (3.1)$$

Equation (3.1) has four distinct terms. On the left hand side are the scalar rate of change and the convection transport performed by the flow. The molecular transport is based on the diffusivity
coefficient $\Gamma$ and sink or source term are placed in the right hand side. In order to solve such as equation (3.1), the approximations of all terms in the equation (3.1) will be shown in the next subsections. By summing all terms in an algebraic equation for each control volume. The achieved equation relates the value of dependent variable $\phi$ at the centre of the control volume to the values at neighbouring control volumes. This equation can be expressed in compact form using the coefficients $A$ and the source term $q$, such that

$$A_P \phi_P - \sum_k A_k \phi_k = q$$

(3.2)

### 3.3.1 Temporal discretization

For unsteady flows the integration of equation (3.1) requires also to accounted for the process that may causes $\phi$ to change with time. Once initial conditions are implemented, the temporal discretization yields an estimate of the scalar value at the next time level. In the present work, an implicit second order three time level scheme is chosen because it is formally unconditionally stable and permits to use arbitrary time step, which is governed only by the accuracy considerations. The second order approximation of the time derivative at time level $t_{n+1}$ is gained by fitting a parabola through the solution at three time level. Then

$$\frac{\partial}{\partial t} \int_{\Omega} \Theta \rho \phi d\Omega \approx \frac{1}{2} \left( 3 (\Theta \rho \phi)^{n+1} - (4 (\Theta \rho \phi)^n - (\Theta \rho \phi)^{n-1}) \right) \frac{\Delta \Omega}{\Delta t}$$

(3.3)

To include the unsteady term, only $A_P$ and $q_\phi$ require modification. The contributions are

$$A_P = \frac{1}{2} 3 (\Theta \rho)^{n+1} \frac{\Delta \Omega}{\Delta t}$$

(3.4)

and

$$q_\phi \Delta \Omega = -\frac{1}{2} \left( 4 (\Theta \rho \phi)^n - (\Theta \rho \phi)^{n-1} \right) \frac{\Delta \Omega}{\Delta t}$$

(3.5)

where $\Delta t$ is the time interval centered around the time level $t_{n+1}$, i.e. from $t_{n+1} - \Delta t$ to $t_{n+1} - \Delta t$. Now, with the inclusion of the temporal term, the main coefficient is guaranteed to take a positive value, so long as $\Delta t$ is sufficiently small (and $\Theta \rho \neq 0$).

### 3.3.2 Spatial discretization

There are two forms of terms in the transport equation namely surface and volume integrals that must be evaluated by numerical methods in order to achieve second order accurate solutions for
any control volume shape. The surface integrals in equation (3.1) are approximated by mid-
point rule, which yields the following approximate face integral as the sum of products of the
variables value interpolated to the cell face and the vector normal to the cell face, thus the flux
of the transported variable across the cell face can be expressed as

\[ F = \int_S f dS = \sum_k \int_{S_k} f dS_k \approx \sum_k f_k S_k \] (3.6)

Where \( S \) denotes the face area, defined as the magnitude of the face area vector \( S \) as shown in
figure (3.1). By following similar method, the volume integral is evaluated by assuming that the
value of the variable \( \phi \) can be averaged over the control volume and multiplied by the volume
of the control volume. Then the mean value of the integrated variable is approximated by the
value of the function at the control volume center \( P \) as shown in figure (3.1) as

\[ Q = \int_\Omega q d\Omega \approx q_P \Delta \Omega \] (3.7)

### 3.4 Convective term

The convective flux across cell faces can be discretized by a number of means of approximating
interpolations for the surface integrals of face values for the convective term within the discretized
domain, many volume centre values which are stored, these methods are outlined below.

**Linear interpolation:** linear interpolation is the most obvious, but in certain conditions
produces unbounded results. It is presented here for completeness, as shown in figure (3.2) but
not used;

\[ \phi_k = (1 - \lambda_k)\phi_P + \lambda_k \phi_K \] (3.8)

where

\[ \lambda_k = \frac{x_e - x_P}{x_E - x_P} = \frac{L_{Pk}}{L_{PK}} \] (3.9)

**Upwind differencing:** Upwind differencing is used to ensure boundedness but results in
excess diffusion, being only a first order accurate scheme. The scheme is used implicitly in
solving transport equations (i.e. the convective contributions in the resulting matrix are based
on this method).

\[ \phi_k = \min(\vec{v} \cdot \vec{n}, 0)\phi_K + \max(\vec{v} \cdot \vec{n}, 0)\phi_P \] (3.10)
**TVD schemes:** To avoid both the unboundedness of linear interpolation and the numerical diffusion of the Upwind differencing, Total Variation Diminishing scheme is used.

\[
\phi_k = \phi_C + \frac{1}{2} \psi(r_f) (\phi_D - \phi_C) \tag{3.11}
\]

where \( \phi_C \) is the volume center value immediately upstream of the face, \( \phi_D \) is the volume center value immediately downstream of the face and \( \psi(r_f) \) is the flux limiter Darwish and Moukalled [2003] as shown in figure (3.3). There are a number of possibilities for the choice of flux limiter, though here only two methods are considered; the first is the Min-mod limiter which is based on central differencing

\[
\psi(r_f) = \max(0, \min(1, r_f)) \tag{3.12}
\]

and the second is the Superbee limiter which is based on the second order upwind scheme

\[
\psi(r_f) = \max(0, \min(1, 2r_f), \min(2, r_f)) \tag{3.13}
\]

\( r_f \) is the \( r \)-factor, defined as

\[
rf = \frac{\phi_C - \phi_U}{\phi_D - \phi_C} \tag{3.14}
\]

where

\[
\phi_U \approx \phi_C - 2 \text{grad} \phi_C \cdot \vec{r}_{CD} \tag{3.15}
\]

**Interface capturing schemes:** For scalar variables such as concentration, convection methods developed for interface capturing are likely to be of use in the transportation of moments. These methods are high order schemes which ensure the concentration remains bounded (so long as the implementation is exact). The method presented here is that by Muzafferija and Peric [1999] and can be used for moment quantities also. Ubbink [1997] offers an in depth analysis of interface capturing methods, though the scheme assumes physical limits to the variable are known (in the case of transporting concentration the lower bound and upper bound are 0 and 1 respectively. For moments, only a lower bound can be defined).

\[
\phi_k = \lambda \phi_C + (1 - \lambda) \phi_D \tag{3.16}
\]

where

\[
\lambda = (1 - \phi_k') \frac{\phi_D - \phi_U}{\phi_D - \phi_C} \tag{3.17}
\]
The angle between the gradient of $\phi_C$ and the face normal vector $\vec{n}$, $\theta$, is a key part of this scheme as shown in figure (3.4). The interpolation constant, $\gamma$ is related to the direction of greatest change.

\[
\tilde{\phi}_k'' = \begin{cases} 
\tilde{\phi}_k & \text{if } Co \leq 0.3 \\
\tilde{\phi}_C + (\tilde{\phi}_k - \tilde{\phi}_C) \frac{0.7 - Co}{0.7 - 0.3} & \text{if } 0.3 < Co \leq 0.7 \\
\tilde{\phi}_C & \text{if } Co > 0.7
\end{cases}
\] 

(3.19)

where

\[
\gamma = \frac{0.7 - Co}{0.7 - 0.3}
\] 

(3.20)

\[
\tilde{\phi}_k'' = \begin{cases} 
\tilde{\phi}_C & \text{if } \phi_C \leq 0 \\
2\tilde{\phi}_C & \text{if } 0 < \phi_C \leq 0.5 \\
1 & \text{if } 0.5 < \phi_C \leq 1 \\
\tilde{\phi}_C & \text{if } \phi_C > 0
\end{cases}
\] 

(3.21)

and

\[
\tilde{\phi}(\vec{x}) = \frac{\phi(\vec{x}) - \phi_U}{\phi_D - \phi_U}
\] 

(3.22)

The Courant number, $Co$, is taken as the maximum of the face Courant numbers over the control volume, $C$, as used by Waclawczyk and Koronowicz [2006].

### 3.4.1 Deferred correction

To avoid losing accuracy and at the same time retain boundedness, a method for implementing higher order interpolation schemes maintaining a compact stencil is to use the lower order scheme to discretize the term and form the matrix and then to include the difference between the higher order scheme and the lower order scheme based on current values on the right-hand side (the source term) of the discretized equation.

\[
F_k = F_k^L + \gamma(F_k^H - F_k^L)^{curr}
\] 

(3.23)

Normally, a value of $\gamma$ is set for each equation, typically in the range (0.5 - 1). However, under certain circumstances at particular cell faces, it may be desirable to modify this value. As can
be seen by equation (3.23) the low order discretization is treated implicitly in order to improve
the numerical stability, whereas the high order term is treated explicitly, therefore is constant
during the iteration loop. If the computations converge, then low order terms will cancel out
and the high order discretization is recovered at the end of the iteration loop.
When solving the moment-averaged momentum equations using a high order convection scheme,
augmentations to the source term by equation (3.23) must be set to zero where the spray does
not exist, as shown in figure (3.5).

3.4.2 Gradient
Calculation of the gradient of a value over its volume is performed by making use of the Gauss’
theorem;

\[
\nabla \phi_P = \frac{1}{\Delta \Omega} \sum_k S_k \vec{n}_k \phi_k
\]  

(3.24)

In order to interpolate to the face centre, values either side of the face are required. For un-
structured grids, the locations of these two points do not necessarily lie along the same line
passing through the face centre as shown in figure (3.6) and so values at auxiliary locations
(P’ and N’) are determined and used instead. To calculate these auxiliary values, knowledge of
the gradient of the variable is required, which in turn requires the face centre values. Thus an
iterative scheme is used to evaluate the gradient accurately. The number of iterations performed
is typically one to three on non-orthogonal grids.
For 2-dimensional cylindrical grids, an additional term is included for \( \frac{d}{dy} \) (where \( y = r \)) when
the gradient is solved using finite volume methods, as detailed in Ferziger and Perić [2002]

\[
\frac{d}{dy}(\phi_P) = \frac{1}{\Delta \Omega} \sum_k S_k n_{y,k} \phi_k - \Delta S \phi_P
\]  

(3.25)

where \( \Delta S \) is the front face area, which is equal to the volume on a 2D planar grid. Here it
is noted that div(\( \vec{v} \)) \( \neq 0 \) if the gradient calculation above is used (for incompressible flow).
However, the gradient is not used to calculate divergence for the FV method.
3.4.3 Convection term

Consider the convection term in the scalar equation. This is discretized in the following manner, using the upwind scheme

\[ A_c^k = \Theta \rho \min(\vec{v}_k \cdot \vec{n}_k, 0) \]  (3.26)
\[ A_c^p = -\sum_k A_c^k + \Theta \rho \sum_k \vec{v}_k \cdot \vec{n}_k \]  (3.27)

The second summation in the above equation is usually assumed to equal zero when dealing with the continuous phase. However, for the discrete phase this summation must be included.

3.4.4 Additional Term

The treatment of the additional term in equation (2.26) needs to be included. This happens to be quite straightforward, being included implicitly.

\[ -\phi \left( \frac{\partial \Theta \rho}{\partial t} + \text{div}(\Theta \rho \vec{v}) \right) \rightarrow -\phi \left( \frac{\partial}{\partial t} \int_{\Omega} \Theta \rho d\Omega + \int_{S} \vec{v} \cdot \vec{n} \Theta \rho dS \right) \]  (3.28)

Discretizing this term then leads to

\[ A_a^p = -\frac{1}{2} \left( 3(\Theta \rho)^{n+1} - (4(\Theta \rho)^n - (\Theta \rho)^{n-1}) \right) \frac{\Delta \Omega}{\Delta t} - \Theta \rho \sum_k \vec{v}_k \cdot \vec{n}_k \]  (3.29)

3.4.5 Main Coefficient

The resulting coefficient from the summation of the above terms reduces to

\[ A_p = A_c^p + A_f^p + A_a^p \]  (3.30)
\[ = -\sum_A A_c^k + \frac{1}{2} \left( 4(\Theta \rho)^n - (\Theta \rho)^{n-1} \right) \frac{\Delta \Omega}{\Delta t} \]  (3.31)

Since there is no pressure-velocity coupling in the discrete phase, the continuity equation (moment equation) is discretized using the above methods. This results in the main coefficient

\[ A_p = -\sum_k A_c^k + \Theta \rho \sum_k \vec{v}_k \cdot \vec{n}_k + \frac{1}{2} 3(\Theta \rho)^{n+1} \frac{\Delta \Omega}{\Delta t} \]  (3.32)

which is the summation of the neighbour coefficients and convection fluxes and the temporal term.
3.5 Algorithm Platform

The presented methodology is implemented into a suitable algorithm for solving continuum fluid flow. The algorithm follows the procedure detailed in Ferziger and Perić [2002], using the SIMPLER scheme Patankar [1980] for pressure-velocity coupling and the $k-\epsilon$ model of Launder and Spalding [1974] for turbulence modelling for high Reynolds number flow. The domain is discretized in an unstructured manner into finite volumes. The solution of the discretized equations is performed using the conjugate gradients type solvers with incomplete Cholesky preconditioning. Time marching is performed using the implicit three time level method for all transported properties. Convergence of outer iterations is defined by the maximum (1-norm) normalized residual of all transport equations dropping to a predefined level (three orders of magnitude). Each residual is normalized by its maximum in the iterative procedure.

3.5.1 Solution Algorithm

The solution algorithm shown in figure (3.7) is made up of two loops, the latter being nested. The outer loop indexes the temporal progression of the solution and the inner loop performs iterations over all the transport equations until global convergence is obtained for a given time step (or until the iteration index reaches a pre-set maximum). Transported scalars are solved after their associated momentum equation. This ordering enables the volume face speed ($\vec{v} \cdot \vec{n}$) to be calculated and stored during the construction of the momentum equation, then used by the scalar equations in the convection terms.

If the momentum is related to the transportation of a volumetric-based quantity, such as droplet volume fraction or mass flow rate, the summated inlet and outlet volumetric fluxes are stored. These quantities are used later to correct the overall volume conservation. The discrete phase precedes the continuum phase and employs a predictor-corrector method; the equations are first iterated to bring the residual down to a certain level, whereby the source terms requiring the solution to the underlying distribution are omitted. Once the maximum of the residuals of the moments transport equation have been reduced to a sufficient level, the source terms requiring the moments closure are included. After the discrete phase is solved, the continuum phase is solved in the order described above, but with an additional procedure performed after the momentum and before the continuity (pressure correction) equation. This procedure summates
the inlet and outlet volumetric fluxes of both phases and calculates the ratio

\[
\frac{(\Theta S \vec{v} \cdot \vec{n})_{in} + \frac{4}{3} \pi (\mu_3 S \vec{V}_{d,3} \cdot \vec{n})_{in}}{(\Theta S \vec{v} \cdot \vec{n})_{out}}
\]  

(3.33)

This ratio is then used as a multiplier for the outlet fluxes used in the pressure correction equation. This ensures that the source term of the pressure-correction equation tends to zero upon convergence. Equation (3.33) assumes that only the continuum phase exits the domain. In addition to the standard boundary conditions of inlet, outlet, wall and symmetry for a generic velocity or scalar, special boundary conditions must be implemented for the turbulence model at the wall and the injection and wall impaction of the spray. For the standard boundary conditions, details are given in Ferziger and Perić [2002].

### 3.5.2 Pressure-Velocity Coupling

Both the SIMPLE and the SIMPLER schemes are implemented in the solution algorithm. Typically, PISO type schemes are used for spray and engine problems Beck and Watkins [2003a] to avoid the need to perform outer iterations, though for the spray methodology presented here, numerical tests have shown that outer iterations are required and so the implemented methods are more suitable.

Jones [2009] compared the performance between the SIMPLE scheme and the SIMPLER scheme for a sample spray case, initial tests showed significant improvement in the rate of convergence using the SIMPLER scheme over the SIMPLE scheme, so the SIMPLER scheme depicted in figure (3.8) will be used as the standard method of coupling velocity and pressure.

### 3.5.3 Linear Algebra Solver

Jones [2009] used a number of linear algebra solvers for sparse systems of equations are available through libraries such as LASPACK and Sparkit 2. However, to use these libraries, the arguments \((\phi, A \text{ and } b)\) must have the proper definition, which is typically

\[
\text{real(kind=wp), dimension(1:N_vol)} :: \phi, b
\]

for the variable and right hand side and

\[
\text{real(kind=wp), dimension(:)} :: A
\]

\[
\text{integer, dimension(:)} :: IJA
\]

for the matrix storage (such as the New Yale Sparse Matrix format).
However, the structure used for the storage of the transported equations is not of this form (for \( \phi \)). To make the CFD code compatible with the libraries, the stored variable, \( \phi \), would have to be copied, the linear system then solved, then update the stored variable with the updated variable.

To avoid this copying of data, a new linear algebra library was written which accepts \( \phi \) in the form of an array of one-dimensional pointers:

```fortran
type::phi_t
  real(kind=wp), dimension(:), pointer :: vc => null()
end type

type(phi_t), dimension(:), allocatable :: phi
```

The one-dimensional pointer enables \( \phi \) to point to a vector so all the components of the momentum equations are solved in a single call. Figure (3.9) shows how the above structure connects with the data structure of the transport equations.

### 3.6 Numerical Integration

Once the probability density function is constructed, moments of that distribution may be required. For a-priori distributions, moments are obtained as functions of their parameters (equation (2.17)). For all other methods, the distribution must be integrated numerically.

Supposing that a group of terms are functions of a single PDF and require integrating between different limits and to different orders (such as the break-up terms in Beck and Watkins [2002]).

To evaluate these terms the normal procedure would be to call a numerical integration subroutine for each moment calculation.

Alternatively, Jones [2009] urged that the numerical integration could be performed once, calculating all integer moments covering the order range and limits of the required moments in a single sweep of the underlying distribution. Coordinates of the constructed PDF (Figure(3.10)) are stored as links on a doubly linked list (Figure(3.11)). Pairs of integration limits are then inserted into the linked list at the appropriate position (Figure(3.12)) and the distribution coordinates (\( \phi(r_a) \) and \( \phi(r_c) \)) are obtained by interpolation, forming a single chain of distribution coordinates. A pass is then made along the list, performing the elemental integration between the current link and the previous link and summating the elemental integrations between the pairs of limits. For example, two moments are required: \( Q_{2.35} |_{r_a}^{r_c} \) and \( Q_{0.78} |_{r_b}^{r_d} \) (Figure(3.10)).

The information then sent to the integration subroutine is calculate moments \( Q_0, \ldots Q_3 \) between the limits \( r_a - r_c \) and \( r_b - r_d \), which would result in an output of eight moments grouped into
two sets \((Q_0 \text{ to } Q_3 \text{ between } r_a \text{ and } r_c \text{ and } Q_0 \text{ to } Q_3 \text{ between } r_b \text{ and } r_d)\). The orders from 0 to 3 for the moments are requested since they span the order range of the required moments. To calculate the actual moments required, interpolation is performed between the nearest pair of integer moments. Geometric interpolation has been performed by assuming consecutive integer moments are available, determining non-integer moments within the range of the available moments can be approximated by

\[
\int \phi(r)r^n r.0.m \, dr \approx \left( \int \phi(r)r^n \, dr \right)^{1-0.m} \left( \int \phi(r)r^{n+1} \, dr \right)^{0.m}
\]  

(3.34)
Figure 3.1: Face centroid and area vector.

Figure 3.2: A typical control volume and the notation used for a structured grid.

Figure 3.3: Convection node notation for unstructured grid.
Figure 3.4: A sector from a simulated scalar variable shows the angle between interface cell face for unstructured grid.

Figure 3.5: \((F_k^H - F_k^L)_{curr} = 0\) in volume N since the spray is not present there.

Figure 3.6: Face value interpolation.
For each set of moments:

- Calculate: PDF and VDF
- Calculate: Hydrodynamics and impaction terms

For each moment:

- Solve: Moment-averaged momentum, $\bar{V}_{d,i}$
- Solve: moment, $\mu_i$

Crop spray

Solve: Liquid film, $\theta$

Calculate: SMR and liq. vol. fraction

Solve: Momentum, $\bar{v}'$

Solve: pressure correction

Solve: Turbulent kinetic energy, $k$

Solve: Turbulent dissipation rate, $\epsilon$

Calculate: Eddy viscosity

Convergence?

Next time step?

End

Figure 3.7: Two-phase flow algorithm.
Solve: momentum equation, $\vec{v}$

Solve: pressure correction equation, $p'$
Calculate: pressure correction gradient, $\text{grad } p'$
Correct velocity, $\vec{v}$
Correct mass flux, $\dot{m}$

Solve: pressure equation, $p$
Calculate: pressure gradient, $\text{grad } p$

Figure 3.8: SIMPLER scheme.

Figure 3.9: Solver variable pointing at the equation variable.
Figure 3.10: Integration of a PDF between sets of limits.

Figure 3.11: Construction of integration linked list.

Figure 3.12: Insertion of limits to the PDF list.
Chapter 4

Sprays hydrodynamics

4.1 Introduction

In this chapter a model for the description of source terms of spray-gas interactions is presented and discussed in terms of a new algorithm for solving the set of moment and momentum transport equations linked with implementation of unstructured grids. This starts with describing the problem of modelling spray with a hollow cone shape and details of the new blended scheme. In addition by considering the kinetic spray effects are taken into account changes in spray properties due to effects such as drag, breakup and collision of droplets. These effects will modify the liquid surface area. According to the mean properties of the spray and the gas phase, the calculation of the moment averaged phase interaction will be determined by taking the integration for the related moment as a function in terms of drop size distribution. The probability density function is investigated and modelled to be used in source terms that are written in terms of the appropriate related moments. The general formula to compute the source terms due to the interaction between the two-phases is calculated per unit volume in terms of gamma distribution as explained in chapter two.
4.2 The problem

4.2.1 Motivation

The work is aimed to develop a robust weighted flux scheme to capture the spray edges in modelling hollow cone type sprays without need to reconstruct the two-phase interface. The moments and momentum transport equations for dispersed phase are solved by using finite volumes associated with unstructured grid topology. The convective flux in each cell face utilises the Weighted Average Flux (WAF) scheme blended with Switching Technique for Advection and Capturing of Surfaces (STACS) scheme for high resolution flux limiters. First of all a test is made on simple comparison between TVD scheme and WAF scheme using the same flux limiter on convective flow in hollow cone spray. Results show the WAF scheme gives a better prediction than TVD scheme. However in the next step, SMART the high resolution scheme is blended with the WAF scheme to provide the sharpness and boundedness of the interface by using switching strategy.

4.2.2 A WAF blended with STACS in spray modelling

The Weighted Average Flux (WAF) scheme was initially proposed by Toro [1989] for the modelling of hyperbolic conservation laws. As cited in Toro [2009] the Total Variation Diminishing (TVD) scheme is a modification of WAF scheme. It is useful to replace the TVD scheme by WAF because it can handle random fluxes that operate on both structured and unstructured grids. Following Darwish and Moukalled [2003], the simplest criterion to assign the centre face value \( \phi_f \) of WAF scheme is to write it in the most convenient way for evaluation via upwind and central difference schemes multiplied by a flux limiter \( \psi(r) \). The flux limiter is set in the form that allows the amplification of the factor applied. In the final formula of WAF scheme the intercell flux takes the form

\[
\phi_f = \frac{1}{2}(1 + \psi(r)\phi_C + \frac{1}{2}(1 - \psi(r)\phi_D)
\]

(4.1)

where \( \phi_C \) is the value at a node upwind of the face (f) (see figure 4.1 (a) and (b)) and \( \phi_D \) refers to the downwind. The flux limiter \( \psi(r) \) is a function that represents the ratio of two consecutive gradients, thus can be written as

\[
r = \frac{\phi_C - \phi_U}{\phi_D - \phi_C}
\]

(4.2)
The value of $\phi_U$ in an unstructured grid can be estimated at a distance of $-2r_{CD}$ away from the node $C$. As a result the solution around the node $C$ is assumed to be distributed linearly. However the value of $\phi_U$ can take the form of

$$\phi_U = \phi_D - 2(\nabla \phi_C) \cdot r_{CD}$$

In hollow cone spray modelling the flow quantities are relatively sharp at the edges due to the effect of centrifugal force that works to push droplets to the outside periphery of the spray structure which makes the conical shape. A special treatment is used in this work via incorporating a modified high resolution algorithm at the interface in order to maintain the sharpness at the edges. The new algorithm comprises the Switching Technique for Advection and Capturing of Surfaces (STACS) scheme suggested by Darwish and Moukalled [2006] which incorporates also blending of two high resolution schemes instead of upwind differencing and also keeps bounded differencing. The upwind scheme is recognized to cause numerical diffusion. In contrast the first order accurate downwind scheme can produce significant oscillations at the interface. In order to take the benefit of the over compression at the interface with no curvature (stepping effect), a switching strategy is constructing based on a blend of high resolution (HR) with bounded downwind (BD) and the angle between the flow direction and the grid lines (see figure (4.1)(b)), where $\theta$ is given by

$$\theta = \cos^{-1} \left( \frac{\nabla \phi_f \cdot r_{CD}}{|| \nabla \phi_f || \cdot || r_{CD} ||} \right)$$

This approach aims to blend the WAF scheme with the STACS scheme because it can handle with fluid status first. The second reason especially applies in this study where the liquid phase (sprays droplets) is treated in Eulerian way as continuum in contrast to the Lagrangian framework. To explain this, when the cell has certain amount of liquid (volume fraction) this comes from the upwind convective flow. If the flow is normal to the grid line the interface is parallel to the cell face as seen in figure (4.2)(a). In this case the bounded downwind (BD) scheme is able to convect the flow downstream through the cell face. However if the liquid flow has filled the cell from the lower part of the cell, thus the interface becomes perpendicular to the cell face. For this state it is more appropriate to predict the convection with high resolution (HR) scheme as seen in figure (4.2)(b). The third case is the closest to modelling spray with hollow cone shape, the flow is inclined with angle as seen in figure (4.2)(c). The strategy takes advantage of the calculated angle that results between the interface and cell face to switch between the two
schemes. Therefore the flux limiter used in this work is normalised after weighting the factor related to the measured angle as explained in Darwish and Moukalled [2006] as

\[ \psi(r_f) = r_f(BD)[\cos(\theta)]^4 + r_f(HR)(1 - [\cos(\theta)]^4) \] (4.5)

With this scheme SMART is implemented here as proposed by Leonard [1990] due to the use of quadratic interpolation, then the SMART is formulated as

\[ r_f(HR) = \max[0, \min(4r, \frac{r}{2} + \frac{1}{2}, 2)] \] (4.6)

\[ r_f(BD) = \max[0, \min(4r, 2)] \] (4.7)

The convection term is discretized using the bounded third-order interpolation scheme. The high resolution sharp and monotonic algorithm for realistic transport (SMART) scheme proposed by Gaskell and Lau [1988] for steady state implicit calculations is implemented. SMART scheme can be considered as bounded version of QUICK scheme. Gaskell and Lau [1988] recommended the use of under-relaxation for the cell faces fluxes which damps the oscillatory behaviour.

The typical ranges are sketched in figure (4.3)

\[ \phi_f = \begin{cases} 
\phi_C & \text{if } \phi_C < 0 \\
3\phi_C & \text{if } 0 \leq \phi_C < \frac{1}{6} \\
\frac{3}{2}\phi_C + \frac{3}{8} & \text{if } \frac{1}{6} \leq \phi_C < \frac{5}{6} \\
1 & \text{if } \frac{5}{6} \leq \phi_C < 1 \\
\phi_C & \text{if } \phi_C \geq 1 
\end{cases} \] (4.8)

The SMART scheme with improved iterative convergence properties is devised by incorporating total-variation diminishing constraints. In order to obtain a sharp edge as in case of hollow cone spray, the SMART high resolution scheme \( r_f(HR) = \frac{3}{2} + \frac{1}{2} \) is known to be responsible for the convection when the interface moves in an inclined direction as explained in equation (4.5). However the high resolution scheme is replaced by the more compressive bounded linear Fromm scheme \( r_f(HR) = \frac{1}{2} + \frac{1}{2} \) which gives reasonable resolution of sharp gradients. Fromm [1968] scheme is inserted here because it is designed to minimize dispersion error and non-equal symmetric with equal weighting given to the centred and upwind gradients. This is not only the main reason to use Fromm’s scheme for high resolution scheme but the SMART scheme recover
4.3 Theoretical perspective

4.3.1 Atomisation models

The transformation of the continuous liquid phase into droplets as dispersed phase through disintegration process is the simplest concept for the atomization. The main purpose for this process is to increase the contact area between liquid-gas interface in the dispersed multiphase system which leads to significantly strengthen the relevant processes such as momentum, heat and mass transfer.

The fundamental of the atomisation model is to describe the spray providing the initial conditions for spray computations, i.e., velocities, temperature and drop sizes at the nozzle exit. The classification of disintegrated liquid depends primarily on the boundary conditions which are classified mainly into jet or sheet. The wave theory is applied to describe the breakup phenomena and regimes, this states that the breakup process originates with the interaction between the liquid surface and the surrounding gas due to the growth of small perturbations.

The jet breakup theory states that the disintegration of a liquid jet emerging from a circular orifice into the stagnant, incompressible gas is caused by amplification to the initial disturbances at the surface. Lord Rayleigh [1878] was first to observe drops breakup as the growth of small disturbances on the liquid jet surface through the interaction with ambient gas. These cause waves ending with formation of droplet with diameter approximately twice the diameter jet orifice. Reitz and Bracco [1982] presented an extension to the jet breakup theory through a solution for mathematical relation between the growth rate with wave length as function of the jet Weber and Ohnesorge numbers:

\[
We \equiv \frac{E_{\text{kin}}}{E_{\text{sur}}} = \frac{\rho U_d^2 v}{\sigma} \quad (4.9)
\]

and

\[
Oh = \frac{\mu}{\sqrt{\rho} \frac{d\sigma}{d\varepsilon}} \quad (4.10)
\]

Four main regimes of liquid jet identified by Ohnesorge [1936] rely on different characteristic numbers, Reynolds and Ohnesorge numbers. These regimes were explained with further detail by Haenlein [1932] and Reitz [1978] as summarised below:
1. Rayleigh regime: the jet breaks up at low Reynolds number results from surface tension effects and drop diameter is larger than jet diameter.

2. First wind induced regime: liquid jet at intermediate Reynolds number breaks up due to aerodynamic drag force with drops diameter of the order of jet diameter.

3. Second wind induced regime: liquid jet at intermediate Reynolds number breaks up also due to aerodynamic drag force of drops at diameter smaller than jet diameter.

4. Atomisation regime: jet breaks up into much smaller drops at high Reynolds number, this occurs close to the nozzle exit.

For prediction of drop size, assumption were made by Reitz and Bracco [1979] for inviscid liquid jet that the radius of the drop varies linearly with wave length, the drop radius \( r \) is given as

\[
r = B \frac{2\pi \sigma}{U^2 \rho_g}
\]

where \( B \) is constant of order unity and \( \rho_g \) is the gas density. Wu et al. [1986] showed that equation (4.11) gave acceptable results when it is compared with the measurement of drop sizes at exit from diesel spray nozzles.

Similarly, studies through employing linear stability analyses to describe the formation and growth of waves development on the surface of the liquid combined with disintegrating of moving film into ligaments have been conducted for the investigation of the breakup of liquid sheets. Squire [1953] was clear in his research, that the breakup mechanism of sheets is caused by the growth of sinuous waves. Experimental results by Van Dyke [1982] showed that in the induced breakup of a liquid sheet from a perturbed fan spray nozzle by supplied external oscillation, the breakup of the sheet into rows of ligaments and droplets were born from the rims of the sheet. Gavaises and Arcoumanis [2001] showed aspects for modelling and experimental validation for transient sprays injected from high pressure -swirl atomizers. The atomization time and the size of the liquid sheet depend on the operating conditions and the nozzle configuration design. They assumed in their derivation for an atomization of a cylindrical liquid sheet that at the exit from the nozzle hole the liquid sheet has an annular cross-section, the flow is one dimensional and the film thickness remains constant together with axial velocity components, the flow is non-viscous and incompressible and no phase change happens whereas the external forces are neglected.
4.3.2 Drag model

The motion of droplets in the dispersed phase can be viewed as chaotic motion where the movement of droplets is determined by computing the forces arising from the interaction motion with the carrier phase. The equation of motion for droplets in fluid is formulated in the Lagrangian approach through solving a set of ordinary differential equations along the droplet path in order to calculate the linear and angular droplets acceleration. From this point, the droplet drag coefficient affects the droplets acceleration and hence its velocity and the change of location as a function of time. Basset [1888] calculated the drag force under creeping flow condition (i.e. for small particle Reynolds numbers) through the equation of motion for one dimensional flow for small rigid particles in viscous and quiescent fluid. Additional work was made by Boussinesq [1885] and Oseen [1927]. Therefore the equations of motion are known as BBO-equation related to them. Clift et al. [1974] applied Basset’s equation in three dimensional flows, with correlation for the calculation of drag coefficient. Compared to experimental results they found an acceptable error of 5 percent. Wallis [1969] suggested the drag coefficient is a function of Reynolds number for thin spray using solid spheres

\[
C_D = 0.424 \quad \text{for } Re > 1000
\]

\[
C_D = \frac{24}{Re} \left( 1 + \frac{1}{6} Re^{2/3} \right) \quad \text{for } Re < 1000
\]

O’Rourke and Bracco [1980] and O’Rourke [1981] developed the above equation for thick spray based on experiments on fluidized bed into

\[
C_D = \frac{24}{Re} \left( \theta^{-2.65} + Re^{2/3} \theta^{-1.78} \right)
\]

where \( \theta \) is the local void fraction. Mostafa and Mongia [1987] implemented in their approach the Lagrangian formula which introduced the drag force in terms of interface friction coefficient as,

\[
\vec{F}_d = \frac{3 \mu}{4 d_k} C_D \mid \vec{v} - \vec{v}_d \mid
\]

where \( v \) and \( v_d \) are the instantaneous velocity of the carrier phase and droplets, respectively and \( C_D \) is the drag coefficient taken from Mostafa and Elghobashi [1984]. Their study for evaporating rate suggested that the drag coefficient be calculated from the standard curve for solid sphere
with the same diameter. This curve is transformed from Clift et al. [1978] into

\[ C_D = \frac{24}{Re} (1 + 0.1315 Re^{0.82 - 0.05 w}) \quad \text{for } 0.01 < Re < 20 \]  

\[ C_D = \frac{24}{Re} (1 + 0.1935 Re^{0.6305}) \quad \text{for } 20 < Re < 260 \]

where \( w = \log Re \) and \( Re \) is the Reynolds droplet number based on the absolute value of the total instantaneous velocity. Moin and Apte [2006] showed that the drag force on a single droplet can be modelled by implementing the drag coefficient of a solid particle with modifications due to internal circulation and deformation,

\[ D_p = 0.75 C_D \frac{\rho g}{\rho_l d_p} |\vec{v} - \vec{v}_d| \]

and \( C_D \) is given in form of nonlinear correlation only for \( Re \leq 800 \) as

\[ C_D = \frac{24}{Re} \left( 1 + a Re^b \right) \]

where constants \( a = 0.15 \) and \( b = 0.687 \) and the modifications were based on the work of Helenbrook and Edwards [2002] for simulation axisymmetric liquid droplets in uniform gas stream. To improve the accuracy of prediction of the drag coefficient, focus was made on the model developed by Henderson [1969], who made a correlation to calculate the drag coefficient in both subsonic and supersonic regions for incompressible flow depending on the local Mach number.

In this present work the dispersed phase, the momentum exchange between the gas-phase and the droplet phase is due to drag force. Assuming spherical droplets, the force acting on a single droplet can be written as Lagrangian formula as presented in Beck and Watkins [2002] who applied in their development an Eulerian framework to describe the rate of change of droplet velocity as,

\[ \frac{d\vec{V}_{d,i}}{dt} = \frac{3}{8} \frac{\rho}{\rho_d} C_D \frac{\rho g}{r} |\vec{v} - \vec{v}_d(r)| (\vec{v} - \vec{v}_d(r)) \]  

where for the drag coefficient the correlation of Wallis which is mentioned above is used. The source term contribution due to inter-phase drag is defined as

\[ \vec{q}_{d,i} = \mu_0 \int_r \frac{d\vec{V}_{d,i}}{dt} \phi(r) r^i dr \]
In order to equate the rate of change of the moment-averaged momentum with equation (4.15), a number of steps are required. First, \( \vec{v}_d \) needs to be replaced by the moment dependent relation, \( \vec{v}_d(r) \) and secondly, the instantaneous continuum velocity, \( \vec{v} \), requires approximating. With the Eulerian dispersion model in place, the gas velocity consists solely of the mean component. However, with the alternative Lagrangian model, turbulent components are added. Here these are defined to be in isotropic form the velocity, \( \vec{v} \), is decomposed into its mean and fluctuating component, whereby the mean velocity is that solved by the continuum momentum equation and the fluctuating velocity is approximated using the turbulent kinetic energy, \( k \), provided by the turbulence model, as
\[
\vec{v}' = (\gamma - 0.5) \sqrt{\frac{2}{3}k}
\] (4.22)
where \( \gamma \) is randomly generated in the interval \( 0 - 1 \). The two equation gaseous turbulence model used in the present calculations assumes isotropic turbulence with the standard deviation of a Gaussian distribution. The drag term can either be evaluated analytically, performing a summation of three integrals (assuming the functional form of the velocity distribution is of a simple form) or numerically by discretizing the PDF and the droplet velocity profile. For analytical integration the conditions relating to the drag coefficient in Wallis suggestions that are rearranged to provide critical radii, \( r_a \) and \( r_b \) respectively. The drag term is then made up of three parts: the integral of equation (4.21) between 0 and \( r_a \), \( r_a \) and \( r_b \) and lastly between \( r_b \) and \( \infty \).

### 4.3.3 Breakup model

The phenomenon of the disintegration of larger drops and ligaments into smaller drops under certain conditions is known as the breakup or secondary atomization. The effect of drop breakup can be summarized as follows. The instabilities that occur for high relative motion between drops and surrounding gas causes a non uniform pressure and shear stress distribution on the drops surface opposed by surface tension and internal forces. These counteracting forces deform the drops. At very low relative velocities the drops are unaffected but when the aerodynamic forces become larger than the force due to surface tension the breakup occurs. A review made by Faeth [2002] at high relative velocities showed that the gas Weber number gives an indication for breakup. When the Weber number exceeds a critical value drops break up. He studied the
viscosity effect and showed that for low viscosity liquid

\[ We_{\text{crit}} = \text{constant} \quad \text{for } Oh < 0.1 \] (4.23)

\[ We_{\text{crit}} = Oh^2 \quad \text{for } Oh > 0.1 \] (4.24)

For high-viscosity liquid Hsiang and Faeth [1992] for high Weber number found that

\[ We_{\text{crit}} = 12\left(1 + 1.077Oh^a\right) \] (4.25)

where \( a \) is the exponential factor given in range 1.6 to 1.64. For diesel sprays the following model encompasses all break-up regimes. Break-up takes place if \( We > 6 \) and the model is valid for Weber numbers less than 1000. The stable diameter is defined as

\[ r_{st} = 6.2r_d \left( \frac{\rho}{\rho_d} \right)^{\frac{1}{4}} \sqrt{\frac{\mu_d}{\rho_d \parallel \vec{v} - \vec{v}_{d,i} \parallel}} \] (4.26)

and the corresponding timescale is

\[ \tau_b = \frac{5}{1 - Oh/7} \frac{r_d}{\parallel \vec{v} - \vec{v}_{d,i} \parallel} \sqrt{\frac{\rho_d}{\rho}} \] (4.27)

A simplified picture of breakup regimes can be mentioned as follows. According to Pilch and Erdman [1987] and Faeth [2002], there are two types of breakup mechanism in sprays, the bag breakdown for low Weber numbers and the shear breakup for high Weber numbers. Break-up occurs if

\[ We = \frac{2\rho \parallel \vec{v} - \vec{v}_{d,i} \parallel^2 r}{\sigma_d} > We_{\text{crit}} \] (4.28)

where the critical Weber number \( We_{\text{crit}} = 12\left(1 + 1.077Oh^{1.6}\right) \). Break-up phenomena are distinguished by their dimensionless breakup time, defined as

\[ T = \begin{cases} 
6(We - 12)^{-\frac{1}{4}} & \text{if } 12 < We \leq 18 \\
2.45(We - 12)^{\frac{1}{4}} & \text{if } 18 < We \leq 45 \\
14.1(We - 12)^{-\frac{1}{4}} & \text{if } 45 < We \leq 350 \\
0.766(We - 12)^{\frac{1}{4}} & \text{if } 350 < We \leq 2670 \\
5.5 & \text{if } We > 2670
\end{cases} \] (4.29)
The break-up timescale then is calculated, using $T$, giving

$$\tau_b = 2T \frac{r}{\| \vec{v} - \vec{v}_d \|} \sqrt{\frac{\rho d}{\rho}}$$

(4.30)

The stable droplet radius is found from

$$r_{st} = \frac{W_{e_{crit}} \sigma_d}{\rho \| \vec{v} - \vec{v}_d \| (1 - V_d)^2}$$

(4.31)

where

$$V_d = (0.375T + 0.2274T^2) \sqrt{\frac{\rho}{\rho_d}}$$

(4.32)

Another identification was made by Reitz and Diwakar [1986]. Their correlation is based on the review of Nicholls [1972]. The bag breakup occurs when

$$W_{e_{bag}} = \rho g \left| \vec{v} - \vec{v}_d \right|^2 r > 6$$

(4.33)

Similarly, shear breakup occurs when

$$\frac{W_{e_{shear}}}{\sqrt{Re}} > 0.5$$

(4.34)

where $Re$ is the Reynolds number given as

$$Re = \frac{\rho | \vec{v} - \vec{v}_d | d}{\mu}$$

(4.35)

where $| \vec{v} - \vec{v}_d |$, $\mu$ and $d$ are the relative velocity, kinematic viscosity and droplet diameter respectively. The time of breakup of drops are

$$\tau_{bag} = C_1 \sqrt{\frac{\rho_d v_d}{\sigma}}$$

(4.36)

and

$$\tau_{shear} = C_2 \frac{r}{U} \sqrt{\frac{\rho_d}{\rho_g}}$$

(4.37)

where the constants in the above equations are of order unity. A model called TAB (Taylor Analogy Breakup) is based on Taylor [1963] (the analogy between an oscillating forced droplet and spring mass system). O’Rourke and Amsden [1987] suggested that when implementing the TAB model, the spring force is related to the aerodynamic force and damping forces are
related to the liquid surface tension and the liquid viscosity force and the breakup time was measured depending on wave stability theory calculations. Linear stability analyses to describe the formation and growth of waves development on the surface of the liquid combined with disintegration of moving film into ligaments have been conducted for investigation the breakup of liquid sheet. Gavaises and Arcoumanis [2001] gave the definition for the breakup length as the distance from the nozzle hole exit to where the bulk liquid disintegrates into droplets. In addition they used the optimum growth rate $\omega_{opt}$ to determine the atomisation time as following

$$t_{atom} = \frac{C_{time}}{\omega_{opt}}$$

Where $C_{time}$ is an empirical dimensionless coefficient to be taken equal to 1.5. In order to determine the droplet formation the flow conditions at the nozzle hole exit should be taken into account at which the following condition is satisfied

$$t - t_{inj} > t_{atom}$$

where $t$ is the time for droplet formation and $t_{inj}$ denotes the time of injection of each individual droplet parcel. An approximation was made by Moin and Apte [2006] based on point-particle to produce a model for secondary breakup in realistic combustor geometry through using subgrid secondary breakup in which the radius of droplets is assumed to be time dependent with the given initial size distribution. The idea of their model that the breakup of large droplets can be viewed as the development of the distribution function around a large droplet in space and time according to Fokker-Planck (FP) differential equation. The distribution function for the breakup frequency and time is denoted as $T(x, t)$ for $x = \log(r_p)$ and $r_p$ is the droplet radius. The condition for breakup occurs when

$$t > t_{breakup} = \frac{1}{\lambda}$$

where $\lambda$ is the breakup frequency. The first production mechanism of surface density occurs when the interfacial surface of the liquid-gas undergoes growth of perturbations. These are followed by the formation into ligaments ending with breakup into smaller droplets. In the latter mechanism the production term is in competition with droplets internal forces, in essence surface tension forces.

The drop break-up models used here are standard ones taken from discrete droplet models Reitz
and Diwakar [1986]. However, for the present method they are re-cast into forms which allow the effects to be manifested in the moment values, and also in terms of the general gamma number size distributions. The bases of the models have been expressed in detail in Beck and Watkins [2002]. Here the methodology used is outlined and the final equations for the components of the source terms \( q_{Q_i} (i = 1, 2 \text{ and } 3) \) due to drop break-up are derived. These are later re-evaluated using the general gamma distribution. There is no source term for the \( Q_3 \) moment equation due to break-up as the total volume of drops is unchanged.

Three break-up models are presented. The first model of Pilch and Erdman [1987] encompasses all the known break-up phenomena. The second model of Hsiang and Faeth [1992] is applicable for diesel spray cases, whereby no categorizations are made regarding the droplet break-up methods. Lastly, the model of Reitz and Diwakar [1986] considers secondary break-up only; that of bag and stripping break-up.

With all the models, the manner in which they contribute to the source terms of the moments equations is the same, only the number of droplets produced, \( N_b \) and the timescale for this process, \( \tau_b \), differs between the models.

The source term contribution to the moment transport equations due to break-up is of the form

\[
q_{Q_i} = Q_0 \int r \frac{\delta r^i}{\delta t} n(r) \, dr
\]

(4.41)

where

\[
\frac{\delta r^i}{\delta t} = \frac{(N_b - 1) r^i}{\tau_b}
\]

(4.42)

The number of droplets produced from the break-up of a single droplet is determined by considering droplet volume conservation, giving

\[
N_b = \left( \frac{r}{r_{st}} \right)^3
\]

(4.43)

where \( r_{st} \) is the stable droplet radius. None of the resultant terms of the break-up models are presented in integral form, although the first model can be integrated analytically Beck and Watkins [2002]. The remaining models must be either integrated numerically or approximated to enable analytical integration. In this work the former method of numerical integration is implemented.
4.3.4 Collision model

The interaction of two or more liquid droplets during their movement because there are differences in velocities, can lead to several collision events such as bounce, coalescence (a combination of droplet masses) or disruption, that what is called collision. The effect of collisions must be modelled as these become important in dense spray, especially in the region near the injection nozzle where the number of droplets is large and the probability to collide is high. Five regimes are have been identified by Orme [1997]. When the surrounding gas between two droplets prevents them to contact the drops bounce. The drop masses combine to form a single drop, at low Weber number where there is enough time to deform the gap between drops, this regime known as slow coalescence. On the other hand, coalescence may occur at higher Weber number where the velocity is capable of overcoming a gas layer. Separation collision refers to temporary combination followed by separation into two or more droplets. Reflex separation regime appears when the Weber number is high and the droplets undergo combination followed by flattening in the normal direction. Surface tension then makes the drop radially inwards end with breakup of the cylinder. Finally, stretching separation occurs just when a part of each droplet interact with other forming a small interconnected region and the rest of the droplets stay in their trajectory unaffected stretching the interaction region. The presented model by O’Rourke and Bracco [1980] implemented in the KIVA computer programme used Poisson distribution method to describe the probability of number of collisions that take place between each parcel in the same control volume in one time step,

\[ P_N = \frac{n}{N!} \pi \]

(4.44)

Where \( \pi \) is the average number of collision given by:

\[ \pi = \frac{c \pi}{V_{cell}} (r_1 + r_2)^2 U_{rel} \delta t \]  

(4.45)

To know whether a collision takes place a random number is taken from a uniform distribution and compared with \( P_N \). If the random variable > \( P_N \) then collision is valid. They also suggested that the probability of collision between two droplets per unit volume per unit time is given by

\[ P_{coll} = \frac{\pi}{V_{cell}^2} (r_1 + r_2)^2 U_{rel} \delta t \]  

(4.46)
Since not all collisions result in coalescence, the probability that coalescence takes place is

\[ P_{\text{coal}} = \min \left[ 2.4 \frac{f(\gamma)}{W e_L}, 1 \right] \]  

(4.47)

where \( \gamma = r_2/r_1 \) and

\[ f(\gamma) = 2.7\gamma - 2.4\gamma^2 + \gamma^3 \]  

(4.48)

and

\[ W e_L = \frac{\rho_d ||\vec{u}_c - \vec{u}_d||^2 r}{\sigma_d} \]  

(4.49)

By generating two random numbers, \( N_{r,1} \) and \( N_{r,2} \), in the interval \((0 - 1)\) the actual occurrence of a collision taking place is if \( N_{r,1} > P_{N=0} \). If collisions take place then coalescence is the result of that collision if \( P_{\text{coal}} < N_{r,2} \) and the number of donor droplets involved is found from the Poisson distribution, such that

\[ \sum_{i=0}^{N-1} P_i < N_{r,1} < \sum_{i=0}^N P_i \]  

(4.50)

In Eulerian models drop parcels do not exist. However, Beck and Watkins [2003a] developed an equivalent form including the drop number distribution moments by multiplying the collision probability by appropriate number of distribution and integrating over all droplets, so they got:

\[ N_{\text{coll}} = \frac{\pi C_{\text{coll}} U_{\text{rel}}}{2V_{\text{cell}}^2} \int \int (r_i + r_j)^2 U_{\text{rel}}(r_i, r_j) n(r_j) \, dr_i \, dr_j \]  

(4.51)

Here \( U_{\text{rel}} \) is the relative velocity between the two drops and it is a function of \( r_i \) and \( r_j \). As a final approximation they used a mean value by assuming the mean value between all colliding droplets. Subsequently they evaluated the number of collision as

\[ N_{\text{coll}} = \pi C_{\text{coll}} U_{\text{rel}}[Q_0Q_2 + Q_1^2] \]  

(4.52)

where the volume of the cell \( V_{\text{cell}} \) cancel out because they measure the droplet number per unit volume. \( C_{\text{coll}} \) is a model constant whose value has been found to be 0.15 by comparison of model results with experimental data on drop size. In Orme [1997], two parameters are required to determine the proportions of drops that collide. These are Weber number \( W e \) and the impact parameter \( (b) \). The latter is defined as the perpendicular distance from the centre of one droplet to the relative velocity vector placed on the centre of the other droplet at impact normalised by the sum of the radii. The collision regimes are explored by Jiang et al. [1992] through a chart
for hydrocarbon droplets where the $x$–axis represents Weber numbers versus impact ($b$) at an ambient pressure of 0.1 MPa.

The most commonly used collision model is based on the work of O’Rourke and Bracco [1980]. This has been used extensively in discrete droplet models of sprays. Here the present work implemented the model that is adapted to the current moments-based approach to spray modelling. In the model the number of collisions, per unit total volume, between a drop of radius $r_2$ and smaller drops of radius $r_1$, provided they are in the same computational cell. The form of the source term contribution is similar to that of the break-up model. Here, the number of droplets undergoing coalescence is determined by empirical and statistical methods in addition to critical radii conditions. The coalescence of $N_d$ donor droplets of radius $r_d$ with a collector droplet of radius $r_c$, results in

$$\frac{\delta r^i}{\delta t} = \frac{1}{\delta t} \sum_{r_d} r_c \left[ (r_c^3 + N_d r_d^3)^{\frac{1}{3}} - r_c^i - N_d r_d^i \right]$$  \hspace{1cm} (4.53)

The number of donor droplets undergoing coalescence is determined by the following method: The probability of a collector droplet undergoing $N$ collisions with droplets of size $r_d$ in the time interval $\delta t$ is assumed to follow the Poisson distribution that is given in equation (4.44).

### 4.4 Presentation of the case study

#### 4.4.1 Description of the experiment

The case consider a non-evaporative hollow cone spray. Spray images and mean drop size were experimentally studied according to Ren and Nally [1998]. The configuration set-up consists of an imaging system and Phase Doppler Particle Analyser (PDPA). A Nd:YAG laser was established as the light source. A CCD camera using back-lighting technique was used to capture, confirm and interpret the results qualitatively. Definitions of the the measurements of spray structures in the axial plane were visualized by Mie scattering images. The measurement principle was based on interfering laser beam through a set of cylindrical lenses to form the light sheet. The flow conditions for the dispersed phase were based on the injection pressure as this parameter is considered the most important in the design of the fuel delivery system. In the present work a 5.5 MPa injection pressure is chosen to be the reference case. N-heptane was injected into air with a uniform injected velocity. The fuel exits from a pressure-swirl injector for a Gasoline Direct Injection (GDI) Spark Ignition (SI) engine to form the hollow cone spray.
The nozzle has a radius of 0.45 mm. The nominal spray cone angle was measured as 80°. The calculated axial and radial velocity components at the nozzle exit were 31.96 m/sec and 80.56 m/sec respectively. The Sauter Mean Diameter (SMD) and the sheet thickness at the injector were 32.2 µm and 38.6 µm.

4.4.2 Description of the simulation setup

The numerical computation of spray moments method are done, to be compared to the experiment described above. Computational calculations require two types of input data. Initial and boundary conditions are required from the experiment for the dispersed phase that is spatially full resolved. In addition the gaseous flow field has to be set as a function of space and time even if there is a lack of experimental data, because the dispersed phase is coupled to the numerical simulations of the gas phase. The spray model presented in this work will be used to simulate the experimental case computationally in order to assess the capability and the accuracy of the modelling method. The main aim is to show the new scheme performance compared to older schemes. The liquid is injected from the bottom left-hand of the computational cylinder. The cylinder of 100 mm x 50 mm is discretized via unstructured grids of polyhedral shape as shown in figure (4.4). The resulting computational domain consists of 7799 volumes, 15787 faces and 7989 vertices. The flow develops after the injection and becomes very complex due to many phenomena occurring. This need to be addressed in the model. An essential way to handle this problem is the refinement of grids around the injector up to five inlet cell faces and up to 15 percent of the whole domain as explained in figure (4.4). The injection duration is set as 2 ms as mentioned in the experiment with a constant time step of 2 µs. The underlying distribution is assumed to be a gamma distribution with a cropping multiplier set to $1 \times 10^{-7}$. The effects of the used schemes will be explained and discussed later.

The case is run at room temperature with an ambient pressure for the gas phase. The gas velocity is initially assumed to be zero while the turbulence model is starting with a very small initial value for turbulent intensity. Only the turbulent kinetic energy and dissipation rate require non-zero domain initialisation. Values of these are sought such that the resulting eddy viscosity is as small as possible without causing the algorithm to diverge early in the solution procedure. Over-estimation of eddy viscosity has been found to excessively resist the acceleration of the continuum phase. The characteristic length scale of the initial turbulence is assumed to be 1 cm with a velocity of 40 m/sec at 5% intensity. Two iterations are performed on all gradient
calculations, dropping the error one order of magnitude. Further iterations of the gradient showed very little gain in accuracy. Pressure and pressure correction are interpolated from the near-boundary CVs to the boundary after the first iteration. Outer iterations are limited to 20 and is assumed to converge once the global maximum normalised (1-norm) residual has dropped three orders of magnitude. Inner iterations (of the linear system) are required to drop the residual one order of magnitude.

4.5 Results and discussions

The comparison with the experimental data is shown in figure (4.5). Here will be included many investigated reasons that may affect the presented results. Although different convection schemes are applied, but the difference is very small due to the definition of the spray tip penetration in hollow cone type compared to Beck and Watkins [2003a] the spray tip penetration is taken to be slightly different in this case as the spray tip does not necessarily travel in an approximately straight line as in solid cone spray. Hence the spray tips are much less densely populated and so the forward most 1% of the liquid volume fraction stretches well back from the spray tip. A useful definition for the spray tip penetration will be dependent in this work. In order to gain meaningful results the definition is the distance from the nozzle orifice to the a position where the liquid volume fraction is 98% of the integrated amount. For producing better results the physical processes that are taking place are taken into account during the spray development. Effects of spray breakup, collision and interface drag are activated. In addition the gas turbulent induction is involved in the computational calculations.

4.5.1 Penetration

Three different TVD, WAF and WAF-STACS schemes have been simulated using identical initialisation and boundary conditions. The last scheme produce better results than the others based on spray structure. The results presented in figure (4.5) reveal that the computational differences are not significantly affected by the application of different convection schemes. This is mainly due to the fact that the thickness of the spray sheet is small 195 µm as measured experimentally at the nozzle exit. Even though the moments method takes into account spray sub-models still the flow is mainly controlled by the momentum exchange between the two-phase as explained later. The results show that at early injection period up to 0.8 ms, approximately half the injection period, an over-estimation of penetration is obtained. This is due to the start-
up conditions for the pressure swirl atomizer used in this experiment. In addition one source of error in the solution appeared here due to use of a dense grid near the injector where the probability of breakup and collision droplets are expected. Near the injector, as the grid density is increased the penetration increased due to increase grid resolution which tends to improve the prediction for the momentum transfer between the gas phase and the spray. This allows to produce a smaller relative velocity (lower drag) leading to higher spray penetration as in Li and Kong [2009]. In addition, the high number of grid points near the injector contains the effective bulk of spray droplets, which in turn tend to increase the convection in spray velocity.

In order to quantify the differences between the experimental data and the new convection scheme predictions, a percentage difference between the two are obtained where the experimental datum is taken as the reference. The results presented in figure (4.5) show that the maximum difference at the end of injection period is about 13%. Therefore with this accuracy there is no need to make a mesh refinement to improve the spray penetration for the reasons which will be explained in details below and in grid analysis section. In both computational results and experimental data. There are uncertainty concerning the actual penetration. This is because in all simulations presented in this work the liquid volume fraction is used in the comparison with the experimental data. The spray volume is cropped when the liquid volume fraction is less than $1 \times 10^{-7}$. While in experimental data, the measurements depend on the visualization tools used.

In this study the in-house code used is able to handle very fine grids with cell size of order $10^{-3}$ m in the downstream volume while the nozzle cells are $O(10^{-6})$m. The effect of refining grids significantly increases the spray penetration. Tonini et al. [2008] found the spray tip penetration to be highly depended on grid resolution. As the number of grids increases and become dense specially in the region near the injector up to 20 mm in the axial direction, so the predictions of spray penetration are improved to record an over-estimation. Here after 1 ms after injection starts the spray enters grids that are relatively coarse so the results are exhibiting an under-estimation of spray penetration values. This difficulty was encountered because of the hollow cone spray shape where the trajectory must be precisely predicted. This is in contrast to the adaptive local grid refinement in selecting zones which is it easy to implement with other types of spray for example solid cone. However the number of computational calculations and time taken increase dramatically with finer grids.
4.5.2 Spray structure

Figure (4.6) contains contours of liquid volume fraction over the range between $10^{-5}$ to $10^{-7}$ at 2 ms after start of injection. Results are obtained using either TVD-Superbee, WAF-Superbee or WAF-STACS scheme. The performance of the schemes will be determined according to the analyses of the spray structure. The spray tips are the leading edge occupied by droplets injected at different times and which have been subjected to different amount of influences either by the entrained gas or the droplets themselves. Greater differences are seen at the spray tips, as illustrated in figure (4.7). As expected the TVD-Superbee produces the most dense tip because of highly compressive scheme as shown in figure (4.7)(a). This deficiency is improved with WAF-Superbee due to WAF scheme using the central difference scheme instead of upwind scheme which is performing worse with unstructured grids because the flow is not aligned with grid line as in structured grids. Figure (4.7)(b) shows this by a slightly less dense spray than TVD-Superbee scheme. The WAF-STACS scheme results in figure (4.7)(c) are less dense than the previous two schemes. The switching strategy that is almost independent of Sweby’s factor \( r \) as explained in equation (4.2) keeps the sharpness at the interfaces. This is not the only reason for this scheme to be the best.

The bulge at the inner periphery of the spray tip provides an indication that at the end of injection period, the droplets tends to move towards the spray core due to the development of induction gas turbulence. The spray thickness at any point and its radial coordinates are considered in this study is essential parameters in the stability analysis. It can be seen that the spray thickness varies with the radial distance. It is not clear to say that the spray thickness is strongly related to the region closest to the nozzle orifice because of a high numerical diffusion for all convection scheme even when schemes are blended with over-compressive scheme (Superbee), which is known to be less diffusive. The proposed scheme tends to reduce the number of computational cells at the interface and the computational cost. Figure (4.8) illustrates that the second-order WAF-STAC scheme produces the thinnest spray tip on the unstructured grids compared to the WAF-Superbee scheme which produces a slight thicker spray tip. The TVD-Superbee scheme is shown to be poor by representing a thicker spray. Figure (4.9) presents results for the narrow region of liquid behind the spray tip. This region is chosen due to the entrained gas effect being very small in this region as shown later in gas velocity profiles. Unfortunately there is a lack in the experimental data about spray thickness. However the interpretation for spray thickness is based on the fact that a large sheet thickness as appearing in TVD-Superbee
scheme means that more liquid is diffused because the TVD scheme is based on upwind scheme which produce diffusive flow. The results for both WAF-Superbee and WAF-STACS schemes produce a higher penetration and velocity (as will be discussed in next paragraph) than TVD-Superbee. That gives an indication that TVD-Superbee scheme is not appropriate for moments transport equations, since the first order upwind scheme tends to be highly diffusive even when blended with higher order compressive Superbee scheme. This normalisation as compared with normalised second order central difference (referring to both WAF schemes) is less accurate. The WAF-STACS scheme exhibits a thinner spray than the others with a thickness of about 2 mm or less. The boundedness is perfectly satisfied because of using the non-linear blending, where the bounded downwind scheme is used when the interface is in parallel with considered face and it is switching with Higher Resolution scheme when the interface is orthogonal to the face.

4.5.3 Two-phase velocity

Other relevant results which are involved in the validation of the mathematical model are obtained through data from the momentum transport equations. Figures (4.10), (4.11), (4.12) and (4.13) show axial and radial velocity profiles in the axial and radial directions. The third moment velocity components are used for this calculations, giving special attention to the differences on the schemes behaviour in the convection term. The WAF-STACS scheme is formulated based on the idea of the donor-acceptor formulation, i.e. as a scheme that varies as a function of the interface-cell face angle. This technique of discretization deforms the interface shape because it does not comply with the local boundedness criteria and depends on the interface velocity direction and the angle it makes with the integration cell face. In all velocity components, the results simulated with TVD-Superbee scheme are higher than WAF-Superbee and WAF-STACS schemes because the prediction method is based on the upwind scheme while the others are based on central difference scheme. Figures (4.14) and (4.15) show both velocity components calculated at x=25 mm downstream after 2 ms. The axial profile shows that the maximum velocity occurs near the inner spray edge. That is because large droplets which are heaviest (biggest momentum) are found here. Whereas in radial profile the maximum velocity value is found in the centre due to the presence of recirculation zone as shown in figures (4.16),(4.17),(4.18) and (4.19) for axial and radial components of the gas velocity at 2 ms, thus the radial component is reduced due to the drag of the entrained gas that tends to oppose the radial liquid velocity component. Furthermore the centrifugal forces affect on the droplets tends to push them away.
from the inner periphery to the outer periphery. The influence of convection schemes on the liquid momentum transport equation can be evaluated. Here in this application, it is important to return to the main drawback of TVD-Superbee scheme that is due to compressive blending. This tends to reduce the accumulation of liquid at the inner spray edge. On the other hand, WAF-Superbee and WAF-STACS schemes exhibit a higher axial velocity at the inner edge. In order to get a full picture contours of axial and radial gas velocity components are shown in figures (4.20) and (4.21) respectively.

The WAF scheme is based on the second order central differencing scheme. Consequently the accuracy of the scheme is proportional to the grid width squared. However the results tend to be more diffusive at the outer spray edge in which the error is increased towards the outer edge because the grids tends to be a less fine. This can be avoided with the WAF-STACS scheme that implements the less diffusive high resolution (HR) which is blended with the bounded downwind (BD) scheme.

It can be seen the difference between the general trend of whole spray behaviour and taking a cross section. This gives an extra indication about the accuracy of the proposed moment method and its treatment to the momentum equation based on drop size classes.

### 4.5.4 Sauter Mean Radius

Figure (4.22) shows the computations of Sauter Mean Radius (SMR) at a location of \( x=30 \) mm downstream of the nozzle for a time of 2 ms. The spray tip penetration and SMR are affected by many physical processes that may occur after the spray injection. This explain why the computed results are selected in a cross section close to the spray tip. The effects of spray hydrodynamics in this study cannot be split into separated single terms to study their effects alone because they represent the source term in moment and momentum transport equations. Figure (4.22) shows a significant difference between WAF schemes and TVD scheme because of using the second order stencil interpolation with unstructured grids. WAF schemes produce oscillatory behaviour near the inner edge of the spray. This unphysical results is a spurious error which can only take place at the discontinuity in phase, concentration ...etc as explained in details in Zhang et al. [2010].

Physically in all computed results, due to the presence of smaller droplets in the inner spray edge which are undergoing extra aerodynamic interactive accompanied by a large amount of droplets breakup, so the peak of SMR that represents the ratio of volume to the surface area
of the spray is found here and gradually decrease towards the outer edge. It can be concluded that for the most part, collision effects are only important in the very near nozzle region.

### 4.5.5 Turbulent flow

Regarding turbulence modelling, the \((k-\varepsilon)\) model has been implemented to characterize the gas turbulent flow field. Figures (4.23),(4.24),(4.25) and (4.26) show both turbulent kinetic energy and dissipation versus the axial and radial distance respectively. These results have been included here to finalize the numerical analyses. From numerical viewpoint, using higher order schemes such as WAF-STACS scheme can lead to minimize the numerical diffusion errors but the computations tend to be less stable. The figures present comparisons between TVD-Superbee and WAF-STACS schemes, to observe if there is over or undershoot in the calculations. Figure (4.27) shows the variation of the turbulent kinetic energy to turbulent dissipation energy where it is not similar to ensure the variation of the eddy life-time is affected by numerical tools in order to provide a stability along the solution. Figures (4.28) and(4.29) show the instability comes about because in the solution some values are including large gradients which can potentially lead to non-physical behaviour. The extreme unstable case in the \((k-\varepsilon)\) model is the exist are of negative values which were not found. The WAF-STACS scheme can be considered a new convection scheme that can produce accurate solution for spray modelling.

### 4.5.6 Grid analysis

GAMBIT software is used for providing criteria for grid refinement based on increase grid resolution at certain places by increase the number of intervals or the compression ratio. Refinement of grids can be used to capture flow details without being excessive as determined by non-zero droplets source terms in a grid cell. One of the basic strategy of grid refinement methods is that increase the compression ratio by increase the number of discretized cell at the axis of symmetry, however the presence of internal grid and the rest of grid boundaries are also affected by this change. Four different computational grids of different grid resolution are made to show the effects of grid refinement. Table (6.1) shows the grid specifications. All calculation are taken at time 1.6 ms.
The axis of symmetry in case A is discretized into 80 intervals with compression ratio of 98%. The coarse grid at case A gives a higher penetration than the others as shown in figure (4.30) but it gives a thicker sheet thickness as shown in figure (4.31)(a). The axis of symmetry is refined by decrease of the compression ratio to 97.5% in case B. Case B produces less penetration than case A as shown in figure (4.30) with a thinner sheet thickness than case A as shown in figure (4.31)(b). More refinement for the axis of symmetry is obtained by decreasing the compression ration to 97%. A slight lower penetration is found for case C than case B as shown in figure (4.30) with a better distribution for droplets inside the sheet thickness than case B with approximately the same sheet thickness as shown in figure (4.31)(c). A problem appears when more refinement is done, the grid shape is distorted to give undesirable shape for the grid specially near the vicinity of the injector. However refinement for all computational domain boundaries has been for case D to give the thinnest sheet thickness compared to the previous cases as shown in figure (4.31)(d). A decrease in the spray penetration by 15% has been observed with finer grids case D because spray penetration depends mainly on the liquid velocity (momentum equation). With a larger number of control volumes, comes an increase of the momentum transferred to the gas phase and consequently increase in the gas velocity. The density of grids is optimised by sensitivity studies to be fine enough to capture the spray sheet thickness.

### 4.6 Conclusions

The results obtained for the three test simulations show that the novel WAF-STACS scheme for handling the construction of interfacial flows in two-phase systems implemented with unstructured grids topology based on a switching strategy is a viable and accurate method. The solution procedure produces accurate results as comparing with standard high resolution schemes. The advantage of the new convection scheme is the blending factor which is a function of angle between the interface and the grid lines. Additionally it can conveniently used the flux limiters to blend high resolution and compressive schemes to calculate the flux through the cell face.
(a) Convection node notation.

(b) Angle between interface and cell face.

Figure 4.1: Unstructured grid notation.
Figure 4.2: Blending strategy for interface-capturing schemes.

Figure 4.3: Flux face with high resolution SMART scheme.
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Chapter 5

Sprays evaporation

5.1 Introduction

One of the primary interests in many engineering applications is the heat and mass transfer processes. Combustion in gas turbine combustors and internal combustion engines is related to evaporation and mixing in desired manner under certain ambient conditions. With growth in computation of two-phase flows nowadays, there has been a great demand for describing the interface transfer of mass, momentum and energy. Also, to overcome the greatest challenges when the spray fuel is injected, the spray structure and trajectory must match the flow field to evaporate in a short time and be distributed in a practical manner under a variety of ambient conditions. The reduction of emissions and improving the combustion efficiency are the most important features for design of next generation of gas turbine engines. Mainly the evaporation process of a single droplet passes through two main phases. Firstly, the separation of fuel molecules from the surface of the droplet into the surrounding gas. Secondly, diffusivity of fuel vapour from the surface into the gas in the vicinity of the droplet. In order to achieve a full scenario, this process starts with two steps needing to be performed. The mathematical modelling for the first point mentioned above, followed by the modelling for the second. Evaporation of droplets is enhanced by higher gas ambient temperature during their motion as well as the droplet residence time which allows the complete vaporization of droplets. The flow in the liquid phase is relatively complicated. Due to the number of different physical phenomena that take place simultaneously, breakup, coagulation and vaporization. Extensive research works in the area of numerical simulation of spray vaporization have been done to improve the further optimisation where the distribution of fuel vapour in combustion chamber is decisive in new
engine concepts. Various models were found to describe the deviation of phase transition on the droplet surface i.e., the transport processes inside the droplet and the two phase interfacial interaction. In many combustion devices such as gas turbine and direct injection gasoline engines, it is strongly required to predict the two-phase flow that results from injection of liquid fuel via pressure swirl atomiser. The latter is widely used to generate hollow cone sprays. It has advantages to produce a thin liquid sheet and well atomised spray at relatively low pressure. Because of the centrifugal force, the fuel injects through the discharge orifice as a thin conical sheet at a certain pressure and velocity. Following its production from the discharge hole, the liquid sheet gradually spreads towards the radial direction while moving it becomes weaker as it flows downstream. It disintegrates into ligaments which eventually further disintegrates into fine droplets and produces hollow cone sprays.

5.2 The problem

5.2.1 Motivation

It is possible to minimize the drawbacks of using Eulerian-Eulerian framework and it will become one of the most important features for this approach. Basically two approaches are used to simulate the flow field in most engineering applications, namely Eulerian-Eulerian and Eulerian-Lagrangian methods where both methods are based on Reynolds-averaged Navier-Stokes equations. The Eulerian-Lagrangian method can only be applied for dispersed two-phase flow which accounts for the discrete nature of individual particles. In contrast, the Eulerian-Eulerian method treats both phases as interacting continua. Focusing on the latest approach, therefore in order to account for the interactions between phases, for example heat and mass transfer and momentum exchange. The characteristics of the flow field such as mass and velocity of particles are averaged over an averaging volume (computational cell). Essentially there are no difficulties in modelling when there are no phase changes in liquid phase, thanks to the conservation of mass. The liquid volume fraction concept can cope with interactions between the two-phases with less computational effort and more efficiently. No longer this concept is validated when there is a change in mass whether increased or decreased due to the interaction with environment. Due to evaporation there are consequently continuous variations of gas and liquid thermophysical properties such as viscosity, density, thermal conductivity, . . . etc. However film temperature is suggested to be used in prediction of thermophysical properties.
5.2.2 Film temperature topology

A simple and explicit formula will be adopted here dealing with calculation of the film temperature. The idea comes from:

1. The accuracy of all heat and mass transfer equations are depending on evaluating the thermophysical properties at a temperature called film temperature. This temperature mainly belongs to the extracted fuel vapour from the surface of droplets due to the evaporation process. To get a full picture evaporation process can be defined as the escape of molecules from the surface of the liquid when they received high energy to form vapour. At a lower energy only a few molecules possess enough energy to release from the liquid surface by overcoming molecular attractions. The method uses the contribution of the fuel vapour mass fraction. The fraction values determine closely the amount of the liberated vapour that enters the gas phase, where fuel vapour mass fraction can give an indication about the reduction in liquid phase.

2. The mixing process between fuel and air is directly influenced by the mass transfer rate. Recently Colin and Benkenida [2003] had proposed a new model for mixing in evaporating two-phase flows. The proposed model consists in constructing two transport equations, one for the variance of fuel mass fraction $Y''$ and one for the scalar dissipation $\chi$. The variance equation depends mainly on the fuel mass fraction leading the approach towards the creation of the film around droplets due to evaporation being related directly to it.

3. The film temperature can be written as

$$T_{film} = T_d + F(f)(T_g - T_d)$$

(5.1)

where $F(f)$ represented any function in terms of the vapour mixture fraction to describe the evaporation process. Numerous past approaches selected a reference value for the temperature which is based on compromise between gas and liquid temperatures through a coefficient of contribution. Sparrow and Gregg [1961] first proposed the value of the coefficient equal to $(1/3)$, whereas a moderate value of $(1/2)$ is recommended by Law and Williams [1972]. A quick glance to all evaporation models that are mentioned below, in general they are sensitive to thermophysical properties value. Therefore through a simple formula which is based on vapour mass fraction, it precisely deals with both local spatial and thermal variations for properties.
5.2.3 Formulation of the problem

Hot gas-droplet flows can be used in a wide range of industrial applications. A common calculation is to evaluate the mass of liquid leaving drops that undergo evaporation. Because of the dynamic interaction by convection around cold droplet, a film is formed in the vicinity of the droplet surface. The discontinuity of liquid temperature is noticed when the droplet surface temperature cannot exceed the boiling point temperature. In order to characterize this layer one parameter is used here, the local film thickness (δ) which is treated as the thickness of the boundary layer.

In this case, a spherical droplet has been assumed subjected to hot environment. The droplet absorbs the heat from the gas and some mass evaporates. The heat conduction equation can be written in spherical coordinates as

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dT}{dr} \right) = 0 \]  

(5.2)

The boundary conditions as explained in figure (5.1) \( r = r_s, T = T_d \) and \( r = r_s + \delta, T = T_g \). The solution of the above after applying boundary conditions is

\[ T(r) = T_d + (T_g - T_d) \left[ 1 - \frac{r_s}{r} - \frac{r_s^2}{r \delta} + \frac{r_s}{\delta} \right] \]  

(5.3)

where \( T_d \) and \( T_g \) are the liquid and gas temperature respectively. \( r_s \) and \( \delta \) are the droplet radius and vapour film thickness. In the spray model, the physical properties in the film are evaluated at the mean temperature of vapour film boundary layer. Integration of the equations of temperature profile across the vapour film thickness yields the following equation:

\[ T_{mean} = \frac{1}{\delta} \int_{r_s}^{r_s + \delta} T(r)dr \]  

(5.4)

\[ T_{mean} = T_d + (T_g - T_d) \left[ \frac{(r_s + \delta)}{\delta} - \frac{r_s (r_s + \delta)}{\delta^2} \ln \left( 1 + \frac{\delta}{r_s} \right) \right] \]  

(5.5)

The vapour film thickness is assumed much smaller than the radius of the droplet, so the expansion of the natural logarithmic function will include only the first two terms, thus

\[ T_{mean} = T_d + (T_g - T_d) \left[ \frac{(r_s + \delta)}{\delta} - \frac{r_s (r_s + \delta)}{\delta^2} \left( \frac{\delta}{r_s} - \frac{\delta^2}{2r_s^2} \right) \right] \]  

(5.6)
$$T_{mean} = T_d + (T_g - T_d)(\frac{1}{2} + \frac{\delta}{2r_s})$$  \hspace{1cm} (5.7)

As mentioned before, the objective of the present work is to develop a more generalized equation for dense spray applications taking account of interaction between the two-phase through a dynamic variable. At each computation time step ($\delta$) depends on the local mass transfer rate in the heat and mass transfer model, thus an approximation for the last in equation (5.7) has been sought to include the vapour mass fraction implicitly. Spray moments theory suggested by Beck and Watkins [2002] can be utilized to describe how the evaporation of droplets are treated in terms of one computational cell using Eulerian-Eulerian framework, thus

$$Volume \ of \ evaporated \ droplet = 4\pi r_s^2 \delta$$  \hspace{1cm} (5.8)

$$Mass \ of \ vapour \ evaporated = 4\pi \rho_v r_s^2 \delta$$  \hspace{1cm} (5.9)

where $\rho_v$ is the vapour density. The fraction of mass evaporated from a single droplet is thus

$$f = \frac{4\pi \rho_v r_s^2 \delta}{4/3\pi \rho_l r_s^3} = \frac{3\rho_v \delta}{\rho_l r_s}$$  \hspace{1cm} (5.10)

where $\rho_l$ is the liquid density. If all drops are evaporated then

$$m_v = Q_0 \rho_l (4/3\pi r_s^3) \ \text{per unit volume}$$  \hspace{1cm} (5.11)

where $Q_0$ is the number of droplets. The maximum value of vapour mass fraction generated by evaporation all drops inside one computational cell can be written as

$$f_{max} = \frac{Q_0 \rho_l (4/3\pi r_s^3)}{\rho_{gas} \Theta + Q_0 \rho_l (4/3\pi r_s^3)}$$  \hspace{1cm} (5.12)

where $\rho_{gas}$ is the gas density and

$$\Theta = 1 - \frac{Q_0 \rho_l (4/3\pi r_s^3) \rho_l}{\rho_v}$$  \hspace{1cm} (5.13)

In order to obtain the value of vapour mass fraction generated by all droplets inside the computational cell the fraction of mass evaporated from a single droplet is multiplied by the maximum
value of vapour mass fraction as

\[ f = \frac{3\rho_v \delta}{\rho_l r_s \rho_{gas} \Theta + Q_0 \rho_l (4/3\pi r_s^3)} \quad (5.14) \]

Rearrangement yields

\[ \frac{\delta}{r_s} (Q_0 (4/3\pi r_s^3)) = \frac{f}{3\rho_v} [\rho_{gas} (1 - Q_0 4/3\pi r_s^3 \rho_l / \rho_v) + Q_0 4/3\pi \rho_l r_s^3] \quad (5.15) \]

The term inside the brackets on the left hand side represents the total volume of droplets. The second and third terms on the right hand side are approximately equal and therefore are cancelled. Then the resulting equation yields an algebraic relation among the local vapour mass fraction, vapour film thickness and droplets radius, per unit volume of the droplets,

\[ \frac{\delta}{r_s} = \frac{f \rho_{gas}}{3\rho_v} \quad (5.16) \]

The fuel vapour mass fraction as the droplet evaporates can be defined as the ratio of the reducing in droplet radius to the reference one, i.e., \((\delta/r_s)\). Therefore the spray film temperature can be expressed as

\[ T_{film} = T_d + (1/2 + f \rho_{gas} / 6\rho_v)(T_g - T_d) \quad (5.17) \]

### 5.3 Theoretical perspective

Four aspects were found to classify heat and mass transfer of droplet into various evaporation models. In order to translate the physical phenomena into a model, two steps are required to describe the gas phase around the droplet and the transportation process inside the droplet assessed by the interfacial interactions between the two phases. All models depend mainly on the liquid phase and with how the interior transporting heat transfer is modelled. The uniform model, alternatively called the infinite diffusion model, assumes that heat and mass transfer processes take place quickly and the thermophysical properties and the chemical composition inside the droplet are uniform.

With regard to turbulence effect, for all models calculations were carried out by most of the researchers in which turbulence effects on the droplets were modelled. Most cases used standard \(k - \varepsilon\) model which is coupled to the evaporation model. Only the film theory approach incorporates the turbulence effect in the model itself. Basically the heat and mass transfer processes
are taking place in a thin region around the droplet core between the droplet surface and the surrounding gas. The fundamental tenet of the film theory is the replacement of the boundary conditions at the droplet surface, with the same conditions moved inward. This type is called a “Two-Temperature Model” and is used in the description of the non-equilibrium models.

5.3.1 First model: classical evaporation model

The simplest model for characterising the evaporation of a droplet is based on the rate of vaporising being governed by the diffusion process. In addition assumptions are used in which the droplet temperature is kept fixed at wet bulb temperature and the gas phase in quasi-steady state. According to this model the effect of convective flow of the mixture and gas out of droplet’s surface (Stefan flow) is ignored. The following articles referenced below, discuss this model with additional specific derivations or assumptions used in each model. Starting with Mostafa and Mongia [1987] applied both Eulerian and Lagrangian approaches separately to simulate a turbulent evaporating model for spray. Hallmann et al. [1995] handled using an Eulerian versus Lagrangian approach for modelling turbulent evaporating sprays, through the solution of two transport equations for droplet temperature and diameter. A uniform temperature model was used which assumes an infinite thermal conductivity Ma and Wang [1993], Kim et al. [2001] and Caraeni et al. [2001] their application of the model were based on a single fuel droplet evaporating assuming that spray droplets are dispersed. Other assumptions include droplets are spherical in shape, constant density and they have homogeneous temperature. The rate of change of droplet radius according to Frossling correlation due to evaporation is given by:

$$\frac{dr}{dt} = -\frac{\rho_w D_p B_M Sh}{2 \rho_l r^2}$$

(5.18)

Spalding [1953] suggested that the mass transfer number is calculated from

$$B_M = \frac{f_s - f}{1 - f_s}$$

(5.19)

and heat transfer number from

$$B_T = \frac{c_p f (T_\infty - T_s)}{L(T_s) - Q_L/\dot{m}}$$

(5.20)

where $Sh$ and $f_s$ denote Sherwood number and the fuel vapour mass fraction at the droplet surface respectively . $Q_L$ and $\dot{m}$ refer to overall heat penetrating to the droplet and mass transfer rate respectively . Using Raoult’s law, assuming that the partial fuel vapour is equal to
the equilibrium vapour pressure, which assumes ideal mixing behaviour, the fuel mass fraction at the droplet surface can be obtained from

\[ f_s = \frac{MW_d}{MW_d + MW_g \left( \frac{P_{\text{total}}}{P_{\text{vap}}} - 1 \right)} \tag{5.21} \]

where

\[ f = \frac{\rho_m}{\rho_g} \tag{5.22} \]

where \( MW, P \) and \( \rho \) are the molecular weight, pressure and density respectively. The subscripts \( d \), \( g \) and \( m \) refer to the droplet, gas and mixture respectively. Thermophysical properties for gas and liquid phase are considered as a function of film temperature, which can be calculated from one-third law as:

\[ T_f = T_i + \frac{1}{3}(T_g - T_i) \tag{5.23} \]

This model has been adopted by Kim et al. [2001] where the droplet evaporation rate is described by Frosseling correlation and dimensionless mass transfer number coefficient introduced by defining the Sherwood number as

\[ Sh = 2 + 0.6Re^{1/2}Sc^{1/3}\ln\left(1 + \frac{B_M}{B_M}\right) \tag{5.24} \]

where \( Re \) is the Reynolds number given as

\[ Re = \frac{\rho Ud}{\mu} \tag{5.25} \]

where \( U, \mu \) and \( d \) are the gas relative velocity, kinematic viscosity and droplet diameter respectively. \( Sc \) is the Schmidt number calculated from:

\[ Sc = \frac{\nu}{D} \tag{5.26} \]

where \( \nu \) and \( D \) are dynamic viscosity and mass diffusivity respectively. The heat transfer between droplets and gas-phase is governed by the energy balance equation. The conduction heat transfer entering to the droplets is given by:

\[ Q_{\text{cond}} = Q_{\text{conv}} + \dot{m}L(T_d) \tag{5.27} \]
where
\[ Q_{\text{cond}} = \frac{k(T_g - T_d)}{d} Nu \]  
(5.28)

where the Nusselt number \( Nu \) is determined from
\[ Nu = 2 + 0.6Re^{1/2} Pr^{1/3} \ln(1 + B_M) \]
(5.29)

where \( Pr \) is the Prandtl number. Modelling poly-disperse sprays by using moments of drop size distribution function was suggested by Beck and Watkins [2003b]. Heat and mass transfer submodel is one of the closures used for modelling. They applied the classical model assuming unity Lewis number. The model was treated with some modifications, especially in the transfer between phases during the evaporation period. An alternative correlation for Nusselt number was used in case of turbulent convection, which could be expressed in terms of Spalding mass transfer number, so the formula is;
\[ Nu = 2 \ln(1 + B_M) \]
(5.30)

Therefore the amount of heat gained by the gas phase is balanced by the heat lost by liquid. Then;
\[ Q_{\text{in}} - Q_{\text{evap}} = 4\pi r_k g \ln(1 + B_M) \left[ \frac{T_g - T_d}{B_M} - \frac{L(T)}{c_{gf}} \right] \]
(5.31)

The stagnant film theory was employed by Zhou [1993] to calculate the droplet evaporation rate in order to solve the energy equation and fuel vapour species mass fraction, the vaporization rate is given as
\[ \dot{m}_k = -\pi d_k Nu_k D_s \rho_s ln \left[ 1 + \frac{f_s - f}{1 - f_s} \right] \]
(5.32)
\[ \dot{m}_k = -\pi d_k Nu_k D_s \rho_s \ln \left[ 1 + \frac{T_g - T_d}{L(T)} \right] \]
(5.33)

where \( Nu_k \) is the Nusselt number of heat convection which is determined from
\[ Nu_k = 2 + 0.5Re^{0.5} \]
(5.34)

and \( Re \) is the Reynolds number of droplet-gas relative motion defined as
\[ Re_k = \frac{\left| \vec{V} - \vec{U}_k \right| d_k}{\nu} \]
(5.35)
with \( d_k \) being the diameter of \( k \)-group of spray droplets. Owing to the assumption that there is a relative motion between the gas phase and the droplet, this sets the droplet evaporation under forced convection. Alternative expression was proposed by Oefelein and Yang [1998] for a droplet in a convective flow field in the form of,

\[
\frac{\dot{m}_p}{\dot{m}_{p,Re_d=0}} = 1 + \frac{0.278 \sqrt{Re_d Sc^{1/3}}}{\left[1 + \frac{1.232}{Re_d Sc^{1/3}}\right]^{1/2}}
\]

(5.36)

where \( Re_d=0 \) is the Reynolds number for droplet at rest. Under quiescent conditions, the equation that described mass transfer rate reduced to

\[
\dot{m}_{p,Re_d=0} = 2\pi d_p D_s \rho_s \ln [1 + B_M]
\]

(5.37)

5.3.2 Second model: Abramzon and Sirignano

Abramzon and Sirignano [1989] revised the classical model in order to take into account the effects of Stefan flow on heat and mass transfer, i.e., the transported convection that result from the relative motion between the droplet and the gas. The model was applied to simulate spray combustion calculations and extended to include the effect of non-unity Lewis number in the gas film; the effect of internal circulation of liquid and effect of thermophysical properties were variant and calculated at reference film temperature. Numerical simulations were performed by Hohmann and Renz [2003] to evaluate the unsteady fuel-diesel vaporisation where the liquid fuel spray was injected into a high ambient temperature and pressure. The effects of non-ideal droplet evaporation and gas solubility through the diffusion of heat and species within fuel sprays were taken as an extension for the model. The Eulerian-Lagrangian approaches were used to model dispersed two-phase flows. In these models fuel-vapour species and energy conservation equations to evaluate mass and heat fluxes can be simplified to quasi-steady droplet evaporation and from the integration of balance equation around the droplet for each species, it can determine the mass vaporization flux as

\[
\dot{m} = 2\pi \rho_g D_{gr} Sh \ln (1 + B_M)
\]

(5.38)

and

\[
\dot{m} = 2\pi \frac{k_g}{c_p} Nuln (1 + B_T)
\]

(5.39)
where \( \rho_g, D_g, c_{pf} \) and \( k_g \) are the density, mass diffusivity, vapour specific heat and thermal conductivity of the gas mixture in the film, respectively. The Sherwood and Nusselt numbers are modified to account for the surface carrying the film which are expressed in non-dimensional parameters as:

\[
Sh = 2 + (Sh_0 - 2)/F_M
\]

and

\[
Nu = 2 + (Nu_0 - 2)/F_T
\]

The forms of Sherwood and Nusselt numbers correlation which included the effect of an enlarged boundary layer due to Stefan flow are calculated from empirical formulations using non-unity Lewis numbers with assuming spherical droplets:

\[
Sh_0 = 2 + 0.6 Re^{1/2} Sc^{1/3}
\]

and

\[
Nu_0 = 2 + 0.6 Re^{1/2} Pr^{1/3}
\]

The correction factors \( F_M \) and \( F_T \) for the Spalding number of the film thickness which accounts for the variation in temperature within the film thickness, is defined by:

\[
F(B) = (1 + B)^0.7 \ln\left(1 + \frac{B}{B_T}\right)
\]

In Hohmann and Renz [2003] the Spalding number due to high mass transfer rate is defined as

\[
B_T = \exp\left(\frac{\dot{m}_{pf}}{2\pi r k_g Nu}\right) - 1
\]

For spray calculations the amount of heat penetrating into the droplets is governed by the energy balance of the droplet at specified boundary conditions where in case of spray convective effects have to be included in the calculations

\[
Q_L = Q_{conv} - Q_{vap} = \dot{m} \left[ \frac{c_p(T_{\infty} - T_s)}{B_T} - L(T_s) \right]
\]
5.3.3 Third model: the equilibrium model

As in the case of classical model, this model does not consider any variation of liquid temperature. That means droplet does not require discretization because it ignores the occurrence of a gradient in the interior of droplets. However, this model does not necessitate a high computing time. Park et al. [2002] implemented the model to improve (TAB) model. The mass transfer rate around the droplet was given by an alternative expression based on Spalding mass transfer number

\[ \dot{m} = 2\pi r \rho_m D_m S_h \frac{\ln(1 + B_M)}{B_M} \] (5.47)

where the modifications of this model are located in two places. First the definition of the surface vapour mass fraction. Since it depends on the vapour pressure which consequently depends on the surface temperature and takes form:

\[ f_s = \frac{MW}{MW - (1 - MW)\theta_{eq}} \] (5.48)

where \( \theta_{eq} \) is the ratio of the molecular weights. Second, thermophysical properties of the mixture of the liquid vapour and air (the film around the droplet) are evaluated by using the one-third law to give the best accuracy. The energy equation is coupled with droplet evaporation rate when the variation of temperature is described through the heat flux penetrating into the droplet as given above. The only difference is the expression of the Spalding energy transfer number. In this case it is determined from a formula related to the Spalding mass transfer number,

\[ B_T = (1 + B_M) \Phi - 1 \] (5.49)

where

\[ \Phi = \frac{c_{pr} S_h}{c_{pm} \text{N} \text{u} \text{Le}} \] (5.50)

where \( \text{Le} \) is Lewis number and same Abramzon and Sirignano [1989] correction factors are used here.

5.3.4 Fourth model: Ra and Reitz

Determination of the unsteady behaviour in a model for droplet vaporization was proposed by Ra and Reitz [2003] and Ra and Reitz [2009]. This model adopted the theory of continuous thermodynamics to model the properties and compositions of multi-component fuels. It considered a
range for droplet evaporation temperature from flash-boiling temperature to normal conditions. They used it to determine boiling and surface temperature. The model was applied to simulate the vaporization of a hollow cone spray of gasoline injected into a cylindrical chamber. KIVA-3V code was implemented for simulation spray sub-models and the mixing of fuel/air mixtures in a constant volume chamber. For more accurate predication for heat and mass transfer rates of the fuel component, when mass transfer rates are large, heat transfer rates are finite therefore the droplet temperature is not uniformly distributed and a surface temperature concept was introduced. The rate of transported mass is calculated via

$$\dot{m} = \rho_g D_g Sh \ln\left(1 + B_M\right) 2r$$

(5.51)

The rates of interface of heat and mass transfer between the droplet and the surrounding gas were calculated in this model from the heat flux to the droplet which is given by:

$$\dot{m} L(T_d) = Q_{in} + Q_{out}$$

(5.52)

$$\dot{m} L(T_d) = h_{in,eff}(T_s - T_{sur}) + h_{out,eff}(T_g - T_{sur})$$

(5.53)

where $h_{in}$ refers to the heat transfer coefficient inside the droplet and is determined from the thermal conductivity and the unsteady equivalent thickness of thermal boundary layer. The last was defined as

$$\delta = \sqrt{\pi D_g \chi t}$$

(5.54)

and

$$\chi = 1.86 + 0.86 \tanh[2.225 \log_{10}(Pe/30)]$$

(5.55)

Where $Pe$ is the Peclet number and the last term in the above equation represents the energy transported by effect of diffusion of species. Then, the surface temperature can be determined.

### 5.3.5 Fifth model: non-equilibrium model

This model accounts for the deviation from the equilibrium due to phase transition which effects clearly appear on the droplet surface. Dushin and Smirnov [2008] introduced a characteristic parameter $I$ which refers to the variations of the non-equilibrium and equilibrium Peclet number. The value of this parameter is zero for the case of equilibrium and it rises to positive values with increase of the deviation from the equilibrium case. This would give an indication in which
range the equilibrium model is applicable. Bellan and Harstad [1978a] and Bellan and Harstad [1978b] adopted the Langmuir-Knudsen law in their evaporation model which incorporates non-uniformity of drop temperature. The model used Lagrangian framework to solve equations for both surface temperature and volume averaged temperature. In non-equilibrium model, the calculation of molar mass fraction, \( \gamma_{s,neq} \) used to determine the vapour mass fraction on the droplet surface \( f_s \) is shown by the following relation:

\[
\gamma_{s,neq} = \gamma_{eq} - \left( \frac{L_k}{r} \right) \beta_L
\]  

(5.56)

where

\[
\beta_L = -\left( \frac{3Pr\tau_d}{2} \right) \frac{\dot{m}}{m}
\]  

(5.57)

Here \( \beta_L \), \( m \) and \( \tau_d \) represent the Knudsen length, mass droplet and the droplet relaxation time, respectively. Subsequent works were done by Watkins [2007] to calculate the local surface area average temperature since heat and mass transfer phenomena are related to this temperature instead of the local value of the volume average temperature. The aim of this calculation is to use it in the energy equation for liquid phase. The procedure mainly starts with two assumptions. First of all the droplets are spherical in shape. The second assumption is that a parabolic profile of temperature exists across any drop from the centre to the surface, given as

\[
T(r) = a + br + cr^2
\]  

(5.58)

where \( a \) and \( b \) are constants to be found from the boundary conditions. In addition, the constant \( c \) is calculated from the definition of the drop volume averaged temperature. Recently, the effect of turbulence on heat and mass transfer have been investigated, Abou Al-Sood and Birouk [2008] developed a three dimensional model to show the turbulence effect on heat and mass transfer rates of a droplet exposed to a hot airstream. This was done by using a correlation of Abou Al-Sood and Birouk [2007] to account for the effect of free stream turbulence on droplet mass transfer, as

\[
Sh(1 + B_m)^{0.7} = 2 + 0.914Re^{0.5}Sc^{1/3}(1 + 1.235I^{0.372})
\]  

(5.59)

where \( I \) is the turbulence intensity of the free stream. Also, the effect of radiation is investigated which is increased significantly as the free stream temperature approaches 1273 K. The shear-stress transport model is used to predict the turbulence term in the conservation equation for the
gas phase. Alternative expression was suggested by Sidhu and Burluka [2008], who modelled the turbulence effect on the evaporation rate, through large variations in temperature and pressure without any need to adjust the model constant. The model used a Eulerian framework based on $Y-\sigma$ for the liquid phase where a transport equation for the average liquid surface area is calculated in which the $Y$ is the mass of liquid and $\sigma$ is the liquid surface area per unit mass.

5.4 Spray heat and mass transfer treatment

5.4.1 Modelling objective

A reactive two-phase flow is characterised by strong non-linear coupling with the fluid flow, turbulence and mass and heat transferred between the phases. Examples are spray evaporation, spray-heated wall interaction and spray flame structure. Due to these complicated phenomena there is certainly a need for a model sophisticated enough in order to capture the complexity of the problem. Inspiration might come from when the droplets have changed their physical state. Obviously, the key parameter is vapour mass fraction. The value and spatial distribution for the latter play an important role because they will accurately give predicted rate. Therefore, a tractable spray evaporation model, based on calculation of film temperature through a simple formula based on the amount of vapour mass fraction is presented here. This stems from several questions that are addressed below:

1. Which computational cells should be affected by evaporation conditions?
2. Should all computational cells calculate with the same film temperature even when it contains different number of droplets?
3. What is the effect of the non-linearity of the evaporation rate?

5.4.2 Proposed spray evaporating modelling

A reacting spray is considered when heat sources due to external field are supplied especially when high temperatures are bound to be encountered. The concentration of fuel droplets sprayed in any combustion chamber or furnace is related to the evaporation rate which represents a decisive process of the fuel preparation. The model described here provides the source terms for both the mass and energy exchanged between phases, based mainly on the work done by Beck and Watkins [2003b] and Watkins [2007].
The conservation equation for liquid phase energy was described above where this equation is for the transport of volume-averaged energy, which results in a volume-averaged temperature locally for the spray. Two assumptions are proposed in order to evaluate the surface average temperature. First of all the droplets are spherical in shape. The second assumption is that a parabolic profile of temperature exists across any drop from the centre to the surface, given as in equation (5.58). The constants $a$ and $b$ are found from the boundary conditions, i.e. $T = T_s$ at $r = r_s$, where subscript $s$ denotes the drop surface, and $\frac{dT}{dr} = 0$ at $r = 0$. Thus $b = 0$ and $a = T_s - cr_s^2$. The constant $c$ is found from the definition of the drop volume-average temperature $\bar{T}_d$

$$\bar{T}_d \int_0^{r_s} r^2 dr = \int_0^{r_s} Tr^2 dr$$

(5.60)

Thus, the form of the parabolic temperature profile expressed in terms of $T_s$ and $\bar{T}_d$,

$$T(r) = T_s - \frac{5}{2}(T_s - \bar{T}_d) \left[ 1 - \left( \frac{r}{r_s} \right)^2 \right]$$

(5.61)

The heat transferred by conduction into the drop is evaluated at the drop surface

$$Q_{in,d} = k_l A_s \left. \frac{dT}{dr} \right|_{r=r_s} = 4\pi k_l r_s^4 \frac{5(T_s - \bar{T}_d)}{r_s} = 20\pi k_l (T_s - \bar{T}_d)r_s$$

(5.62)

where $k_l$ is the liquid thermal conductivity. The total heat transfer rate into all the spray drops locally is evaluated by integration over all the drops in a control volume by means of the number size distribution, hence

$$\dot{Q}_{in} = \int_0^{\infty} Q_{in,d} n(r_s) dr_s = 20\pi k_l \int_0^{\infty} (T_s - \bar{T}_d)n(r_s)r_s dr_s$$

(5.63)

where surface-area-averaged liquid temperature $T_{l2}$ and volume-averaged liquid temperature $T_{l3}$ are defined from the equations

$$T_{l2} Q_1 = \int_0^{\infty} T_s r_s n(r_s) dr_s$$

(5.64)

and

$$T_{l3} Q_1 = \int_0^{\infty} \bar{T}_d r_s n(r_s) dr_s$$

(5.65)
Thus the liquid surface averaged temperature is expressed as

\[ T_{12} = T_{13} + \frac{\dot{Q}_{im}}{20\pi k_1 Q_1} \]  

(5.66)

Hence once \( T_{13} \) can be obtained from the liquid phase energy transport equation, \( T_{12} \) can be evaluated, as long as \( \dot{Q}_{im} \) can be found. The latter is done by evaluating the heat transfer by convection from the surrounding gas. Consequently in case of evaporation takes place from the surface of the droplet. The heating of the droplet due to the energy gained from the hot gas starts to change the state of liquid droplet into vapour with losing some of its mass which has to be taken into account. Small droplets evaporate faster than big droplets because of the higher surface curvature which leads to reduced forces between the molecules directly at the surface. The heat penetrates into the liquid phase during the heat up period when the liquid is not at the saturation temperature.

The particular model adopted here is that due to Beck and Watkins [2003b] in which the convective heat transfer for a single drop is given by

\[ \dot{Q}_{c,d} = \dot{m} \left[ \frac{c_{pg}(T_g - T_s)}{B_m} \right] \]

(5.67)

where \( \dot{m} \) is the mass transfer rate defined below and this equation can be integrated locally over all droplets. Subscripted values \( s \) denote drop surface conditions and \( g \) denote conditions in the surrounding gas. The convective heat transfer rate must be equal to that entering the drop; therefore \( \dot{Q}_{in,d} = \dot{Q}_{c,d} \). Some of the energy that enters the drops is lost back to the gas due to evaporation. When mass transfer occurs at a certain conditions the gas phase properties should be evaluated. It is not precisely predicted. However, a good prediction of evaporation mass rate gives an indication of the rate at which the drop size decreases and most importantly for this study, the amount of vapour which enters the gas phase. Hopefully the level of validation that is obtained agrees with the equations that express the mass rate. For the model presented here, it is restricted to the case of one-component liquid. Also, this model is used to describe a part of spray evaporation model rather than droplet mass transfer. The evaporation rate is expressed through the drop Nusselt number \( \text{Nu}_d \)

\[ \dot{m}_d = 2\pi \left( \frac{k_g}{c_{pg}} \right) r_s \text{Nu}_d \ln(1 + B_M) \]  

(5.68)

Therefore the heat transferred between phases during the heat-up period when the liquid is not
at saturation temperature is given by equation (5.67) can be integrated locally over all droplets to give

\[ q_E = \int_0^\infty 4\pi k_g \ln(1 + B_M) \left[ \frac{(T_g - T_s)}{B_m} - \frac{L(T_s)}{c_{pg}} \right] r_s n(r_s) dr_s \] (5.69)

Note the presence of the minus sign due to the source term being the energy gained by the gas phase in equation (5.69) and lost by the liquid phase in equation (2.32). Care must be taken when the temperature difference is very small but the liquid is super-saturated. For this type of mass transfer, it is assumed that the liquid gains from the gas exactly the energy it requires to evaporate the appropriate amount of mass. Hence the source term \( q_E \) becomes zero in this case as the net transfer of energy to the liquid is exactly zero. By using the similar procedure, the equation (5.68) can be integrated over all droplets at a local level to obtain the desired mass source term in terms of underlying drop size distribution

\[ q_m = \int_0^\infty 2\pi \left( \frac{k_g}{c_{pg}} \right) Nu_d \ln(1 + B_M) r_s n(r_s) dr_s \] (5.70)

The forms of the Nusselt number correlation suggested by some authors are rather too complex for use within the current model. This is because of the need to integrate the convective heat transfer over the drop size range locally, as illustrated below. Thus, for this first derivation of the new model, a simpler form of correlation is adopted, due to Ranz and Marshall [1952]

\[ Nu_d = 2 + 0.6 Re_d^{0.5} Pr^{0.333} \] (5.71)

where \( Re_d \) is the Reynolds number as defined by equation (5.25) and the Prandtl number is independent of drop size. The source term for the liquid surface area can also be derived from the same starting point. The loss in mass can be related to a change in radius by

\[ \delta m = 4\pi r^2 \rho_l \delta r \] (5.72)

The change in the square of the droplet radius is related to the droplet radius change by using the following equivalently

\[ \delta(r^2) = 2r \delta r \] (5.73)

Therefore the change in the square of the droplet radius per unit mass lost is given as

\[ \frac{\delta(r^2)}{\delta m} = \frac{1}{2\pi \rho_l r} \] (5.74)

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by using equation (5.68) to replace in equation (5.74), hence the change in square of the radius can be set as

\[ \frac{\delta(r^2)}{\delta t} = \frac{2}{\rho_l} \left( \frac{k_g}{c_{pg}} \right) \ln(1 + B_M) \]  

(5.75)

Integrating the above equation over all droplets locally, the contribution to the source term for \( Q_2 \) from the change in the equivalent source term, due to mass evaporation, for the surface-area moment \( q_{Q_2} \) is given by

\[ q_{Q_2} = \int_0^\infty \frac{2}{\rho_l} \left( \frac{k_g}{c_{pg}} \right) \ln(1 + B_M) n(r_s) \, dr_s \]  

(5.76)

In this model an extension is made where the source term of droplet radii due to evaporation. The rate of change droplet radius is determined from using the Frossling correlation, as in Lefebvre [1989]

\[ \frac{\delta r}{\delta t} = \frac{\rho_g D_g B_M Sh}{2 \rho_l r} \]  

(5.77)

The same procedure is repeated here, following the same steps to calculate the surface area moment source term, the source term for the drop radii moment can be written as

\[ q_{Q_1} = \int_0^\infty \frac{\rho_g D_g B_M Sh}{2 \rho_l r} n(r_s) \, dr_s \]  

(5.78)

As appear in above equation, to avoid the negative moment, it can be replaced by equivalent moments through applying equation (2.14) by setting \( j = -1 \)

\[ Q_{-1} = \frac{(k + 2)Q_0}{(k - 1)r_{32}} \]  

(5.79)

5.5 Presentation of the case study

5.5.1 Description of the experiment

Recent experiment work by Shim et al. [2008] on high-pressure swirl injector in the GDI engine has shown spray characteristics under evaporation conditions. The experiment was performed to investigate the main features of hollow cone spray resulting from high pressure swirl atomiser in the GDI engine. The experiment was conducted by means of an intensified-CCD camera where spray images were recorded digitally. The configuration camera system contains a computer
with an image grabber, a shutter controller and a pulse generator. The injector was installed vertically in a constant volume chamber. The swirl-type injector employed in the test was of 0.1 mm diameter. The operating conditions were 5.1 MPa pressure for a hexane injection into nitrogen. Nitrogen was used as an ambient gas instead of air in order to purify the chamber to avoid the quenching of liquid fluorescence by oxygen. The injection duration and the fuel mass flow were 2 ms and 15 mg respectively. The experimental conditions were up to 0.1 MPa for the ambient pressure and 473 K and 293 K for gas and liquid temperature, respectively.

5.5.2 Description of the simulation setup

The spray moments methods proposed by Beck and Watkins [2003a] treats the injected bulk of liquid as three consecutive moments of underlying droplet size distribution in order to simulate their interaction with the gas phase. The main structure of the model is based on constructing three transport equations cast with the gas phase in term of Eulerian-Eulerian approach. In this approach the two-phase fields are treated as a single incompressible continuum with an effective variable moments which are inseparable across the liquid-gas interface. The spray moments methods is based on introducing a set of transport equations for the flow field where spray moments (volume, surface area, drop radii and number of drops) in definition and flow field are in general correlative. The inclusion of the physical processes relating to the moments and their momentums is not closed, therefore to close the equations a underlying probability density function is presented. The closure method was revised by Yue and Watkins [2004] through extending the model to evaluate the first four moments and assumed the underlying distribution is of the form of a gamma distribution. The numerical computations were performed in a new in-house code Jones [2009], based on current methods in Ferziger and Perić [2002]. A finite volume method for arbitrary cell-shapes in combination with a collocated arrangement is used for discretization the equations. Higher order differencing schemes were implemented with conjunction of an unstructured grid topology to improve the accuracy of the solution. A cylindrical coordinates system is adopted because the flow in a hollow cone swirl atomizer appears to be nearly axisymmetric.

In the present study, the computational domain was subdivided into a finite number of non-overlapping control volumes. The variables were stored at the centre of each control volume following a collocated arrangement of variables in the grid. The control volumes were constructed to be taken as polyhedral (unstructured grids), that means that the cells could have
any number of neighbours. Here, attempts at improving both schemes are presented. For temporal discretization, the three time level method is adopted Ferziger and Perić [2002], which is a second order implicit scheme and has no time step constraint. For spatial discretization, the high resolution interface capturing (HRIC) scheme developed by Muzaferija and Peric [1999] is implemented here for moments quantity with only one adjustment; that one can define the lower bound. The main reason to use this technique is because the moment in a control volume can be formulated algebraically without reconstructing the interface. For the continuum, since it is entrained and accelerated by the spray interaction. The upwind and central differencing scheme is implemented explicitly Ferziger and Perić [2002] for all transported properties and blended with the implicit trim scheme. The present heat and mass transfer models are applied to simulate hollow cone spray vaporisation. The objective was to achieve an accurate model to capture all characteristics of hollow cone spray and the effects due to hot gases. The calculations were performed by representing the computational domain of 50 mm x 100 mm using an unstructured grid topology.

The grid analysis has been carried out to ensure the obtained results are independent of the grid used where full details are mentioned at the end of this chapter. The case (A) is selected because it produces a less spray thickness. The computational domain contains 7799 control volumes, 15787 faces and 7989 vertices as shown in figure (5.2). For the calculations, the initial time step used is 2 µs.

5.6 Results and discussions

This section features the description of numerical results that have been obtained from the application of the presumed model to simulate spray evaporating as well as the validation of both one-third rule and film equation for reactive two-phase flows. These are presented by comparisons with experimental and available numerical data. The purpose of using such an atomizer is to generate fine droplets spread over a relatively wide angle. The pressure swirl atomizer feeds liquid tangentially giving it high angular momentum, thus an air cored vortex would be formed. The mechanism of the resultant sheet at the outlet of the orifice starts when the liquid rotates inside a swirl chamber and emerges through orifice due to the action of centrifugal force to form a hollow cone sheet. The vortex motion establishes a low pressure regime and an air core is formed. The cone angle is governed by average tangential and axial velocity components at the outlet. In order to correctly model the influence of heat and mass transfer
on hollow cone spray injected into hot gases, firstly the capability of the basic computational method of spray modelling without segregation into drop sizes was tested. The capturing of spray dynamic behaviour and interaction processes were evaluated and presented as a comparison with experimental data on spray tip penetration.

5.6.1 Penetration

This part deals with the computation of spray tip penetration. In this context, an accurate prediction of spray penetration depends mainly on the droplet size and velocity distribution as outlined in Mondal et al. [2004]. Consequently the heat and mass transfer models proposed in section (5.4.2) give an insight on the thermo-physical properties of the vapour fuel and spray droplet size distribution at gas-droplet interface. The only source of energy for liquid fuel evaporation is the hot air entrained into the spray droplets trajectory. The accuracy of the results allows some assessment of the overall mass evaporation rate and spatio-temporal velocity and distribution of droplets. The first part of calculation of spray penetration depends on the prediction of injection velocity and droplet velocity profile. The initial spray injection velocity is determined based on injection pressure and is calculated via a Bernoulli argument as explained in equation (2.36). Comparisons for evaporating cases were made using numerical and experimental data obtained by Shim et al. [2008]. In order to achieve as good an agreement as possible with the data, the injection conditions were made as closely as possible to the data given by Shim et al. [2008]. The measured spray angle from images was used in order to set the temporal variation of radial component of the liquid velocity at injection.

Figure (5.3) shows the predicted spray tip penetration versus time for the presented models compared with experiment at the ambient temperatures of 473 K. For both one-third rule and film equation the results show over-predication in the early period up to 0.8 ms. This is due to the start-up conditions for the pressure swirl atomizer used in this experiment. In addition one source of error in the solution appeared here due to use of a dense grid near the injector where the probability of breakup and collision droplets are expected. Near the injector, as the grid density is increased the penetration increased due to increase grid resolution which tends to improve the prediction for the momentum transfer between the gas phase and the spray. This allows to produce a smaller relative velocity (lower drag) leads to higher spray penetration as in Li and Kong [2009]. In addition, the high number of grid points near the injector containing effective bulk of spray droplets is found, which in turn tend to increase the
convection in spray velocity. The above reasons can be used for general investigation, however to insert the effect of evaporation, the amount of fuel vapour mass fraction at the earlier stage of injection is high because of small amount of mass is injected into the hot gas. However the fuel vapour is dense which tends to reduce the droplets dispersion and hence increasing spray penetration. The results show there is a small difference between one-third rule and equation (5.17) where one-third rule has higher penetration than film equation at the begin of the period where both evaporating cases show under prediction spray penetration because of the effects of gas density and evaporation. Evaporation reduces the drop sizes which may lead to lower spray penetration. Also the reduction in penetration might be due to the presence of smaller droplets due the accumulated effects of hydrodynamics at the spray tip which evaporate faster. The gas density increases due to reduction in temperature (equation of state) that affects directly on spray dispersion i.e., decreases the angle of the cone where less entrained air would be found within the spray. The lower amount of entrained mass causes increase in penetration. In addition the effect of evaporation clearly appears after the injection due to its accumulation which results in the reduction of droplets dispersion and consequently the over penetration by as much as 10% relative to the experimental data. Another reason has to be mentioned here related to the under-predictive results for spray penetration after 2.5 ms. The swirl atomiser is used to generate fine droplets within a thin sheet, and the smallest amount of droplets are found at the tip due to the dispersion process compared with other parts of the spray body as will be described in figures (5.4) and (5.5). For this reason, the accuracy of calculations will be less due to modelling error even though this may be alleviated somewhat by using the integrable method of the probability of all droplet sizes. Also, the probability of breakage and collision droplets would be less because of the effect of dispersion. The predicted results are close to each other partly due to the short period of the injection, so that differences in evaporation are not so significant.

This does not allow an investigation of the effect of film equation. At the early stage of injection, the film equation exhibit less penetration compared to the one-third rule because of the high amount of fuel vapour released. At the end of injection time both the film equation and one-third rule approach tend to produce an identical trend closer to each other because of the highest rate of evaporation at the end of injection time. The reduction in spray penetration rate at the late injection time is expected due to decrease in drop sizes in which the momentum is lower. In addition the amount of fuel evaporation becomes small due to reaching the saturation state in the gas phase compared to the the amount produced at the earlier stage of injection.

The experimental spray tip penetration was evaluated by measuring the visible leading edge of
spray images. The spray tip penetration was determined in the calculations by using the leading edge from the fourth spray moment, the volume fraction of the liquid phase. The explanation of reduction of the axial penetration of fuel sprays due to evaporation is because it reduces the drop size. As a consequence there is over-prediction of the penetration from about 0.1 ms up to 1.35 ms, followed by under-prediction thereafter from 2.0 ms up to 3.0 ms. However, the error is within range from 5% to 10%

\[ \text{Error} = \frac{X_{Exp} - X_{Calculated}}{X_{Exp}} \times 100 \quad (5.80) \]

where \( X \) represent the value of spray tip penetration at time \( t \).

Figure (5.4) includes spray topology at a cross section \( x=20 \text{ mm} \) at different times. It shows the reduction in liquid volume fraction as the time proceeds. To figure out the distribution of the liquid volume in axial direction, the radial direction was chosen to illustrate the way in which the liquid droplets are spread out. From the plots in figure (5.5) for the axial and radial profile of liquid volume fraction the liquid volume or concentration increases at the front of the spray whilst the peak of liquid volume fraction is concentrated near the injector. Because of the recirculation region downstream, the spray tends to spread towards the core of the spray as shown later by gas velocity vectors. Further downstream the air induced by spray impedes these undesirable movements towards the centre line which cause collapse of the sheet and work to weaken the tip penetration. Figure (5.6) (a) and (b) show the comparisons between simulated liquid volume fraction and the direct photographs of experimental spray development processes after 1 ms and 1.6 ms respectively at ambient temperature 473 K. These liquid volume fraction results are obtained at the early and approximately mid section of the simulations because the spray characteristics are substantially modified during these stages due to the high injection velocity. As illustrated in figure (5.6)(b), the spray penetration is determined by droplets in the middle of the spray and not the edges boundary of the spray. This is because the penetration is governed by the motion of large droplets and also the droplets at the edge experience more drag. So the physical spray edges are retarded while the core of the spray moves more quickly downstream. In general, the comparisons of predicted distribution has an adequate shape compared to the Shim et al. [2008].
5.6.2 Sauter Mean Radius

Comparisons of the droplet Sauter Mean Radius (SMR) obtained using the one-third rule or the film equation are shown for different downstream distances at different times with the simulation work of Shim et al. [2008] implemented with the KIVA code. After the start of injection of liquid, the smaller droplets are seen to move towards the centre of spray because of the drag induced by the entrained gas velocity drawn into the spray. The larger droplets continue to travel to the outer edge of the spray (spread out in their original direction) due to centrifugal force effect. Therefore the drop size in the central core region gives an indication that there are very small droplets here or no droplets. The SMR reduces continuously downstream because of the evaporation. It has been noticed in previous section how the spray tip penetration and liquid volume fraction are affected by evaporation due to reducing the mass of liquid fuel. Figure (5.7) shows overall changes in drop size, illustrated by calculating the profile of SMR at x=30 mm and 40 mm from the injector orifice at 2 ms and 3 ms. At a distance of 30 mm downstream of the spray nozzle, it is important to observe that the large droplets are positioned on the inner edge of the spray where the peak of SMR is found. Additionally the turbulent mixing (entrained hot gas) controls the evaporation process. Figure (5.7)(b) at time 3 ms, it is important to observe that the sheet thickness is reduced from 18 cells at x=30 mm at 2 ms to 16 cells because large droplets are convected downstream to x=50 mm at the inner edge of the spray as shown in figure (5.7)(c) where the peak of SMR is found. The results of the predicted variations of these dynamic effects are not matched with obtained results cited in Shim et al. [2008]. The results can be analysed according to the deformation in hollow cone spray construction. Before making any investigations about the comparisons with KIVA results, it is important to note that such comparisons are referring to two different techniques. In the original KIVA code, it is assumed that after droplets breakup and evaporate the distribution of droplets is presented in terms of Rosin-Rammler distribution. The characteristic mean droplets size is expressed straightforwardly in terms of Sauter mean diameter \(d_{32}\) as

\[
d = d_{32}\Gamma(1 - q^{-1})
\]

where \(\Gamma\) and \(q\) are the gamma function and the distribution parameter respectively. The assumed method here uses an Eulerian treatment and due to the higher order numerical tools that have been used in this code, has the potential to handle fine grids. In fact the last characteristic is shared with model capability and the accuracy of sub-models. The initial value of SMR is 25 \(\mu\)m.
and the full details about the number of grids that have been used in each comparison are shown in figure (5.7) in order to analysis the over-prediction in the simulated results. The number of cells at 2 ms are 18 at x=30 mm and 16 at x=30 mm at 3 ms respectively. At 3 ms the number of cells is 16 at x=40 mm. One of the most interesting observation is the difference is two cells between 3 ms and 2 ms at x= 30 mm because the spray droplets dispersion is increased with injection time and at 3 ms calculations is recorded higher value than 2 ms due to the increased the rate of evaporation. At 2 ms there is an increase in SMR towards the centre of the spray. The outer edge of the spray has relatively lower values than the centre as shown in figure (5.8), where the smaller droplets are found in which their evaporation rate is low and the effect of turbulent is weak due to lower gas velocity. The inner edge of spray has considerably higher values than the centre as shown in figure (5.8), where the smaller difference can be seen at the inner edge and grows as are proceeds from the edge. However the second difference is the predicted sheet thickness at x=30 mm at 2 ms and 3 ms is thinner than that calculated using KIVA because of the higher order numerical techniques that were used in this work. At 3 ms the difference between the simulated results and those simulated with KIVA code is considerably greater due to the constraints mentioned above in contrast to the Eulerian framework that is considering the whole effects that may change the geometrical distribution for both surface and volume of the spray. Two cross sections are taken downstream at x=30 mm and x=40 mm. Figures (5.9) and (5.10) show the radial profile of Sauter Mean Radius. At x=30 mm figure (5.9) shows that due to development of spray downstream the net effect caused by evaporation and other submodels like breakup and drag do not be clearly appear. However at x=40 mm shown in figure (5.10), the trend effect can be observed better. The effects of development of the gas entrained which enhances heat transfer and causes the drop size to decrease results in the dispersion being increased. So at the inner edge of the spray, the SMR increased substantially because from its definition it is the ratio of the volume to surface area of the spray. Evaporation made a diminution in surface area faster than in volume. Therefore this is one of the potentials of the moments method that describes spray in terms of volume, area, radius and the number of droplets. The SMR values simulated with the film equation in the cases are higher than the SMR values simulated with the one-third rule because all comparisons are made with relatively advanced time 2 ms and 3 ms. At these time the amount of evaporated mass transferred in the film equation case is larger than one-third rule case because it is based on half rule. However the evaporation rate is low (increased in the liquid temperature and drop in the gas temperature) as shown in figure (5.5) where the liquid volume fraction simulated with the film temperature is
higher than the liquid volume fraction simulated with one-third rule. This means the reduction in liquid mass is less and will be explained in more details in the liquid and gas temperatures part.

Furthermore, to assess the effect of drop size in the spray on heat and mass transfer rates, figure (5.11) (a) and (b) are presented, figure (5.11)(a) explains the temporal diminishing in surface area at $x=20$ mm measured at four different times and figure (5.11)(b) shows the overall behaviour of the spray second moment in order to investigate the influence of the accumulation of heat on the size of the droplets. Figure(5.11)(a) and (b) show at the earlier stage of injection the second moment simulated with the film equation recorded lower values because the film equation is firstly based on the half rule and secondly on the highest values of vapour mass fraction at this stage. There is not a large amount of reduction in surface area just at the earlier stage of injection and because it will be compensated by spray development as breakup and collision of droplets increased with time. In addition the obtained results from film equation is lower with respect to the one-third rule because the highest values of surface droplet temperature are obtained from the finite conductivity evaporation model as explained in Watkins [2007], resulting in higher amounts of fuel vapour being released during the transient heating. In fact there is another reason has to be explained here. The ratio (one-third) is fixed which gives a linear relation during the temperatures variation. Whereas in film equation the quadratic formula is able to tune with drop size distribution which is crucial. This is investigated in more detail in next parts.

5.6.3 Vapour mass fraction

This paragraph deals with the computation of overall mass transfer rate within the spray region. The mechanism of turbulent mixing governs evaporation along with the gas temperature by determining the rate of energy entrainment which is directly related to the hot gas entrainment mass flow rate. In this situation the net reduction in the injected fuel mass flow rate due to the evaporation process will have to be matched by an increase in the entrained gas mass flow rate to add a new amount of energy needed to evaporate the new quantity of spray droplets. The bulk of mass transfer rate is calculated from integrated equation (5.70) which is related to the ensemble averaged mean droplets evaporation rate. In the proposed model presented in this work the same source term which is used to represent the total reduction in liquid phase mass flow rate is used in the transport equation of vapour mass fraction introduced in chapter two.
equation (2.45) but with the opposite sign. Now in more advanced details, owing to the active heat and mass transfer rates between droplets and ambient gas, there are many smaller droplets that evaporate quickly. Additionally, droplets with small momentum are diffused toward the ambient gas that results from the growth of the vortex area, this enhances the heating processes. Hence high vapour mass fraction regions always appear along the centre of the spray and in the vortex area. There are locally higher distributions of vapour fraction regions in the middle and near the edges of the sprays. These area are where induced entrained gas flow mixes with vaporized fuel just below the recirculating vortices.

The predictions of the development of fuel vapour mass fraction at different times are presented in figure (5.12). Figures (5.12) (a) and (b) show the radial profile of the local concentration of fuel vapour mass fraction calculated at two different axial locations at x=5 mm and x=20 mm respectively at different times. Figures illustrate the proceeding of the value of $f$ throughout the lifetime of the spray and show how it is convected downstream by the gas flow. In addition the profiles show that the radial dispersion of the gas phase is evident at downstream locations. Figure (5.12)(a) shows $f$ values at x=5 mm relatively close to the injector orifice at time of 0.4 ms and 0.6 ms respectively. A higher mass evaporation rate is produced with the film temperature than the one-third rule because the higher difference between the gas and liquid velocity. Also higher mass evaporation rate is found than at axial locations downstream at time of 1 ms. In addition to the momentum transfer mentioned above, the droplets size decrease while moving downstream, so the released amount of vapour will be less as can be observed at x=20 mm linked with time 2 ms and 3 ms as shown in figure (5.12)(b). Figure (5.12)(c) shows the temporal behaviour of vapour mass fraction in axial direction at time 2 ms and 3 ms respectively. At 2 ms with film equation, a higher amount of vapour mass fraction is produced than with the one-third rule due to the high gas temperature resulting in a significantly higher film temperature. Whereas at 3 ms the highest values of vapour mass fraction are found while the film equation produces less amount than the one-third rule equation. This is because when the liquid temperature rise at the end of injection period therefore the difference between the gas and liquid temperature is small compared with previous time.

Figure(5.13) (a), (b) and (c) show contour plots of fuel vapour mass fraction, at time 1.0 , 1.6 and 3.0 ms at ambient temperature 473 K. In figure(5.13) (a) and (b), the left sides of the contour show the simulation of vapour mass fraction in the present work and the right sides show the KIVA code simulation results Shim et al. [2008]. The comparisons of predicted vapour mass fraction with KIVA code are generally good. Figure(5.13) (c) contour plot shows the
distribution of vapour mass fraction at 3 ms with the local values of vapour mass fraction at
different locations. Here the simulated results of vapor mass fraction with one-third rule are not
included because there is a small difference as compared with film equation. Gas flow velocities
were lower than liquid velocities throughout most of the spray, particularly near the injector
tip. Therefore the vapour shown here is both that just produced at the position in question plus
that accumulated over time due to convection from upstream. This is why it is important to
recognize the effect of mass transfer rates that vary both in position and time.

5.6.4 Two-phase temperature

As with all numerical work, it is important to explain all sorts of temperatures that influence the
 evaporating two-phase flow. As shown by Watkins [2007] the surface area-average temperature
can be significantly higher than the volume average temperature. This has an important impact
on heat and mass transfer rates. Unfortunately, there are no experimental works by which to
judge the accuracy of these predictions. Therefore, the results shown and discussed here depend
for their explanation on the natural behaviour of the structure of the hollow cone spray. The
concept of two moment liquid temperatures introduced by Watkins [2007] is implemented here.
Figure (5.14) (a) and (b) show profiles comparisons between liquid volume and surface average
temperature along the axial and the radial direction at time 2 ms for film equation and one-third
rule. Film equation results are exhibiting a slightly higher value than one-third rule. Figure
(5.15) shows the predicted results calculated at x=40 mm and 50 mm from the injector hole
at 2 ms and 3 ms after start of injection for the liquid surface average temperature and figure
(5.16) shows the liquid volume average temperature at x=40 mm and 50 mm at time 2 ms and
3 ms respectively. Just away from the injector there appears to be little difference between the
volume averaged temperature and the surface averaged liquid temperature.

In regions near the injector tip, the difference was slightly noticeable. This is due to the cold
liquid droplets exposed to high gas temperature, so the gap between surface and volume liquid
temperature is greater. Near the spray tip, as the spray proceeds further downstream, the
liquid will have been heated for a longer time. Hence the difference between the surface and
liquid temperatures becomes smaller. Both temperatures calculations are implemented with the
two technique for applying the film temperature. The film equation exhibits generally lower
temperature prediction but gives the same trend with one-third rule along the cross section.

The gas phase temperature must clearly be examined to assess the ability of this model and
to successfully predict the mass transfer and vapour distribution. Figure (5.17)(a) shows the calculations at two different location x=20 mm and x=40 mm downstream after 2 ms and 3 ms respectively. Figure (5.17)(b) explains the effect of using film equation and one-third rule on gas temperature at different time. The plots in figure(5.17)(a) demonstrate the large increase in heat transfer rate due to convection. This can be seen as the drop in gas phase temperature because relatively close to the injector many droplets will have not heated up yet. With increasing in the depth and time most of the spray parts were heated so the rate of heat transfer lowers (the difference between the gas and the liquid temperatures is small) as shown at x=40 mm at 3 ms. The drop in gas temperature is due to convection process between the gas phase and the droplets which appears significantly decreased with time as shown in figure (5.17)(a) at 3 ms.

5.6.5 Film temperature

The unsteady-state heat and mass transfer rates and the fluid thermodynamic properties at gas-liquid interface are studied in this part in terms of comparisons made between the proposed film temperature equation and the well known one-third rule. The procedures described above for modelling the spray provide all information that are required in the film equation such as vapour mass fraction, liquid and gas temperatures. The fuel vapour mass fraction that forms can have important consequence on the performance of the heat and mass transfer mechanisms which are related to it. The most obvious disadvantage in evaporation modelling is the required accuracy of prediction of thermophysical properties for both phases. Precise determinations of local fuel vapour mass fraction have significant implications on exchange processes between liquid and ambient gas. The applicability of the equation (5.17) is shown in figures (5.18) and (5.19). It can be seen in figure (5.18) that the proposed equation results in larger film temperatures at both location at time equal 2 ms compared to the one-third rule. The maximum difference for both predication is 20 K. At x=20 mm, the obtained results were over estimated as comparing with one-third rule because of high evaporation rate in regions close to the injector due to existence of a relatively high mass of fuel vapour. This increased downstream where the heat transfer rates were enhanced. In other words there is increased fuel vapour concentration due to heated up liquid droplets. The film equation agrees with natural behaviour of moving droplets in a hot chamber. It establishes a coupling between the phases through linkage of a transported parameter related to both heat and mass effects.
In figure(5.19) comparisons of predictions of film temperature between one-third rule and film equation at axial distances of x=20 mm and x=40 mm respectively are shown at time of 3 ms. In addition to the above investigation, an observation at x=20 mm at time 2 ms is of the trend of one-third rule and film temperature to increase towards the outer edge of spray where smaller drops may be found but the film temperature decreased in one-third rule while in film temperature equation it increases gradually until they met at outer edge to record high film temperature due to high gas phase temperature. Alternatively the observation at x=40 mm at time 3 ms is the trend of one-third rule and film temperature should be increased towards the outer edge of spray where smaller drops may be found but the film temperature decreased in one-third rule while in film temperature equation it seems to be fluctuated due to the cross section has been taken at the tip of the spray where less evaporation is produced because of higher mass concentration.

To illustrate the justification of using the film equation requires a simple example to show the potential of equation (5.17) through its treatment of changes in position and state for sensitive regimes where the spray calculations need to be more accurate. Consider extracts from the calculations that have been done in this case study. Shown in figure (5.20) are contour plots for vapour mass fraction at time 2 ms where A, B and C three sections are selected in which the local values of fuel vapour mass fraction are pointed out in order to implement in the proposed equation. From previous calculation of gas phase temperature as shown in figure (5.17) the range at x=20 mm is between 461 K- 468 K and the surface-average liquid temperature within 293 K-340 K where the liquid boiling temperature is 355 K whereas the vapour mass fraction is varying as shown in figure (5.20). This variation induces a great variation in the film temperature when calculated with the new equation in contrast to one-third rule parameter which is depending only on the gas and liquid temperatures. There is substantially more vapour produced near the nozzle where the gas temperatures are high and the differences between the two liquid temperatures are a maximum. The vapour mass fraction shown here is both that just produced at the position in question plus that accumulated over time due to convection of the gas phase. This is why it is important to recognise the effects of mass transfer rates that vary both in position and time. Thus the maximum differences between the film equation and one-third rule equation are seen near the spray edges. The droplets would have received heat from the gas phase by convection during a significant time period and thus the droplets have had time to conduct it to reduce temperature variations within droplets. Equally the gas temperature has dropped significantly from its initial condition. Due to these variations, the film temperature would be the local value
of liquid temperature plus one third the difference between gas and liquid temperatures for the computational domain if the one-third rule was applied. In fact this formula does not take in consideration the actual amount of liquid or gas inside the computational cell. As in case of two-phase flow non-evaporating case the volume fraction of liquid is the key to solve the coupling, here using similar concept namely vapour mass fraction. Actually the numbers of droplets are certainly different in each cell which matches the theory of dispersed phase. The major reason for using vapour mass fraction as the crucial parameter in the film equation is because of the large effect of droplet evaporation on the pressure of the vapour in the film around the drops. More specifically, the mass transfer rates, as expressed through equation (5.70) is proportional to \( \ln(1 + B_M) \), where \( B_M \) is the Spalding mass transfer number, defined here as

\[
B_M = \frac{f_s - f}{1 - f_s} \quad (5.82)
\]

Using Raoult’s law, assuming that the fuel vapour partial pressure is equal to the equilibrium vapour pressure, which assumes ideal mixing behaviour, the fuel mass fraction at the droplet surface can be obtained from

\[
f_s = \frac{MW_d}{MW_d + MW_g \left( \frac{P_{\text{total}}}{P_{\text{vap}}} - 1 \right)} \quad (5.83)
\]

where \( f, MW, P \) and \( \rho \) are fuel vapour mass fraction, the molecular weight, pressure and density respectively. The subscripts \( d, g \) and \( m \) refer to the droplet, gas and mixture respectively. These equations show \( B_M \) to be proportional to the pressure of vapour in the film. The vast majority of the gas surrounding the drops is composed of air so that the partial pressure of the air is much greater than that of the vapour. Consequently, values of \( B_M \) are much less than 1, and \( \ln(1 + B_M) \) is proportional to \( B_M \) and hence the mass transfer rate is proportional to the partial pressure of fuel vapour. From Watkins [2007], the equation for the pressure of vapour in the film is given by

\[
p_{v,s} = Ae^{(f_{\text{film}})} \quad (5.84)
\]

where for n-hexane the partial pressure is taken from Yaws [2003] in terms of the film temperature is given by

\[
p_{v,s} = 465.2 xe^{(0.01735xT_{\text{film}})} \quad (5.85)
\]

Due to the dispersion of particles or droplets the outer cells of the spray has to be diluted for
two reasons, first because different events take place within the spray like breakup, collision and coalescence which means different velocities result in chaotic dispersive behaviour. Second in case of evaporating flow the hottest regimes are encountered here. It is easy to estimate the gas and liquid temperatures in order to calculate the film temperature using the two methods. Simple calculations are shown below at section B at time 2 ms in order to gain clear comparison, so

\[ T_{film} = 340 + \frac{1}{3}(461 - 340) = 380.333K \]  
(One−third rule)  

\[ T_{film} = 340 + \left( \frac{1}{2} + \frac{0.01}{6} \right)(461 - 340) = 400.7K \]  
(Film equation)

The only justification for using a new formula instead of using one-third rule is based on volume fraction in the computational cell. Actually figures (5.12) and (5.13) give an indication of the fuel vapour mass fraction that occupies each cell approximately.

Going further take other cells in section B near the inner spray edge, which is thicker due to the presence of larger droplets. With one third rule a lower value is obtained near the inner edge followed by an increase towards the centre and then dropping near the outer edge of the spray. In figures (5.18) and (5.19), the calculations that are done with proposed equation are tuned with drops distribution, at the inner edges there is a drop in film temperature due to thickness of the edge even when the vapour mass fraction is relatively high near the centreline as shown in figures (5.13) and (5.20) then there is a gradual increase in film temperature towards the outer edge for two reasons. Figure (5.21)(a) shows the temporal behaviour of film temperature in axial direction at different times. The highest values can be found at 2 ms using the film equation because of the higher amount of vapour that is produced than using one-third rule, due to the high gas temperature. Whereas at 3 ms are found the lowest values of film temperature. This is due to the distributive effects of convection and diffusion processes. In addition if substantial amounts of vapour exist in the vicinity of the drops then the driving potential for mass diffusion of the vapour is diminished and less liquid can evaporate. While in figure (5.21)(b) the one-third rule equation produces lower values at 2 ms and the highest values at 1 and 3 ms respectively. This is because when the liquid temperature rises at 2 ms a smaller difference between the gas and liquid temperature is predicted as compared with 1 ms and 3 ms. From the prediction of Sauter mean radius shown in figure (5.8) the inner edge is thicker than outer edge which causes naturally more vapour mass fraction as shown in figure (5.13) that means higher film temperature at the spray edges than the core of the spray which is considered as a dense regime.
where the concentration of liquid droplets are relatively high. In this region of the spray the reduction in gas temperature is substantial due to presence of high number of droplets while the liquid temperature is relatively increased.

5.6.6 Two-phase velocity

In this study, after investigation of the drop size distribution behaviour, the droplet velocity profiles are presented here to increase the understanding of spray droplets characteristics under the effect of evaporation and dispersion. Most of the droplets are influenced by the entrained gas mixture; it redirects their trajectories according to the induced recirculating flow. Generally axial and radial liquid velocity profiles show a non-linear decrease with increasing axial and radial distances downstream. Figures (5.22) and (5.23) show the predicted variations of the axial and radial liquid velocity components after 1, 2 and 3 ms. The third moment velocity components are used for this comparison. The axial and radial velocity profiles exhibit a half bell-shape, that is due to the effect of interface drag mainly and maybe to the other hydrodynamics effects that causes a change in droplet size and specially increases in gas temperature can affect the drag model because the gas density is changing. The hollow cone sprays are predicted to spread radially as long as the injection proceeds. As expected with time the evaporation process tends to reduce the radial liquid velocity component along both the axial distance due to consuming droplets, as shown in figure (5.23). As shown in figures (5.22) and (5.23), in any cross section there is a decrease in axial and radial velocities with axial and radial distances towards the outer edge of the spray. In the central region is recorded the maximum value, followed by a gradual decrease towards the outer edge of spray where smaller droplets were found as mentioned before due to the centrifugal force. Generally speaking the drop size difference between the inner and the outer edge of the spray is large and the drop sizes seem to increase with increasing radial distance. This is related to the effect of the centrifugal force. Thus, the large droplets have higher velocities than the smaller drops and are expected to have a tendency to move toward the inner edge of the spray due to the centrifugal force. As time elapses further, the drop sizes decrease due to the effects of hydrodynamics and evaporation process leading to reduction in droplets velocities specially near the outer edge of the spray as shown in figures (5.22) and (5.23). The calculated velocity at different cross sections is considered here, figure (5.24) shows the axial liquid velocity component after a short period from start of the injection to include some effects of changing spray structure due to interaction with gas phase. The maximum axial velocity
can be found at the injector hole. Moving away downstream the reduction occurs because the droplets are losing their momentum further increased by the evaporation process. It should be noticed that the variation of the liquid axial velocity component appeared slightly reducing in velocity between x=14 mm and x=19 mm associated with the developed recirculation gas region downstream. While from the observation of radial liquid velocity there is a smaller decay because droplets are spread out radially and the induced gas velocity are accelerating it in some part of the spray. Examination of the droplet radial velocity plot in figure (5.25) confirms this. The tangential velocity values increase from the inner edge towards the maximum value near the outer edge of the spray due to the effect of swirl on the droplet velocity. In general the maximum liquid velocity is found near the inner edge of the spray because of the concentration of largest droplets.

The development of the recirculation region downstream of the nozzle inside the cone comes from the negative droplet velocities in the core area for the hollow cone spray. The computed profiles of axial and radial gas velocity components are presented in figures (5.26) and (5.27) respectively at three different axial cross sections at time of 3 ms after start the injection. These velocities are generated by the recirculation of the gas due to droplets movement in it. The obtained results were predicted using the k-ε turbulence model. These results clearly show that the film equation produced nearly identical results as compared with one-third rule in axial component calculations at x=10 mm and x=25 mm respectively, with a very small difference at x=35 mm because the high rate of evaporation at the top points in spray where the effect of evaporation tends to reduce the gas velocity. Differences in calculations are more noticeable in radial gas velocity profile shown in figure (5.27) specially at x=25 mm and x=35 mm due to the recirculation induced by swirl combined in this case with vaporisation affect. The calculations of axial gas velocity show that the maximum value of axial velocity was found near the injector and that shows in figure (5.26) at x=10 mm approximately as 52 m/s and decreased due to the effect of expansion and dispersion of droplets. In radial profile because the presence of recirculation zone near the injector for example at x=10 mm result in negative values, whereas at x=25 mm reduced negative values were found. It was found that the maximum radial velocity was 5 m/s away from the inlet.

In all velocity profiles the film equation results give a good agreement with one-third rule as shown in figures (5.28) and (5.29). The reason why earlier period and closest cross section were selected in velocity calculation is to prove that the earlier stage of evaporation the amount of reduction in mass is small so the velocity is high as in film equation results.
5.6.7 Grid analysis

The most desirable solution for an asymptotically grid independence test is attained by means of refining grid. The computational two-dimensional domain with a symmetry axis along the centre line of the cylinder, is discretized using unstructured grids. The unstructured grids system has been generated using GAMBIT software to achieve the desired level of numerical analyses that can be obtained from a sufficient resolution of fine grids. In addition two treatments are performed to assess the grid independence test. First, the number of injection cells at the nozzle are discretized from five cells for cases A, B, C and D and two cells for case E. This has been done to show the effects of inlet conditions like liquid velocity and spray injected moments on the general solution. It is not the main reason to do this treatment for the simulation of hollow cone spray. In this work, the treatment shows the effect of radial velocities applied to the spray at inlet, given that the liquid velocities are applied at cell faces, and that there are no droplet groups. The radial grid resolution is uniform only in the orifice that gives a minimum grid size of 0.1 mm. Second, the purpose of the finer and inhomogeneous region due to unstructured grid topology near the injector (in the area of interest), is to capture the chaotic behaviour, steep gradient of the flow and rapid changes in spray droplets due to hydrodynamics effects such as break-up, collision and coalescence of droplets. The case E is set for the spray computation to show the injected drop sizes (injected spray moments) are not effected by the number of injection cells. So the change in spray penetration and spray sheet thickness are effected due to the change in the entrained air amount. The grid specification is shown in table (5.1).

<table>
<thead>
<tr>
<th>Case</th>
<th>No. volumes</th>
<th>No. faces</th>
<th>No. vertices</th>
<th>No. injection cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>7799</td>
<td>15787</td>
<td>7989</td>
<td>5</td>
</tr>
<tr>
<td>B</td>
<td>4729</td>
<td>9587</td>
<td>4853</td>
<td>5</td>
</tr>
<tr>
<td>C</td>
<td>4019</td>
<td>8147</td>
<td>4129</td>
<td>5</td>
</tr>
<tr>
<td>D</td>
<td>2831</td>
<td>5757</td>
<td>2927</td>
<td>5</td>
</tr>
<tr>
<td>E</td>
<td>2605</td>
<td>5310</td>
<td>2706</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure (5.30) shows the effect of the number of volumes in the computational domain on the spray tip penetration. All data are calculated at time 2 ms. A decrease in the spray penetration is observed with finer grids. Spray penetration depends mainly on the liquid velocity (momentum equation). With a larger number of control volumes, comes an increase of the momentum transferred to the gas phase and consequently increase in the gas velocity. Due to momentum
conservation there is a consequent decrease in the liquid momentum and velocities. This leads to a reduction in penetration length. In hollow cone spray the droplets movement are oriented due to the effect of centrifugal force. It is interesting here to mention the effect of the shape of the unstructured grid on the results. It works to drift the direction of the droplets because the liquid velocity is dependent on the angle between spray axis and grid.

Figure (5.31) shows the calculated liquid volume fraction at \( x=40 \) mm at time 2 ms for the cases. The outer edge of the spray appears to be relatively insensitive to the grid structure with the results of the two finest grids almost coincidental. However, the inner edge of the spray shows a significant variation with grid refinement.

### 5.7 Conclusions

In this chapter, the spray evaporation modelling is assessed by an extensive evaluation of computationally efficient treatment for liquid phase. A significant progress has been made in the moment method proposed by Beck and Watkins [2003a] to capture the structure of hollow cone spray. The method with all hydrodynamic sub-models (drag, breakup and collision) is tested first and the results are compared with experimental work of Shim et al. [2008]. Then, the evaporation model is included and the obtained results are compared with experimental and calculated data cited in Shim et al. [2008]. Next, with the success of these model validations, the model was applied to investigate the heat and mass transfer effects to assess the feasibility of applying this model to a realistic spray. A novel equation for calculating thermophysical properties has been used. The comparisons of spray penetration and vapour mass fraction that have been carried out, for both one-third rule and film equation evaporation model and then the non-equilibrium evaporation model with experimental and available numerical data, demonstrate the ability and the potential of these models as they show a good agreement. The stability and robustness of the performance of the in-house code was tested by obtaining converged solutions for both test cases run. In addition the accuracy of the method and the model has been proved and assessed through presentation of different comparisons related to spray characteristics. Detailed explanations are described for the reasons to use a new film equation. A comparison with well known (one-third rule) equation is based on the analysis of their values according to structure of the spray. The fuel vapour mass fraction areas are classified and investigated. The largest values are found near the axis due to the presence of the vorticity of the gas, while the lowest values are found around the droplets. Finally this equation provides combustion models with
an accurate prediction for the temperature of the unburnt fuel vapour. In general this equation can be used to couple the evaporation model with combustion models.
Figure 5.1: Representation of evaporation from a single spherical droplet

Figure 5.2: Computational domain
Figure 5.3: Comparisons of predicted penetration with experimental data

Figure 5.4: Radial variation of liquid volume fraction at x=20 mm different times
Figure 5.5: Comparison of predicted liquid volume fraction at different times.

Figure 5.6: Comparison of predicted liquid volume fraction with Shim et al. Shim et al. [2008] experimental data.
Figure 5.7: Sectors of SMR contours show number of cells at $x=30$ mm and 40 mm $t=2$ ms and 3 ms.
Figure 5.8: Comparison of predicted SMR with KIVA code at x=30 mm at time=2 ms

Figure 5.9: Comparison of predicted SMR with KIVA code at x=30 mm at time=3 ms
Figure 5.10: Comparison of predicted SMR with KIVA code at x=40 mm at time=3 ms

Figure 5.11: Radial variation of liquid surface area at different times

(a)x=20 mm 
(b)Radial profile
Figure 5.12: Radial and axial variation of vapour mass fraction at different times
Figure 5.13: Contour plot of vapour mass fraction at different times.

(a) Time=1.0 ms

(b) Time=1.6 ms

(c) Distribution of vapour mass fraction in a contour plot at time=3.0 ms.
Figure 5.14: Comparisons of simulated surface and volume average temperature at time=2 ms.

Figure 5.15: Prediction of liquid surface temperature
Figure 5.16: Prediction of liquid volume temperature

(a) Radial at x=20 mm and 40 mm
(b) Axial profile

Figure 5.17: Prediction of gas temperature at different times.
Figure 5.18: Comparisons between proposed film equation and 1/3 rule at x=20 mm and x=40 mm at time=2 ms

Figure 5.19: Comparisons between proposed film equation and 1/3 rule at x=20 mm and x=40 mm at time=3 ms
Figure 5.20: Distribution of vapour mass fraction at time=2 ms

Figure 5.21: Prediction of film temperature at different times.
Figure 5.22: Comparisons of simulated axial liquid velocity at different times.

(a) Axial
(b) Radial

Figure 5.23: Comparisons of simulated radial liquid velocity at different times.

(a) Axial
(b) Radial
Figure 5.24: Prediction of radial profile of axial liquid velocity component at different axial cross sections and times.

Figure 5.25: Prediction of radial profile of radial liquid velocity component at different axial cross sections and times.
Figure 5.26: Prediction of radial profile of axial gas velocity component at different axial cross sections at time=3 ms.

Figure 5.27: Prediction of radial profile of radial gas velocity component at different axial cross sections at time=3 ms.
Figure 5.28: Prediction of axial profile of axial gas velocity at different times.

Figure 5.29: Prediction of axial profile of radial gas velocity at different times.
Figure 5.30: Penetration of spray with variation of number of control volumes.

Figure 5.31: Radial profiles of liquid volume fraction with variation of number of control volumes.
Chapter 6

Sprays combustion

6.1 Introduction

Combustion definition states that either by the accumulation of heat or by catalyzing reaction, products in a system are due to the development of the chemical reaction under conditions of self acceleration growth. Typical combustion phenomena involve turbulent fluid flow, heat transfer, radiative heat transfer and chemical reaction. It is considered one of the most important processes in engineering applications. Consequently it is essential for any combustion system to be capable of predicting the temperature, flow characteristics, concentration of resulting products and emissions for the design and improvement of combustion equipment. Two main sub-divided types of combustion are classified. They include non-premixed or diffusion and premixed combustion. This division is based on how the two streams meet to mix and burn. The combustion is of either individual droplets or groups of droplets, when the liquid fuel is taking the form of discrete liquid ligaments during atomization process. A wide range of sizes, trajectories and velocities will be found. The dependency of unburnt mixture on the non-uniformity causes irregularities in the ignition and propagation of flames through the spray. In principle, the gas turbine engine combustor performance increases the enthalpy of the working fluid by combustion. Modern gas turbine engines tend to improve combustion efficiency through better temperature distribution to the turbine from the subsequent air dilution of the resulting combustion products. The recent technology is based on the strategy of avoiding high consuming rate and reduction of the $NO_x$ to the lower level. In order to meet these requirements, two concepts are introduced for advanced combustor technology, Rich-Quench-Lean and Lean-Premixed-Prevaporize. Due to the enormous interest in numerical simulation of the turbulent reactive flow in gas turbine
combustors, research has become very intensive in the last two decades. It can be considered the most helpful technique to find an optimised solution and development phase of a new engine. Physical and chemical interactions of two-phase flows lead to reaction under certain conditions. Complexity of all these phenomena needs to be demonstrated in which experimental testing become prohibitive. In addition drawbacks of experimental techniques are falling into some inherent limitations in terms of resolved small-scale details and experimental costs are considerably large. In real gas turbine engine, the liquid fuel is injected into the gaseous phase. In fact, the chemical process is often in many real configuration occurring in a highly turbulent and unsteady flow where temperature and composition are subjected to large fluctuations.

### 6.2 The problem

Spray combustion remains one of the most complex phenomena to describe and simulate because of the chaotic behaviour for the droplets during their motion and interactions with outer media. In practice, the burners of both gas and liquid fuelled gas turbine and diesel engines are considered the main applications for turbulent flame. In diesel engine, the high injection velocity for the liquid transforms the continuous liquid phase into droplets as dispersed phase through disintegration process into droplets by atomisation leads to increase the dispersed phase surface area. When droplets are subjected to the hot gas, this accelerates the evaporation and consequently combustion rates. Before spray auto-ignition takes place or out of the reaction zone, in some parts droplets are evaporated and burnt in a sequential process. The only reason that can be seen is the insufficient mixing of the liquid droplets and fuel vapour with surrounding hot gas which leads to heterogeneity in the mixture that may increase the auto-ignition delay time. Unfortunately experiment lacks to provide the information about these zones because of small scales and short life time. Beside the modelling error arises from the simulation of the chemical reaction in order to achieve a good compromise between calculations of the chemical reaction rate and justifiable fuel vapour mass fraction consumption.

Numerically, when the droplets have been evaporated completely due to high temperature, then the source term due to mass transfer become zero. In this case the gas velocity will initiate gradients in scalars due to the convection term while the molecules are spreading via the diffusion term. Therefore the calculation for chemical reaction would be incorrect because in fact there is no fuel vapour to burn. Becker et al. [2004] identified two parameters Arrhenius parameter and diffusion coefficient for combustion problem and will be adopted in this work.

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6.2.1 Lumped spray combustion

Motivation

A lumped spray combustion model concerns the numerical investigation of spray combustion using the concept of dynamic thickened flame LES model but in terms of the two-equation turbulence model to simulate the turbulence in reaction zone. Dynamic thickened flame LES model was proposed by Legier et al. [2000] to evaluate mixing, diffusion and premixed flames for combustion regimes which cannot be identified as perfectly premixed nor non-premixed. The main objective of modelling is to develop a combustion model capable of handling the effects of mixing and turbulent reaction which is very important in most engineering applications like diesel engine and gas turbines. Secondly the basic idea of scaling (artificially thickening) flames is to reduce the ability of vortices to wrinkle the flame front and increase the diffusion speed of propagation. This is used here for damping any fluctuation in gas temperature during the evaporation period before the auto-ignition delay time or out of the reaction zone after the auto-ignition delay time. Practically scaling flames mean that in terms of Arrhenius equation in order to reduce the modelling error arises between the chemical reaction rate and mass transfer due to fuel consumption. So the chemical reaction rate shown here is both for the fuel vapour that has just been produced at the position in question plus that accumulated over time due to evaporation droplets to generate fuel vapour. This is why it is important to recognise the effects of chemical reaction rate that vary both in position and time:

1. Enhancing the molecular diffusion. As mentioned before mixing is the governing physical phenomenon in non reactive zone and it is usually preferred to investigate the structure of the flame, not in the physical space but in the mixture fraction space.

2. Decreasing Arrhenius parameter in the chemical reaction rate equation.

For successful simulation and optimisation of the chemical reaction rate, an algorithm for two parameters provides identification of the strain zone. The treatment is based on the physics of incomplete mixing process in order to interpret the uncertainty in the prediction for the chemical rate. This is achieved by introducing a local scaling factor which is active during spray droplets evaporation stage or where large gradients of reaction rate values are found outside the reaction zone and relaxes to unity inside the reaction zone. This is because the spray flame can be captured in terms of micro-scale procedure. These limitations work to suppress the scaling to prevent any modification for mixing process and lumping the modelling error that may occur
which eventually can be used to correct the chemical reaction rate prediction. However the innovative treatment made here of scaling the diffusion term and reducing the reaction rate by the same factor only occurs when the reaction flame thickness become less than the diffusion layer thickness. Therefore the model has two processes, first is to capture the zone and the second is to eliminate the zone in order to compensate the error in modelling. Also this model takes on the role of modelling both mixing process through using transported mixture fraction and scalar dissipation rate and the turbulent reaction process through identifying two concepts for diffusion flame thickness in addition to the main reason for using such a model which is scaling the diffusion flame. This increase in diffusion term and decrease in Arrhenius parameter can appear in different ways where these changes can be observed such as increases in the surface flame front and increases in speed of heat transfer and distribution of active species and the homogeneity of the reactants by enhancing mixing process.

Mathematical modelling

The mixing efficiency can be defined as the part of the fluid in the layer that has been mixed at a certain molecular level. In turbulent combustion, if the chemical reaction is fast the mixing efficiency can be deduced from the products formation. The present work follows Freund et al. [2000] to define the upper and lower bounds of mixing efficiency. In addition the proposed model uses direct measurement for the bounds instead of using scalar probability density function measured at different transverse positions as stated in Freund et al. [2000]. Thereafter there is no need to use a probability density method to generalize the solution. The choice of reaction thickness as small parameter influences the resulting mixing efficiency. This is because the higher reaction thickness values mean that more mixture is considered burned. From this theoretical analysis the mixing efficiency is formulated as a scaling factor $F$ set to vary from maximum value inside the lumped zone and takes the form

$$ F = \frac{t_d}{t_r} \quad \text{(6.1)} $$

where $t_d$ is the diffusion flame thickness and $t_r$ is the reaction flame thickness. Here $F$ cannot be set as a fixed value within a range depending on the application (spray type) but can be computed according to the turbulence model used. Legier et al. [2000] calculated a thickening factor according to the number of cells used to resolve the flame front and to local grid size based on large eddy simulation with an appropriate value for the laminar flame thickness. The
ratio of the diffusion layer thickness to the reaction zone thickness means the use of local mixing zone which is considered the largest zone because reaction zone is very small and in some cases such as for infinitely fast chemistry the thickness is equal to zero. A general transport equation is used to evaluate reactive species, written in the form of

\[
\frac{\partial}{\partial t} \int_\Omega (\rho Y_f) \, d\Omega + \int_S (\rho Y_f \vec{u}) \cdot \vec{n} \, dS = \int S \Gamma_\phi \nabla (Y_f) \cdot \vec{n} \, dS + \int_\Omega \dot{q}_m \, d\Omega + \int_\Omega \frac{\dot{w}}{F} \, d\Omega
\]  

(6.2)

Chemistry modelling

There is a need to introduce an accurate chemistry model while accounting for the flame thickness in combustion zones using the effects of turbulence to integrate combustion modelling; such a model requires mainly two things. First identification of combustion regimes supports the model development by comparing the characteristic mechanical and chemical scales. This task is difficult in turbulent non-premixed combustion for two main reasons. First, non-premixed flames do not exhibit a reference flame speed because propagation of flame can be in any direction depending on flow conditions. Second as mentioned above, flame thickness cannot be defined as diffusive thickness because it mainly depend on the local flow stretch and may take a wide range of values. The idea comes from Peters diagram for turbulent diffusion flames and the notes mentioned in Hollmann and Gutheil [1996] where the regime of distributed reaction zone is separated from flamelet regime at Kolmogorov time scale. Classification of length scale in non-premixed flames is still difficult due to the clear scales to be recognized, two well known length scale are defined here. A length scale for molecular mixing may be shown as the thickness of the zone where substantial changes can occur for mixture fraction and reactants; this is named as diffusion layer thickness. Then the typical diffusive thickness can be identified and assumed to be controlled by the Kolmogorov scale \( \eta \) Vervisch and Poinsot [1998]

\[
t_d \approx \eta
\]  

(6.3)

Second, the reaction layer where the chemical reaction takes place and the layer thickness is lower than Kolomogorov scale. Corresponding to these, reaction zone thickness \( t_r \) may be defined. In addition within these constraints a problem may arise, Vervisch and Poinsot [1998] used asymptotic results to estimate reaction zone, hence

\[
t_r = t_d Da^{-1/(v_f + v_O + 1)}
\]  

(6.4)
here $D_a$ and $v$ are Damkohlar number and molar stoichiometric coefficient for fuel and oxidizer respectively. According to Peters [1983] the local expression may be written as

$$D_a = \frac{2A_\rho st v OZ_{st}}{\chi_{st} MW_F}$$  \hspace{1cm} (6.5)$$

where $A$, and $MW_F$ are the Arrhenius preexponential factor and fuel molecular weight respectively. $\rho_{st}$ and $Z_{st}$ are the density and mixture fraction at stoichiometric conditions respectively. Here $\chi_{st}$ is the mixture fraction scalar dissipation rate for stoichiometric value of $Z$. Following Pitsch [2000] the instantaneous scalar dissipation rate is defined as

$$\chi = \chi_{st} Z^2 \ln(Z) Z_{st}^2 \ln(Z_{st})$$  \hspace{1cm} (6.6)$$

where $\chi$ can be obtained from

$$\chi = \frac{a}{\pi} \exp \left( -2 \left[ erf c^{-1}(2Z) \right]^2 \right)$$  \hspace{1cm} (6.7)$$

where $a$ is the strain rate.

**Turbulence modelling**

The second requirement is inserting a suitable turbulence theory to assist physical and chemical changes during the combustion process. This work uses the intermittency theory where the boundaries for any turbulent flow have an intermittent character and the anomalous scale is a measure of it. Since spray droplets are evaporated preparing for combustion, they evaporated and then ignited completely or partially in some parts until they reach a region where it is not easy to capture the flame because the chemical reactions break down. Therefore the length that is used for characterizing the chemical reactions in the flamelet structure is diffusion flame. More accurately this length is measured just when the flamelets are ignited and increases until the chemical reaction is stopped as mentioned above. As a conclusion the diffusion flame thickness in turbulent reactive flow field has similar behaviour as spray combustion and is characterized as a local phenomenon rather than integrated variable (as in mixing regime). In order to put a correct representation for the diffusion flame thickness, the benefit comes from the analogy of spray combustion and the intermittency models as outlined in Frisch [1995].

The proposed intermittent beta-model is implemented in this work, where two aims are achieved through using this approach. First is capturing the thickness of diffusion flame. Second is
to prevent the overprediction for scalars only in the flamelet regime by applying the lumped hypothesis to the mixing scalar as will be described below. In terms of this model, Richardson cascade is applied at each stage. Due to the nature of turbulent flows a large range of length and time scales can be characterised. The theory states that the large eddies that have a high Reynolds number break up into smaller eddies that in turn break up into smaller ones and so forth. This proceeding does not stop until the viscous force dominated over the convection forces and the smallest eddies are dissipated. Numerically the number of smaller eddies formed from a given large eddy is chosen such that the function of fraction of volume occupied by the operative eddies is decreased by a factor $\beta (0 < \beta < 1)$. The factor $\beta$ is an adjustable parameter of the model where the intermittency is presented in a power function. The largest eddies have the initial scale size of the length scale that is generated by induction of droplets. The smallest eddies have scales approximately equal to the Kolmogorov dissipation scale $\eta$. Here, the number of eddies per unit volume is assumed to be varied (increase or decrease) with diffusion layer thickness to ensure that the appropriate number of small eddies will be generated. The fraction $P_l$ of the space which is active within a smaller eddy of size $L = r^n L_0$ decrease with the power of the length scale $L$ and $L_0$ the initial length scale.

$$P_l = \beta^n = \beta \frac{\ln (L/L_0)}{\ln (r)} = \left( \frac{L}{L_0} \right)^{3-D}$$

(6.8)

where

$$3 - D = \frac{\ln(\beta)}{\ln(r)}$$

(6.9)

the exponential marker $D$ is related to the Hausdorff dimension, which can be interpreted here as a fractal dimension of the considered turbulent regions. If $D$ is a dimension of a structure, in order to cover the probability of being within a distance $L$ one needs $(L_0/L)$ for a line, $(L_0/L)^2$ for a plane and $(L_0/L)^3$ for a volume. Therefore for small length scale of $L$, the probability of being within a distance of $L$ in a structure of dimension $D$ is the fraction of the number of volumes coating the structure. Thus,

$$P_l \propto L^{3-D}, L \rightarrow 0$$

(6.10)

where the term $3 - D$ is called the co-dimension of the structure. The energy per unit mass of the velocity $u_L$ of the active eddies of size $L$ fill just the fraction $P_L$ of a total volume. The
energy $E_L$ can be computed after inserting equation (6.8) that yields

$$E_L \sim u_L^2 \left( \frac{L}{L_0} \right)^{3-D}$$  \hspace{1cm} (6.11)

The energy flux $\pi_L$ at the scale $L$ to smaller scales is

$$\pi_L \sim \frac{E_L}{\tau_L} = \frac{E_L u_L}{L} = \frac{u_L^3}{L} \left( \frac{L}{L_0} \right)^{3-D}$$  \hspace{1cm} (6.12)

where $\tau_L$ is the eddy turnover time. Through this approach one could use the common argument that in the inertial range, the range flux does not depend on the length scale $L$, in another form

$$\pi_L \sim \epsilon = \frac{u_L^3}{L_0}$$  \hspace{1cm} (6.13)

where $\epsilon$ is the dissipation rate of the kinetic energy. From equation (6.12) and (6.13) with some algebra, the eddy turnover time can be written as

$$\tau_L = \frac{L_0}{u_{L_0}} \left( \frac{L}{L_0} \right)^{\frac{2-D}{3}}$$  \hspace{1cm} (6.14)

In Beta-model, the viscous cutoff time scale is obtained by equating the turnover time and the viscous diffusion time given by

$$\tau_d = \frac{\eta_d^2}{\nu}$$  \hspace{1cm} (6.15)

therefore the dissipation scale can be expressed as the derivation in Frisch and Sulem [1978].

$$\eta_d = L_0 Re^{\frac{3}{3-D}}$$  \hspace{1cm} (6.16)

and

$$Re = \frac{u_0 L_0}{\nu}$$  \hspace{1cm} (6.17)

where $Re$ is the Reynolds number. $u_0$ and $\nu$ are the initial velocity and dynamic viscosity respectively. The crude assumption of the diffusion layer thickness is equal to the micro-mixing Kolmogorov is treated by the exponent $D$. Santavicca et al. [1990] implied a relation depends on flame speed to estimate the increase of the parameter $D$ as the flame speed transits from laminar to turbulent as,

$$D = 2.0 - \frac{s_l}{u' + s_l} + 2.35 \frac{u'}{u' + s_l}$$  \hspace{1cm} (6.18)
For $D = 3$, the Kolmogorov definition is recovered and the intermittency is ignored. For $2 < D < 3$, this closed range is used to accommodate the factor $D$, due to the geometrical constraints mentioned above. Flamelet is valid only when the local reaction zone thickness is smaller than the turbulent dissipative length scale.

6.3 Theoretical perspective

Datta and Som [1999] studied numerically spray characteristics of spray combustion inside gas turbine combustor. They focused on the fuel preparation in gas turbine combustor. In such an engine the combustion efficiency is depending on the evaporation rate and the mixing of fuel vapour with the surrounding gas. They used a simple model to characterize the chemical reaction rate with Arrhenius form. Thereafter, for the single-step reaction, the chemical rate can be formulated as:

$$
\dot{\omega} = A \left( \frac{\rho_g Y_f}{MW_f} \right)^a \left( \frac{\rho_g Y_O}{MW_O} \right)^b \exp \left( \frac{-E_a}{RT} \right)
$$

(6.19)

Wang and Baek [2007] applied Arrhenius equation to investigate the unsteady behaviour of spray combustion in a relatively high pressure regime. In their work the comparisons were made with normal pressure environment. The higher temperature of the spray flame due to high pressure was created faster than the normal pressure spray; therefore the lifetime of spray would be shorter. In that case, the spray penetration depth would also be shorter and the maximum drag force was found at initial stage of injection. The influence of both evaporation and combustion process due to high pressure were observed to be taken placed more rapidly and the reaction occurred in a more compact zone as compared to normal pressure case. Their study does not account for turbulent effects and assumed spray is considered as dilute in which droplets interactions such collision and breakup were ignored. Moreover Boileau et al. [2008] implemented Arrhenius formula to simulate steady spray combustion in a realistic aeronautical gas turbine combustor. The spray combustion computation has been performed by using a parallel large eddy simulation Eulerian-Eulerian solver. Two cases were carried out reacting and non-reacting flow one dimensional laminar two-phase flow and a swirled non-reacting flow which is related to turbulent dispersion of the particles. For reacting case a simple one-step chemical reaction for kerosene surrogate was used.

Compressible large eddy simulation code was used with unstructured mesh by Boudier et al. [2008], their implementation was on a sector of a realistic helicopter chamber to capture the
characteristics of reacting flow. The results showed that the unsteady behaviour for flame and the
flow field characteristics i.e., velocity, temperature and reaction rate were relatively insensitive to
mesh resolution. Arrhenius equation was applied to represent the chemical kinetics of one-step
chemistry model. The combustion of $C_{10}H_{10}$ with air involved 43 species and consists of 174
steps. An adjustment for the exponential constant in terms of equivalence ratio was practically
applied in order to reproduce a proper flame speed. Accurate prediction for flame speed is
only in lean regimes where the equivalence ratio is less than unity. The dynamic thickened
flame approach was used by Legier et al. [2000] to handle the flame/turbulence interaction.
This approach is based on the theory of laminar premixed flames and applied just for large
eddy simulation model. The details of this model are describing in the following section where
modifications were made in terms of using a different turbulence model and application. Owing
to the complex geometry of gas turbine combustor, a fast-chemistry and partial-equilibrium
model with a number of modifications like changing the values of the constant of the standard
model or by adding a new term due to the effect of streamwise curvature and swirl flow had
been used to reduce some of deficiencies in $(k-\varepsilon)$ model and was applied by Shyy and Braaten
[1988].

Hybrid kinetics/eddy break-up (EBU) model is one such approach which had been adopted in
computational study for Datta and Som [1999]. The work applied for gas turbine combustor
where their investigation was on gas-droplet flows. They focus on the influences of operating
parameters like temperature, pressure and inlet air swirl and spray parameters mean drop size
and spray cone angle on the occurred chemical phenomena. The results showed that increasing
both sprays parameters or one of them increases combustion efficiency. They reported that the
higher combustion efficiency can be achieved in a gas turbine combustor depending mainly on the
effective mixing process between air and fuel vapour. Consequently Sharma and Som [2002] used
the same approach with further investigations. These investigation specially included the fuel
volatility that leads to a rise in combustion efficiency only in case of high pressure. A modified
version of eddy break-up eddy dissipation model was implemented by Klose and Zarzalis [2001]
with joint-PDF combustion model to simulate methane liquid fuel spray flame in low-emission
aero engine combustor. The comparisons with experiments explained that joint-PDF combustion
model preformed better than eddy dissipation model predicting a detached reaction zone while
eddy dissipation model predicted an attached reaction which was contrary to the experiments.
Moreover, they denoted that the proposed combustion model in combination with $(k-\varepsilon)$ model
produced good results and appeared to have numerical stable behaviour.
Till recently, the rate of heat release was predicted by using methods require only evaluation of averaged species mass fractions to describe the combustion process in a very simple form. However, there is a need for an explicit formula to couple chemical kinetics with rate of combustion in turbulent mixing controlled regime. With regard to numerical simulation Guo et al. [2002] in a pure Eulerian-Eulerian approach used a hybrid kinetics/eddy break-up (EBU) model for modelling propane and kerosene spray combustion in an axisymmetric sudden-expansion combustor. Turbulent interactions between gas-droplets were simulated by applying \((k - \varepsilon)\) model. The model showed the effects of recirculation zone on enhancement of spray evaporation and flame stabilization. Another application for Eulerian-Lagrangian approach for turbulent reactive two-phase flows inside an industrial tubular burner was implemented by the ONERA’s MSD numerical in-house code to perform a modified version of EBU model. The modification takes into account the variation of hot products compositions where the local air-fuel ratio plays an important role and to ensure that there is no overpredictions for the mean temperature in the reaction zone. The two-equation model was utilized to characterise the induction of turbulent flow due to droplet dispersion and to simulate the turbulent flame structure.

Menon and Patel [2006] made two contributions to the large eddy simulation for spray combustion. The evaluations were done by using subgrids for fuel-air mixing and the rate of chemical kinetic beside spray-turbulence. Using such low scales below LES resolution for two models showed that the laminar reaction rate gave flame stabilization and better physical prediction downstream rather than EBU model, where the flame at inlet upstream was unphysical. Also, they pointed out to use laminar reaction rate approach is computationally more expensive than EBU model because the computations for the finite rate of kinetic were done for every subgrid cell. Byun and Beak [2006] extended their numerical model to investigate soot formation at high temperature and pressure and the heat transfer by radiation for liquid kerosene-oxygen spray combustion in the liquid fuel rocket engine at all speeds. To account for the existence of turbulent intermittency on the chemical reactions, \((k - \varepsilon)\) turbulent mixing time and chemical species mass fractions were used for modelling. Furthermore a considerable study for three-dimensional arbitrary curvilinear coordinates in a gas turbine combustor was presented by Yan and Liu [2008]. An Eulerian-Lagrangian approach was used to simulate gas-liquid two-phase turbulent combustion flow. EBU subgrid model was employed to calculate the finite rate of chemical reaction and k-subgrid equation was used to simulate eddy viscosity. This study was focused on the effects of primary holes position and air-fuel ratios on the turbulent reactive two-phase flows field. Three combustion models with large-eddy simulation were implemented by Zhou
et al. [2008] in different simulation for jet diffusion, swirling diffusion and premixed combustion behind a bluff body. The aim of this study was to make comparisons between the second order moment (SOM) combustion model proposed by the authors with EBU model and presumed probability density function (PDF) combustion model. From the obtained results the presented model is able to produce qualitative statistical results when it is comparing with the other two models. Advanced model used for simulation turbulent combustion is the flamelet model. Many researchers have been used this model in their modelling. For example, a comparison has been made based on mathematical modelling between non-equilibrium, mixedness-reactedness flamelet and eddy dissipation model where the natural gas in a cylindrical combustion chamber is used by Gran et al. [1994] and Ma et al. [1999]. In these numerical investigations the turbulent field was introduced in terms of Reynolds stress model based on four equations for the stresses. The finite volume approach linked with body-fitted curvilinear non-orthogonal coordinates and a non-staggered grid arrangement was used together with the high Reynolds number \((k − \varepsilon)\) model. The flamelet model produced a good agreement in general as compared with the experimental data. While the eddy dissipation model produced an overpredications for the temperature and underpredications for the oxygen concentrations near the axis. Thus in order to improved that model, they had two suggestions either by adding the extinction model or by reducing the model constant.

Abraham and Gopalakrishnan [2004] applied flamelet model to study the effects of multicomponent diffusion on the predicting of autoignition of spray combustion. The thermal diffusion coefficient were calculated by TRANSPORT library from the CHEMKIN code Kee and Miller [1993]. Similar to diesel engine conditions were used and the obtained results were compared with those of unity Lewis number. Inhomogeneity in turbulence effects on the diesel auto-ignition process were observed. Zhang et al. [1995] studied transient laminar flamelet model with \((k − \varepsilon)\) model in cylindrical chamber. The method calculated the chemical reaction rate source term depending on the progress variable, scalar dissipation rate at stoichiometric conditions and the pressure. The calculated local value has linked with joint pdf to determine the mean value. The experimental work of Friedman and Renksizbulut [1999] was modelled by Kim et al. [2001] to simulate a steady hollow cone spray flame of methanol interacting with an annular air jet. The stationary laminar flamelet model with a low strain rate of \(1 \text{ sec}^{-1}\) is applied for modelling turbulent combustion. Recently Ge et al. [2008] experimentally and numerically simulated a turbulent ethanol spray flame. Spray flamelet model has used combined with a transported probability density function (PDF) method to describe the two reaction zones in the spray flame.
Flamelet model in diffusion flame has been included the effect of turbulent Prandtl/Schmidt numbers on the flow field modelled by Jiang and Campbell [2008]. This concept uses the well known Reynolds analogy where turbulence scalar transfers in flow field and characterizes on the basis of momentum transfer. Combustor modelling was their application and to describe the turbulent flow field Reynolds stress model was used. One flaw of this model is need to construct four transport equation to represent Reynolds stresses whereas in case of two-equations model needs only two equations for the description of turbulent field.

6.4 Chemical thermodynamics and kinetics

Chemical kinetics is the study of reaction mechanism with respect to reaction rates, formed species and formation of new intermediate products. Chemical reactions generally take place when pairs of molecules collide. Because of collision chemical bonds are broken during impact and new bonds are created. For the duration of this process many intermediate species and bonds are formed. The points of interest are chemical kinetics concepts joint to how these reactions occur and amount of reacted and formed species as well as speed of their formation. In other words the rate of change of their concentration i.e., rates of reactants consumption and products formation. One of the theoretical tools to describe combustion calculations is the chemical reaction. A chemical reaction between the reactant species \( A, B, \ldots \) that forms the product species \( C, D, \ldots \) can be written in a general form

\[
 v_A A + v_B B + \ldots \ldots \rightarrow v_C C + v_D D \tag{6.20}
\]

here the \( v_i \) are termed the molar stoichiometric coefficients. The above equation is considered as a single-step irreversible chemical reaction i.e., direct progress rates due to consuming and forming. In fact the chemical reaction has more than one step such is called elementary reaction which allows many possible reaction mechanisms that make the chemical kinetic more complicated. Therefore combustion modelling is required to determine rates of consumption and production for species. However a complete mechanism is necessary, where it is specified at which molecular level the reaction proceeds and gives precise details about each stage of the chemical reaction transformation. The above equation is identified as a forward reaction which is not sufficient to illustrate a chemical reaction then a backward reaction is presented to involve unstable and high reaction intermediate species. Then a system of equations can be expressed in compatible
form as
\[ \sum_{i=1}^{n} v_{ij} A_j \rightleftharpoons \sum_{i=1}^{n} v'_{ij} P_j \] (6.21)
where \( j \) represents the number of species. Every chemical reaction can proceed in both directions.
The mass conservation equation is enforced in the above equation which should be satisfying
the balance equation. The mass conservation can be written as :
\[ \sum_{i=1}^{n} v_{ij} MW_i \rightleftharpoons \sum_{i=1}^{n} v'_{ij} MW_i \] (6.22)
where \( v'_{ij} \) and \( MW_j \) represented the molar stoichiometric coefficient for the products and molecular weight of species respectively. As it seen the mass balanced equation does not provide any information about how the reactants become products and how long it will take to reach equilibrium state. This information of the overall process can be evaluated through one or more steps in reaction kinetics. The temporal mass reaction rate of \( (i) \) species in the reaction \( (j) \) is:
\[ \dot{\omega}_{ij} = s_{ij} MW_i v'_{ij} \] (6.23)
here \( s_{ij} \) refers to the rate of progress of reaction \( j \). If reaction mechanism is involved for all reaction that were taken place, then the mass reaction rate, \( \dot{\omega}_{ij} \), can be expressed as the sum of reaction rates. Hence the sum takes the form of
\[ \dot{\omega}_i = \sum_{j=1}^{n} \dot{\omega}_{ij} = MW_i \sum_{j=1}^{n} s_{ij} v'_{ij} \] (6.24)
As mentioned above the sum of all mass reaction rates for all species obey the law of mass conservation, so equation (6.24) takes the form of
\[ \dot{\omega}_i = \sum_{j=1}^{n} \dot{\omega}_{ij} = MW_i \sum_{j=1}^{n} s_{ij} v'_{ij} = 0 \] (6.25)
It expresses the variation of products formation with time where there are four aspects that can be affected:

1. Existence of catalyst.
2. Concentrations of products.
3. Reactant type phase.
4. Temperature.

The declaration of the law of mass action, states that there is a proportionality between the rate of consuming reactants and the production of the product species. The rate would be raised to the powers related to the stoichiometric coefficients of the reactants. The temporal variation of species concentration is related to the reaction rate because the slope of concentrations of products plot against time gives a local value for that reaction. Therefore the reaction for the considered reaction rate is written as:

\[ R_i = K_f \prod_{j=1}^{n} \left( \frac{\rho y_i}{MW_i} \right)^{v_{ij}} - K_b \prod_{j=1}^{n} \left( \frac{\rho y_i}{MW_i} \right)^{v'_{ij}} \]

(6.26)

where the expression \( \left( \frac{\rho y_i}{MW_i} \right) \) is termed as molar concentration of species. \( K_f \) and \( K_b \) are forward and backward rate constants respectively. The rate constants can be obtained from experiment for each reaction because firstly they are difficult to calculate. Secondly they are related to the temperature of the system. There is an expression that is known as the Arrhenius equation:

\[ K = AT^{b_j} e^{\exp \left( \frac{-E}{RT} \right)} \]

(6.27)

where \( R \) is the universal gas constant (8.314 J/mole.K), \( E \) is the activation energy and \( T \) is the temperature with exponent \( b \). The constant \( A \) is called frequency which is related to the collisions between reactants. Consequently due to the huge number of reactions required for using a detailed mechanism, these have been tabulated for many chemical reactions, to capture the numerous physical and chemical phenomena that are involving in a combustion process. The macroscopic viewpoint is introduced through convection, diffusion, heat exchange and chemical interaction processes investigation. In general three main combustion systems can be classified depending on the introduction of reactants to the combustion zone. Their identifications are:

1. Non-premixed combustion:

   It is also known as diffusion flames, the principle of this system is based on the fuel and oxidizer are supplied to the combustion zone as two streams spatially separated. According to this the flames are unable to propagate upstream but the reaction rate is controlled by the degree of mixing of reactants. This is governed by convection, molecular diffusion and turbulent transport.

2. Premixed combustion:
Contrast to non-premixed combustion, the reactants, the fuel and oxidizer are completely mixed before entering to the combustion zone. The molecular mixing level is favourable in terms of high intensity turbulence and the dispersion of the molecules to raise combustion efficiency. This kind of flames are capable of propagating in premixed reactants upstream, leading to unsafe situation.

3. Partially premixed combustion:

This is a middle situation between the two previous kinds mentioned above and it applies in a few cases. This happen only when the non-premixed reactants are mixed by turbulence before combustion and the resulting flames can propagate through the forming mixture.

Essentially this work is based on non-premixed combustion and will be explained in more details in a separate section below.

6.5 Non-premixed combustion

The phrase diffusion combustion is often used to identify non-premixed combustion, when the subsequent mixing between two spatially separated streams of fuel and oxidizer meet in the reaction zone before the chemical reaction is initiated. Indeed the mixing process is governing the behaviour of this combustion type and the reaction rate is often controlled by mixing rate. Examples in industrial applications are combustion in gas turbine combustor, diesel engine and aero engines. Numerous complex processes occur in diffusion combustion including mixing, pre-combustion, combustion and flame propagation. In case the fuel is liquid the evaporation process is involved that takes place before mixing, and volatilization when the fuel is solid.

When combustion occurs only three zones can be constructed within the structure of non-premixed combustion. A mixture region (reaction zone) is separating a fuel-rich side and an oxidizer-rich side. Both fuel and oxidizer are transported toward the combustion region. During their motion interactions through convection and diffusion may be occurring between them which lead to heat up and mixing within the reaction zone. Eventually rapid reaction takes place. It is, however quite useful to explain non-premixed combustion when the fuel is in liquid state.

A bulk of liquid or droplets of fuel does not combust as such. It should be first evaporated and the resulting vapour is mixed with oxidizer to form a combustible mixture. The rate of evaporation is significantly influential and even governs the overall reaction rate. Many relevant factors are controlling the evaporation phenomena, the most important of which are discussed.
The liquid is dispersed in which the atomized liquid fuel is commonly broken up into droplets to form a cloud of fine droplets. As a result the rate of evaporation in general will increase as the surface area of liquid increases. Thereby a higher intensity of combustion would be achieved. Evaporation of liquid is an endothermic process. That is because the received energy from the surrounding converts liquid to vapour. This energy is often referred to as the latent heat. The extracted mass from the liquid to the surrounding is the process termed as evaporation. The evaporation process is also influenced by pressure at which a liquid fuel evaporates. In case of pressure increased, higher temperatures are required to evaporate. The probability of liquid decomposition due to increased temperature is expected to increase. In addition the evaporation is affected by whether the pressure of the surroundings exceeds the critical pressure of the fuel. Using high hydrostatic pressure as the liquid fuel emerges from the nozzle during injection period to form fine droplets is also accomplished with dispersion as discussed before.

After the evaporation process, the fuel vapour has to be mixed with surrounding gas before combustion can occur. The mechanism of mixing process is dependent on the liquid situation. Perhaps the liquid is completely evaporated prior to combustion or individual droplets are enveloped by diffusion flames. Each case has different features for non-premixed combustion. For example, when droplets evaporate completely as flow occurs prior to entering the combustion zone, the resulting flame can be regarded as premixed. The radiation from combustion zone may increase the rate of evaporation for the rest of liquid fuel as it approaches the flame. Practically the forming mixture cools down as the rate of evaporation increases. The rate of evaporation is influenced by boundary layer around the drops. Small droplets offer a large area per unit mass of liquid to evaporate. Lower masses mean that they are more probable to be accelerated to the gas velocity in which they are enclosed. Therefore the diffusion due to the thicker boundary layer will be less than for heavier droplets because it has larger relative velocity. The other situation exists when individual droplets as they instantaneously vaporized are enveloped by diffusion flames. Explanation of this starts from the driven convection and radiation heat transfer supplied to the droplet by the ambient gas. The droplet surface decomposes to liberate fuel vapour which fills the volume between the droplet surface and inner bound of the concentric diffusion flame. Combustion takes place when a thin layer of fuel vapour and oxidizer flows towards the combustion zone.
6.6 The mixture fraction

The fundamental approach for modelling non-premixed combustion phenomena is using the well known concept of the passive scalar mixture fraction concept. This conception it based mainly on two assumptions which are:

1. The diffusion coefficients are equal for all species.
2. Heat capacities and their independence are equal for all species.

The mixture fraction $Z$ can be introduced as a dimensionless conserved scalar where its value ranges from unity in fuel side to zero in oxidizer side. As a starting point to define the mixture fraction, a one-step irreversible reaction between fuel and oxidizer is assumed

$$v_F F + v_O O \rightarrow v_P P$$

then the mixture fraction $Z$ can be defined as

$$Z = \frac{SY_F - Y_O + Y_O^0}{SY_F^0 + Y_O^0} = \frac{\dot{m}_F}{\dot{m}_F + \dot{m}_O}$$

here $S$ refers to the stoichiometric ratio given by

$$S = \frac{v_O MW_O}{v_F MW_F}$$

where $Y$ and $\dot{m}$ are the mass fraction and mass flux, respectively. The superscript 0 refers to initial values while subscripts $F$ and $O$ denote fuel and oxidizer species, respectively. The passive scalar changes due to convection and diffusion in a transport equation without chemical source term. It was first suggested by Shvab and Zeldovich as a simple conserved scalar which is varying linearly with x-coordinate as,

$$\rho \frac{\partial Z}{\partial t} + \rho v \frac{\partial Z}{\partial x} = \frac{\partial}{\partial x} (\rho D \frac{\partial Z}{\partial x})$$

where $D$ is diffusion coefficient. This element (mixture fraction) is used to perform a transformation for unburnt and burnt mass fraction and enthalpy (sensible and chemical), in other words it simply refers to the mixing process in reactive case which involves burnt and unburnt gases. A mixture fraction is called stoichiometric mixture fraction if the ratio of the concentration of fuel and oxidizer in the unburnt mixture is equal to $S$. In reality it is utilized to study combustion
response variation phenomena in Z-space. In contrast to a two-inlet gaseous streams system, the transport equation of mixture fraction for a liquid fuel has a source term due to evaporation of liquid which is transferred to the gas phase, so the equation (6.31) become as

\[ \rho \frac{\partial Z}{\partial t} + \rho_l \frac{\partial Z}{\partial x} = \frac{\partial}{\partial x} \left( \rho D \frac{\partial Z}{\partial x} \right) + \dot{q}_m \]  

(6.32)

Where \( \dot{q}_m \) refers to the mass evaporation rate transferred to the gas phase. For an arrangement of diffusion structure, in the case where the heat lost by radiation and change of enthalpies due to extra mixing process are both ignored, then the temperature, density and species concentration all become a function of mixture fraction. In fact, real diffusion flames have more complicated behaviour and the structure is more complex to determine. The simplification of mixture fraction is essentially to achieve reasonable results at least for thermochemical elements. However the difficulty is initiated after solving equation (6.32) with appropriate boundary conditions. For example, if the enthalpy variation is considered, then extensions for the independences have to be included. An extra transport equation is needed to be solved with boundary conditions to involve radiation effects. For these reasons different approaches exist with sophisticated assumptions to determine the diffusion flames structure depending on the mixture fraction.

6.7 Combustion modelling

The starting step of all kinds of combustion modelling is a formulation of mathematical model for chemical species to simulate physical and chemical interaction processes. The mathematical models are different in their complexity. For the solution, the chemical reaction rate needs to be modelled. The chemical reaction rate can be regarded as one of the most challenging topics for the numerical and theoretical aspect of non-premixed combustion modelling. According to this the modelling of chemical reaction rate falls into two categories:

1. An implicit model which benefits from transport of mixture fraction and its variance to calculate temperature and chemical species.

2. An explicit model based on transported species mass fraction, therefore the reaction has to be modelled.

Both techniques are used in the frame of this work to analyze their performance. The combustion model computes the chemical kinetics that may happen within the reactive species. The spray
combustion model is used since the spray droplets are introduced into the reactive medium. The autoignition and combustion models implemented in the present work are characterised by one combustion model. This model has the ability to represent the two separate processes in contrast to the commercial softwares like STAR-CD. The overall combustion rate is given by

\[ \dot{\omega}_t = R_{turb} + R_{lam} \] (6.33)

The combined combustion model (CCM) consists mainly of combining two combustion models. Eddy breakup (EBU) model is considered as the simplest version that can be handled for turbulent combustion modelling with flamelet assumption. The principle of EBU model is that the combustion rate is evaluated by the rate at which groups of unburned mixture within the turbulent flame brush are broken into smaller ones, these create a sufficient interfacial area between the unburned mixture and the hot gases to allow reaction. In addition the EBU model was initially developed for when the reaction time scale is small as compared to the micromixing time scale. According to the model, the fuel consumption rate is expressed on the base of a single step reaction as

\[ R_{turb} = \frac{\rho E}{k} A_{ebu} min[Y_F, \frac{Y_O}{s_O}, B_{ebu} \frac{Y_P}{s_P}] \] (6.34)

where \( A_{ebu} \) and \( B_{ebu} \) are empirical coefficients. The parameter \( s_O \) is given by

\[ s_O = \frac{n_O MW_O}{n_F MW_F} \] (6.35)

and

\[ s_P = \frac{n_P MW_P}{n_F MW_F} \] (6.36)

The second term in CCM is from the theory of laminar combustion flows. The theory is based on combustion being a combination of transport phenomena and chemistry. More clearly, any reacting flow is instantaneously determined by both fluid dynamics (such as pressure, temperature and velocity) and the chemistry (such as concentration of species). However it is more conventional to present the laminar reaction rate in terms of the standard Arrhenius equation as

\[ R_{lam} = AT^{bj}[F]^{m}[O]^{n} \exp \left( -\frac{E}{RT} \right) \] (6.37)

where all parameters were previously defined.
6.8 Computational contributions

6.8.1 Turbulence model

The nature of turbulent flows is presented in most realistic flow modelling. Turbulence in flow is associated with the flow can being seen as irregular, random and chaotic. This can be prescribed by eddies characterised by a large range of length and time scales. The large eddies with scale sizes according to the order of the flow geometry extract their energy from the mean flow. As a matter of fact, the large eddies may undergo a number of breakage into smaller eddies if the Reynolds number is exceeding the turbulent limit. This process is known as energy cascade because it continues until viscous forces dominate over convective forces, ended with dissipation of smaller eddies. As mentioned above the mean flow imposes the large scale whereas the smaller eddies would not have the capability to retain their origin and orientation. It will behave independently to their direction i.e., isotropic.

Unfortunately reactive two-phase flows add more difficulty to the use of a single turbulence model which can be adopted for all sorts of flow and its transition. In this work the main effort will be concentrated on the use of intermittency theory for the turbulent spray flame. Moreover, this theory will try to help to capture spray flame configuration. A \((k - \varepsilon)\) model can be considered as cited in the literature as sufficiently appropriate to use for a successful simulation of non-reactive spray, where a relatively large scale of eddies are generated by induction of the gas phase through droplets motion. Therefore a standard two-equation model can be joined to a intermittent turbulent conception to identify the two reaction zones for the spray combustion modelling. In addition the model offers a great advantage due to solving the fluctuation problem which is the main task for the lumped model.

6.8.2 Mass and heat transfer model

In addition to spray dynamics interactions, the mass and heat transfer processes also have significant influences on combustion, ignition and pollutants formation. The foundation of simulation of spray combustion is based on the formation of fuel vapour due to evaporation which is necessary for the subsequent chemical reaction. Here due to the injection of a liquid into relatively hot air or other gas, a liquid droplets starts to evaporate. Therefore the interaction phenomenon between cold spray droplets is needed to be modelled. In this work, using the spray moments approach proposed by Beck and Watkins [2002] and Beck and Watkins [2003a], the drop sizes would be changing due to the reduction in mass. Hence, the order of the moment is imposed
on the treatment of mass transfer equation according to volume, surface area or drop radii. In spray combustion, the heat transfer process gives an indication about spatial distribution of equivalence ratio and therefore strongly affects both time and location for the ignition. In order to describe the evaporation process physically, the energy is transferred from the hot combustion chamber gas to the cold droplets by convection and radiation and due to conduction within droplets. These cause diffusive and convective mass transfer from the boundary layer at the droplet surface due to forming fuel vapour. This again changes velocity, temperature and vapour concentration in the gas phase. Therefore for this reason mass and heat must be calculated.

6.8.3 Mixing controlled combustion

The main title for this part is to prove there exists a relationship between mixing process and combustion through inserting two poles of a new mixing model inside a modified combustion model. The poles are vapour mass fraction and scalar dissipation rate. The mixing model starts from a transport equation for fuel vapour mass fraction for which it is clear how to assign all terms inside the transport equation including the external effects. On the other hand, the scalar dissipation rate is evaluated via transported mixture fraction. Although there are many researches were made and many suggestions for modelling the transported scalar dissipation rate but still these attempts are under development. The decisive reason to choose the vapour mass fraction instead of using scalar fluctuation variance is because it can be calculated from the amount of consumption directly through the chemical reaction formula. The scenario starts when the spray droplets are evaporating to generate vapour which in turn mixes with surrounding air. The forming vapour mass fraction is bounded between $[0,1]$. This parameter can provide information about the evaporation and mixing states. Now the question is posed, if there is such a parameter as mixture fraction ($Z$) that can be used for describing the proceeding of mixing process as found in the literatures, why should we use a different one? As mentioned before, the mixture fraction can handle the reduction of mass due to evaporation, which is still not enough to give a full picture about the components inside the combustion zone. However when the case is spray combustion, it is certainly correct to use vapour mass fraction. Previous works were investigated by several researchers with the focus on spray mixing models. Since the topic is multi-faceted and affected by many physical phenomena, their work can be classified into three groups by giving the priority to the reacting two-phase flow only. The first group
adopted the fuel droplet evaporation model. This model assumes that combustion is controlled by evaporation rate. Thereafter spray hydrodynamics changes are taken into account. The actual spray computational calculations are divided into zones and the droplet evaporation rate is calculated in each time step because mainly the model is depending on the time history of consumption as documented in Hountalas et al. [1997]. The second class was based on transient gaseous flow modelling. These models assumed that droplets are evaporated instantaneously due to rising pressure in the combustion chamber where the gaseous phase is dominating and where combustion modelling utilized the vapour mass fraction which is in fact inaccurate as implemented by Kuleshov [2005] in diesel engine. The last group lays behind two-phase evaporation modelling. In CFD calculations, the droplet concentration may be reduced in each time step depending on the entrained air as stated in contribution paragraph and explained in more details in chapter five. In order to provide full information about mixing modelling, McCracken and Abraham [2002] is selected as an example from the first group just to illustrate the concept. When spray droplets are injecting into the combustion chamber, they mix with chamber air. The chamber has divided into three zones, rich, flammable and lean to explain the mixing approximately. The rich zone had a local equivalence ratio of $\phi > 2$, the flammable zone had an equivalence ratio between $[0.5, 2]$ and the lean zone had an equivalence ratio of $\phi < 0.5$. It may be useful to know that all these values were arbitrary.

### 6.8.4 Auto-ignition

Ignition of droplets can be essentially classified into two types according to the process that may be accomplished. The first is thermal ignition (auto-ignition) which occurs when cold droplets are exposed to hot gases in diesel engine. The second is network ignition which takes place when spray flame is in contact with cold droplets. The heat of combustion which is emitted from hot gases is transferred to droplets and ignition results. In diesel engine, after the start of injection auto-ignition may occur after a certain time. The period of auto-ignition characteristic of diesel engine may be defined as the time for a significant increase of temperature to be observed.

This definition is subjective just when there is a quantifiable increase in gas temperature. The slope has a very sharp curve of gas temperature versus time due to the nature of exponential process, that can help for the resolution of the problem. The auto-ignition of hydrocarbons in diesel engine is proceeding in terms of three consecutive steps that occur during this time delay. These steps are as follows:
1. The surface temperature of the droplet receives a sufficient amount of heat by convection and radiation due to the contact with the hot surrounding as a result the fuel vapour is released.

2. The fuel vapour mixes with the oxidizer in the hot chamber, hence the temperature of the mixture fuel vapour-oxidizer is increased.

3. The mixture becomes within the inflammability limits, and, when the temperature exceeds the ignition temperature, ignition occurs.

Precisely at this point, the amount of heat released by the reaction is higher than the heat lost by the surrounding, resulting in auto-ignition.

6.9 Presentation of the case study

6.9.1 Description of the experiment

In this section application is made of the complete model for the simulation of non reactive and subsequently turbulent reactive submodels in diesel engine. The different submodels represent the complex phenomena which include high injection velocity, breakup, collision, evaporation and combustion. Typically, a spray combustion model implemented in diesel engine has mainly two modes classified according to the time of reaction. They are auto-ignition and combustion mode because combustion process is accumulative over time. However validation of the spray combustion model includes comparisons with auto-ignition delay time at different initial gas temperature, gas velocity and penetration with experimental and numerical data available to support the model and provide a full picture for spray combustion modes inside the combustion chamber. This study is dedicated to investigate the ignition mechanism and accommodates a proper establishment to distinguish spray combustion in diesel engines.

The experimental configuration of the open reactor reported by Koss et al. [1992] consists of a vertical closed vessel of 90 mm diameter and a nozzle. The nozzle is of 0.1 mm radius and uses n-heptane as liquid fuel and the injector is placed along the centerline in the direction of the flow. The hot air is blown in the direction of the co-flowing injected liquid. The air pressure is set to be 50 bars. The initial air temperatures were confined between [763K-823K]. The simulated liquid flow injection conditions correspond to experimental data. The injected fuel mass and temperature at the injection stage were 6 mg and 300K respectively. The injection duration was
1.4 ms. A perforated plate was positioned in the axial direction associated with a laser optical device in order to initiate turbulence in the flow by rapid flow through the plate.

6.9.2 Description of the simulation setup

The computational domain for the geometry of the open reactor has been taken from Koss et al. [1992]. The reactor contained a cylinder of 90 mm diameter and the liquid fuel was injected through a nozzle placed along the centerline in the direction of the co-flowing of the hot gas resulting in a full cone spray. Figure (6-1) shows the overall grid for the cylinder plus the nozzle orifice. The numerical accuracy can be obtained here by using unstructured grids which provided the desired level of accuracy for the computational calculations. By taking into consideration the use of a very fine grid around the injector forming four injector cells. In addition a very fine grid along the centreline is used where the spray droplets are expecting to be dispersed. This avoids a fine grid in the regions where there are no interaction hence decreasing the computational time. The domain is divided into 10738 finite volume cells which consists of 21656 faces and 10919 vertices. The grids are generated using GAMBIT, the mesh generating software which is linked with the in-house code for solving two-phase flows with unstructured mesh Jones [2009]. Computations are based on using the unstructured grid arrangement, which provides the solution to resolve the high gradient combustion regions along the stoichiometric line. The grid analysis is explained in more details at the end of this chapter.

The lumped spray combustion model proposed here is incorporated into the open reactor using n-heptane liquid fuel. At three different ambient temperatures the engine operates with same initial conditions at the injection stage. Under these conditions, the time required to achieve nearly complete mixing is proportional to the ambient temperature. As a result the mixing time becomes shorter when the temperature is increased.

6.10 Results and discussions

6.10.1 Penetration

In order to validate the present simulation calculations, two parameters are compared with available experimental data in separate paragraphs. Spray tip penetrations obtained from the experiment were measured either by Phase Doppler Anemometry (PDA) or photographically. It is simple to define the spray penetration as the furtherest distance that liquid droplets reach.
through a certain time. For the calculations it is determined as the axial position behind which 99% of the liquid volume are contained. Included are most of the relative interactions between spray droplets and ambient gas as modelled in spray submodels.

Figure (6-2) shows the calculated results on spray tip penetration compared with experiment. Two combustion models are included in this comparison, combined combustion model (CCM) and the proposed Lumped spray combustion model (Lumped). The models show a good agreement with experiment. CCM after 1.3 ms appears to relatively match the data until 1.5 ms, this because there is no mixing process in earlier stage which tends to enhance the vaporising effects and CCM produce a later auto-ignition point than does the Lumped model. Therefore precisely at time 1.2 ms Lumped model starts to produce a higher amount of heat sufficient for self-ignition as will be explained later in auto-ignition paragraph below. This amount of heat will increase the gas temperature and consequently increase the evaporation rate which is leading to decrease in spray penetration due to extra heat subjected to the spray droplets. Alternatively the modified mixing which is the main reason for using Lumped treatment clearly appears in figure (6-2) and it takes effect between 1.2 ms to 1.5 ms, keeping the reduction for fuel liquid penetration below that of the experiment approximately constant. The spray flame produced here is considered as a diffusion flame since the propagation of the flame takes place both down and up stream. The consumption rate of vapour mass fraction and droplets in the combustion zone is high but the Lumped model shows better results than the CCM model at late time of injection specially at the auto-ignition point where it works to accommodate the higher reaction rate, this observation will be discussed in mixing sub-model later. In fact that leads to a long lifespan of droplets in CCM model which needs a long time to prepare the mixture of fuel vapour and air for ignition.

6.10.2 Auto-ignition

The second part of the comparison deals with auto-ignition points and gas temperatures of solid cone sprays injected into air at different initial gas temperature. Three two-dimensional simulations of auto-ignition of n-heptane liquid fuel sprays in hot air have been performed by changing only the initial air temperature. In order to improve the accuracy of the results and ensure numerically sensible results the length and time base units are scaled up by a factor 1000. The Lumped model details described in section (6.2) enables to study the auto-ignition phenomena and beyond it. To have a better understanding behind the concept of using Lumped
treatment the comparisons are validated with the conditional moment closure model which has features similar to the flamelet model. The only difference is instead of using conventional averages conditions are set for modelling reactive scalars depending on discretization of the mixture fraction by using the conditional probability density function Wright et al. [2005]. Alternatively in Lumped model not all fluctuations of the reactive scalars are associated with the mixture fraction fluctuations specially in the reaction zone. More clearly as explained in section (6.2) and repeated here in more details, the main reason is the fact that the transport equation of the mixture fraction does not contain the effect of non-equilibrium turbulent chemistry. The auto-ignition delay period is calculated by simple relation according to vapour mass fraction and the oxidizer (Arrhenius equation), that explains the reason behind selecting vapour mass fraction directly in the presented model. However a more subtle way to characterise and capture the turbulent reacting zone during the evaporation stage or outside the main reaction zone which is spatially and temporally found before the end of injection period and then eliminated it to keep the generality in the solution. Lumped treatment is based on scaling properties used for identification of flame surface geometry. A review of the existing theories were applied to model spray auto-ignition point in terms of the original model. For example shell model, the extended shell model and look-up table methods. The shell model was originally developed using the idea of solving system of ordinary differential equations for all chemical kinetics. It is computationally expensive due to intensive calculations. Alternatively look-up table methods are also producing extra computational effort because of search and extrapolation techniques that have been used to match the case. However CCM and its modification (Lumped model) treat auto-ignition by coupling with other physical sub-model involved in the calculations without separate calculations. Numerically the energy equation for the gas phase is considered the source to extract the results for the gas temperature and auto-ignition point. The latter is evaluated from the CFD calculations as the time develops in the spray modelling.

In figure (6.3), the predicted auto-ignition delay times of n-heptane are compared with experimental work of Koss et al. [1992]. Figure (6.3) shows that the auto-ignition delay time decreases with an increase in ambient temperature at the same ambient pressure. The location of auto-ignition point (can be observed where the gas temperature is rapidly rising) is just downstream of the injector in the contour plot of the gas phase temperature. Auto-ignition of any mixture of fuel vapour and oxidizer with the presence of droplets occurs through complex physical and chemical processes so that it is not simple to define exactly the onset of ignition in both numerical and experimental investigations. Although many researchers have suggested various
methods, there is still no definite or universal criterion for an auto-ignition point. In some applications, the point when the second order time derivative of maximum reaction rate in gas field become zero was selected as the autoignition point. In the present work as realized from the experimental literature, the auto-ignition point is always inaugurated in a lean mixture zone and from modelling when the scalar dissipation rate is low. The location of ignition point mostly depends on injected fuel velocity, initial gas temperature and turbulence. The effect of initial gas temperature on spray auto-ignition delay is shown in figure(6.3). The effect of turbulence obviously appears as eddy break up model is implemented and compared with experimental data and other models.

The auto-ignition period can be divided into two parts according to the previous experimental and theoretical investigation. In order to analysis the auto-ignition point more deeply, each term will be investigated separately. The first term is an implicit expression related to the time spent for reducing the velocity gradient below the critical value near or at the spray tip. Ignition delay will be determined from Arrhenius equation as:

\[
\tau_{\text{chem}} = A^{-1} T^{-bj} [F]^{-m} [O]^{-n} \exp \left( \frac{E}{RT} \right) \tag{6.38}
\]

The calculation of ignition delay time due to proceeding chemical reactions comes from a simple estimation for a single global Arrhenius formula expressed above. Because of evaporation of droplets, the heat release equation gives negative values before combustion. Here in the original model, CCM, the standard \((k - \epsilon)\) model is implemented to characterise the gas velocity field development. The second term is an explicit expression which involves the chemical reaction rate for the same velocity gradient. Developing this phenomena states that chemical reaction time is much smaller than the former term named as micro-mixing time (the physical delay time required for spray interaction without chemical effect). Coupling between chemistry with turbulent reactive flow by using this approach is only useful when the turbulent mixing time scale is very small as compared with chemical time scale. For the present case, this occurs only for mixing time less than 1/1800, Mura and Demoulin [2007]. The EBU model is considered to describe the integral turbulent length scale conjugated with Beta intermittency model to capture the smallest scale of turbulent dissipation separated flamelets. The eddies that may generate secondary reaction zone (extinction zone) can be converted into extra heat by modified mixing process. This method is more useful than using multiple time scale turbulence model that needs a restricted domain and large computational time and cost. The turbulence time scale is related
to the eddy turnover time and written in the form of

\[ \tau_{\text{tur}} = A_{\text{ebu}}^{-1} \left( \frac{k}{\epsilon} \right) \]  

where in Mura and Demoulin [2007] the constant is proportional to the ratio of turbulent kinetic energy to flamelet propagation velocity as

\[ A_{\text{ebu}} = A_{\text{ebu}}^{0} \left( 1 + \frac{4.4}{1 + 4 \cdot \frac{k_{0.5}}{S_{t}}} \right) \]  

where \( S_{t} \) is the flamelet propagation velocity. Alternatively the way chosen by Patterson and Reitz [1994] was by introducing a delay coefficient multiplied by the presented equation above. The coefficient was chosen to simulate the reaction progress variable as increasing influence of turbulence on combustion after ignition has occurred, the coefficient was expressed by

\[ f = \frac{1 - \exp(-c)}{0.632} \]  

where \( c \) is the reaction progress variable. In contrast to the other models, Lumped model is related to the dissipation rate of the kinetic energy where as documented in turbulence modulation part in section (6.2.1), the viscous cutoff time scale expressed in equation (6.15) is representing the residence time in the fine structure and in addition related to the flame production. Actually the emphasis on implementing Lumped treatment only to the first term comes from the perspective models mentioned above and in fact after auto-ignition point the value of vapour mass fraction tends to be zero as shown in figure (6.4). Normally the auto-ignition delay is decreased as the initial gas temperature and pressure are increased inside the chamber. Consequently the location of auto-ignition is very important and it can exist below the outer spray edge. Under the assumption of enhancing the mixing process by the effect of Lumped strategy, evaporation and mixing processes are directly affected through parameters that are controlling the case, namely the amount of fuel injected and the entering temperature. The mixing process generates a wide range of equivalence ratio, (the ratio of stoichiometric air/fuel ratio to the actual air/fuel ratio). The Lumped model depends on the intermittency theory, the results illustrate that auto-ignition takes place after micro-mixing process that can modify the smallest length scale (or larger according to the fractal theory). The model adopted this special treatment because chemical reactions are only occurring when the reactants become molecularly mixed, assessed by mixing efficiency. The latter here is defined as the ratio of diffusion flame thickness
to the reaction thickness at the molecular level. The adjusted ratio is to ensure that the scaling is referring to parameters related to the reactive zone. Returning to the CCM advantage, as known the auto-ignition phenomena may occur within a wide range of equivalence ratio. CFD calculations starts with zero value of mixture fraction and fuel vapour mass fraction. In the earlier injection period, the physical mode is dominating over chemical mode that is supporting the implementation of CCM.

Figure (6.4) shows the temporal variation of vapour mass fraction. At the earlier stage of injection, the amount of liquid that has been injected into the hot chamber is relatively small compared with total injected mass thus the highest value of vapour mass fraction appears at 0.19 ms approximately. The figure (6.4) does not give an indication about the accumulation of vapour mass fraction as the contour plots do. This is because the calculations that have been extracted are representing selected points downstream. But it clearly shows the values of vapour mass fraction are zero for both models at auto-ignition point where the combustion starts. The accuracy for CCM and Lumped are calculated according to the reference line which has been set to illustrate the experimental auto-ignition point.

6.10.3 Gas temperature

The results in figure (6-5) show the mixing time before the chemical reaction where an ascent in temperature curve is observed. The rise in temperature is related to the amount of fuel vapour forming during vaporising of spray droplets. Of course the gas temperature is slightly reduced before auto-ignition point because fuel vapour temperature generated around droplets is proportional to film temperature (1/3 rule). By using the same reference line as shown in figure (6.4), the results that have been produced by Lumped model are higher than CCM. The maximum temperature in CCM model is recorded as 2031 K while in Lumped model is 2963 K up to time \( t=1.6 \) ms. However it more interesting to know that modifying the mixing process gives rise to the combustion efficiency which match the postulation of enhancing mixing process. The jump from negative to positive values in the exponential term in equation (6.37) means the accumulation is changing the state from mixing to combustion. In order to check the reliability of this auto-ignition criterion the variation of maximum temperature in gas field is shown in figure (6.6) for both models at four different cross section \( x=13, 28, 43 \) and \( 44 \) mm at \( t=1.63 \) ms. The present criterion seems to be reasonable to estimate auto-ignition point where the Lumped model result is closer to the experimental data than that of the CCM model. If there
are fluctuations this is because the maximum value of gas temperature and reaction rate in the gas field do not appear at the same position as the time goes on, which is the aim of this model and can be seen in contours plot in figure (6.7). Results for the Lumped and CCM models have been validated and compared at three times with CMC model results presented by Wright et al. [2005]. The Lumped model shows a better agreement with CMC model, as shown in figure(6.7) the auto-ignition takes place in a small region at a certain radius below the outer edge of the gas temperature contours. When the turbulent mixing becomes more intensive by Lumped model, the auto-ignition will take a short time to take place since the quantity of fuel vapour is increased. When analysing the results it was observed that the auto-ignition occurs below the outer edge of the spray. In experimental configurations it has been found that auto-ignition occurs in the rich mixture downstream of the end of the liquid phase penetration length. The simulation performed here show thus the same behaviour as seen in experiments. Figure (6.8) compares the gas temperatures against the mixture fraction at t=1.6 and 1.65 ms respectively. The main purpose to calculate the gas temperature after the auto-ignition point is to prove that the chemical reaction has occurred at the stoichiometric conditions. In fact this theory has been applied only on the gaseous phase and slightly will be different in case of presence of droplets as will be discussed later in mixture fraction investigation. Figure (6.9) shows the gas temperature against the axial distance at four different times. To extract gas temperature calculations, a cross section at the axis of symmetry has been chosen to determined the gas temperature with 20 selected points downstream. Notice the reaction zone in the figure (6.9) where it is initiated in a small region and then grows downstream at t=1.5 ms and downstream and upstream at t=1.7 ms.

6.10.4 Mixture fraction

Physically mixture fraction can be used to describe the local mixing of reacting species. Numerically it is defined as a non-dimensional parameter that can be introduced as a conserved scaler modelled with a transport equation. The source term that has been added in spray combustion case is the rate of droplets mass evaporation only. The molecular diffusivity of mixture fraction gives an indication about the gaseous mixing but not due to chemistry which means that mixing process could be introduced as a separated process from the chemical reaction. The variance of mixture fraction is used to describe fluctuations of the fuel consumption by the flame. Figure(6.10) shows profiles for the mixture fraction at three different times. These results are
taken along a cross section parallel and close to the axis of symmetry. At time $t=0.6$ ms, the rate of evaporation and mixing is relatively higher than the other times due to the amount of liquid that has been injected and the higher injected velocity at this stage. At $t=1.4$ ms and 1.6 ms, because the combustion has started an amount of fuel vapour has been consumed. It is interesting that because the Lumped model ignites earlier than CCM model it exhibits a lower mixture fraction specially after the auto-ignition time at 1.4 and 1.6 ms due to consumption of the mixture of fuel vapour and air. The accuracy of the mixture fraction transport equation is demonstrated as both models were ignited near the stoichiometric value of $Z$ at $x=42$ mm downstream.

Combustion process not only affects the droplet evaporation but also the droplet dispersion. Dispersion of droplets refers to the ability of droplets to characterise local variations of the gas phase velocity. Figure (6.11) shows the radial evolution of the mixture fraction at the same three times. At $t=0.6$ ms, the rate of mixing in Lumped model gives rise to greater droplets dispersion than CCM model whereas at $t=1.4$ ms they show the same trend. At $t=1.6$ ms, as the combustion is proceeding the additional mixing effects works very well as the rate of dispersion is higher and less evaporation takes place.

6.10.5 Scalar dissipation rate

The scalar dissipation rate $\chi$ is a parameter which can be used to describe the strength of diffusion process through the coupling of mixing and chemical reaction. Usually this critical element depends on the mixture fraction and the strain rate. In the present model this quantity as in equation (6.7) is used to calculate the local Damkohler number represented by equation (6.5) where the effects of turbulence and chemistry are included. The local spray flamelet is represented by flamelet equation in terms of mixture fraction as

$$\frac{\rho\chi}{2} \frac{\partial^2 Y}{\partial Z^2} + \dot{\omega} = 0 \quad (6.42)$$

where the effects of turbulence and mixing on flamelet are mapped only on the mixing term (first term) which governs the characteristic diffusion time within flamelet. Therefore it is interesting to make comparisons with conditional scalar dissipation rate using the contour results cited in Wright et al. [2005] at different times. The main objective of these comparisons is to show that the increased reactive diffusion process method has different results to those obtained from the conditional moment closure model due to the different technique and numerical tools used.
The two methods are calculating in different ways but rather similar results on distributions are produced as shown in figure(6.12). Another reason to not include these comparisons in this work, because the conditional scalar dissipation rate is evaluated at stoichiometry conditions while in Lumped model it is used as a sensor for capturing regimes before it reaches to the stoichiometric conditions. However an attempt has been made here to investigate the general behaviour of the scalar dissipation rate at all conditions. At the injection stage of the spray droplets, the scalar dissipation rate increases dramatically and reaches to the maximum value due to the high amount of evaporation that occurs and the intensive turbulence initiated by droplets due to the high injection velocity. The high injection velocity increases the rate of liquid disintegration, breakup and evaporation. On the other hand it also enhances the turbulence of the gas phase. Due to this high velocity the scalar dissipation rate increase suddenly because there are large gradients in both the spray and the gas phases. Then after the injection period a gradual decrease for the scalar dissipation rate continue due to the dissipation of turbulence and spread of fuel vapour. Figure (6.13) shows the temporal evolution of the scalar dissipation rate at five different times. At t=0.6 ms the scalar dissipation rate is rapidly increasing and reaches to a maximum value of 24 $sec^{-1}$ due to the highest gradient of mixture fraction (highest rate of droplet evaporation) and the high injection velocity that generated intense turbulent field close to the nozzle exit. After the initial stage, the scalar dissipation rate at the rest of the time intervals rapidly decreases to the relatively slow varying values as the dissipation of turbulence is continuously decreased. When the scalar dissipation rate decrease, diffusive losses become small so that heat and radicals produced by chemical reactions can build up and lead to auto-ignition. The scalar dissipation rate appears in this model in the separated flamelet regime, the smallest dissipation rates are found due to the diffusive losses becoming small so that heat and radical species are continuously increased then the corresponding mixture may be ignited. To examine the scalar dissipation rate behaviour along spray flame regimes, figures (6.14) and(6.15) show seven axial and four radial cross sections along the body of the spray flame at t=1.8 ms. Recall that factor $F$ represents the ratio of the upper and lower boundary of the flamelet regime in which the scalar dissipation rate is used mainly to determine these boundaries. Therefore it can be regarded that $t_r$ the smallest length scale at flamelet regime can balance the chemical reactions otherwise the factor $F$ will be used. The factor $F$ can be considered as a combustion index, which is used to distinguish the reaction zone from before the auto-ignition takes place or the separated flamelet regime after the auto-ignition. The factor is based on the local ratio
of the extent of diffusion flame thickness to the reaction zone thickness as

\[ F = \max \left( 1, \frac{t_d}{t_r} \right) \]  

(6.43)

If \( F \) is less than 1, the combustion occurs in the reaction zone where the Damkohler number is small. The reaction zone is usually called the distributed regime. Whereas if \( F \) is greater than 1, then combustion occurs in flamelet regime. Therefore instead of solving equation (6.42), both chemical reactions parameters are calculated to capture the flamelet regime and also the extinction regime is identified when Damkohler number is exceeding the critical value. The latter refers to the characteristic residence time in the fine structures is given by equation (6.15). In more detail about using factor \( F \) in the calculations, the factor is used only when the reaction flame thickness is so small that it cannot be captured. From running three different cases, it is found that the scaling factor is applicable with a constraint up to 1.5 in order not to get a significant changes of the spray flame structure. To prove that, the axial and radial gas velocity components are presenting in figures (6.16), (6.17), (6.18) and (6.19). Figures (6.16) and (6.17) show the axial and radial profiles of the axial gas velocity along the centreline at different times. At time 0.6 ms the axial and radial profiles of the axial gas velocity is higher than the axial gas velocity profiles at 1.2 ms because of the increase in the gas density due to the effect of evaporation. At time 1.4 ms and 1.6 ms the axial gas velocity profiles are increased because of the effect of the chemical reaction which tends to increase the gas temperature and consequently reduction in the gas density. Figure (6.17) shows the radial profile of the axial gas velocity which it increases with time and tends to move towards the centreline because the flame propagates downstream and upstream due to the presence of mixture of the fuel vapour and air. Figures (6.18) and (6.19) show the axial and radial profiles of the radial gas velocity along the centreline at different times. Figure (6.18) shows the axial profile of the axial gas velocity which is increased with time along the centreline towards the reaction zone especially at time 1.4 ms and 1.6 ms where the gas temperature is increased tremendously due to the effect of auto-ignition at the reaction zone. Figure (6.19) shows the radial profile of the radial gas velocity which it increases with time and tends to move towards the centreline because the flame propagate downstream and upstream due to the presence of mixture of the fuel vapour and air. It is also found at the earlier stage of injection 0.6 ms the turbulent gas velocity for both axial and radial components decrease as the axial distance increased due to the effect of evaporation.

Comparisons for axial and radial gas velocity are shown in figure (6.20) between results from
Lumped model and CMC model at different times. At time 1.2 ms in figure (6.20) there are less differences between axial and radial gas velocities because both Lumped and CMC models have not ignited the mixture yet. Whereas at time 1.42 the differences between axial and radial gas velocities are significant due to the difference in the auto-ignition delay time and location. At time 1.52 ms the differences are reduced because of the dominating effect of spray flame velocity. In the various existing models of combustion, it is important to differentiate between the velocity of spray flame and gas velocity. The gas velocity is basically a kinematic quantity for the gas phase and spray flame velocity is considered as a quantity characterizing the rate of reaction of the flame. In models where the combustion of the spray flame is considered as an infinitely thin surface, the gas velocity is a fundamental kinematic quantity called velocity of movement, within the spray flame velocity, which allows the description of chemical processes. This velocity is defined precisely in the reaction zone from the increase in turbulent kinetic energy due to the chemical reaction and it is through this that the linkage is made between the rate of local reaction of the spray flame and the flow and formation of the flame. It has the advantage of being locally determined where the characteristic spray flame velocity is a measure of reaction rate per unit area of spray flame. This rate, commonly called consumption rate (or burning) then represents the consumption of mixture and characterizes the intensity of local combustion. There is no such relationship approximated between the gas velocity and spray flame velocity because the spray flame speed is a quantity not well defined and remains dependent on the experimental configuration studied.

The inspiration of factor $F$ comes from Charlette et al. [2002] who developed a model for turbulent premixed flame for unresolved flame surface density in terms of cutoff scale. The model adopted large eddy simulation and they argue that the model can be applicable with RANS models by replacing the filter size by turbulence integral scale.

$$\frac{S_t}{S_l} = \left(1 + \frac{\Delta}{\eta}\right)^\beta$$  \hspace{1cm} (6.44)

Where $\Delta$ is the filter size. $S_t$ and $S_l$ are turbulent and unstrained laminar flame speed respectively. A model for premixed turbulent flame proposed by Watkins et al. [1996] has been implemented with RANS models. The model uses the flame thickness calculation as

$$t_r = C t_d \left(\frac{S_l}{S_t}\right)^n$$  \hspace{1cm} (6.45)
where $C$ and $n$ are model constants. Finally by comparing between sub-grids scale wrinkling factor and flame thickness calculation in above equation with mapping conditions allows to prevent the change in spray simulation. Thus the scaling factor takes the form in equation (6.1). Mathematically and physically that means the mixing is too slow to balance the chemical reactions.

6.10.6 On the Lumped zone

In order to represent the Lumped zone, the turbulent diffusion flame is used where the structure of the diffusion flame is approximately close to the turbulent spray flame. This is according to Borghi [1988] who classified turbulent diffusion flames into three regimes based on the relation between the turbulent and chemical time scales. Since chemical reactions can only takes place when the reactants become molecularly mixed, here are considered only separated flamelet regime to avoid the universal mapping that may change the structure of the spray flame. The new computational model benefits from the scaling ratio to artificial thicken this regime to a limit that is captured by the proposed procedure. Normally this is determined by the vapour mass fraction which is considered the source of proceeding of the chemical reaction. Similarly the mixture fraction is subjected into mathematical steps to generate the scalar dissipation rate. In more advanced analysis the latter is commonly know as small-scale mixing rate. The reaction zone is characterised in terms of multi-scale reaction structure. Again the proposed ratio is activated only when the reaction flame thickness is below the diffusion flame thickness when this ratio leads to generation of fluctuations. Therefore the mixing works to smooth the fluctuation by local mapping to the diffusion flame thickness up to 1.5.

The planar diagram in figure (6.21) uses the laminar flame parameters $u_l$ and $e_l$ the characteristic velocity and length scale respectively. The parameters $k$ and $l_t$ are the turbulent kinetic energy and the integral turbulent length scale respectively. The Lumped zone can be found in the intermediate regime (perturbed flamelets). The structure of the flame will become more complicated due to the rise in local and instantaneous gradients of vapour mass fraction and oxidizer. In fact the reason is that the rate of stretching fluctuation is decreasing that causes extinction regime, as the turbulence level increases further and the chemistry becomes slower. The length scale associated with the smallest turbulent mixing scale eventually becomes similar to the diffusion flame thickness. The use of combined combustion model in the body of Lumped model is justified as to achieve the following point, in the eddy break-up model the physical
processes are playing important role in the flamelet regime. Peters [1988] suggested a new theory to describe turbulent premixed flames. The theory, named thin reaction zone regimes, is used instead of distributed reaction zones regimes proposed before. The identification of the new regime should satisfy the condition as mentioned above. In this regime small eddies can transport away from the hot gases out of the spray evaporation zone to create a small separated zone. The Lumped zone is a thin zone which is affected by turbulence mixing field and can be found in flamelet regime. The model is trying to utilized the well known micro-mixing and reaction elements to fill the gap between mixing process that controlled the combustion process. As expected the Lumped zone cannot be found in reaction zone because the reaction flame thickness is larger than the diffusion flame thickness. As shown in figure (6.22) the Lumped zone may be found as separated flamelets. The Lumped zone is separated from the evaporation zone at length scale less than Kolmogorov length scale, where the vapour mass fraction and oxidizer are not intensively mixed before combustion. If the case turbulence is generating characteristic scales associated with the turbulent spray flame which may be locally extinguished when they are subjected to local strain.

6.10.7 Can turbulence model identify strained zones?

Unfortunately there is no single turbulence model that can be used to characterise all types of flow. However the presented model is aimed to use an extra procedure to identify the fine structure inside the interacting two-phase flows instead of using multiple time scale model. The latter needs to construct two other transport equations for fine structure which is more computational effort but this not the only problem. Till now the effect of heat reaction are not modelled explicitly in the model. Therefore the results to be shown in this section are just to prove the accuracy of the selected turbulence model to predict the characteristics of the turbulent (non-reactive or reactive) flow and if it is capable of being used as a sensor to identify whether there is a strained zone or not. The impact of the turbulence modelling on the gas phase is introduced here in terms of \((k-\epsilon)\) model. From the continuous phase viewpoint, the turbulence is related to the high Reynolds number and can modify the effective viscosity that causes wake phenomena and consequently increase of velocity gradients. In fact it describes the chaotic fluid motion (fluctuations) and properties, thus it produces a wide range of scales structures ranging from large to small scales. In case of presence of dispersed phase, for example droplets, the case will become slightly more complex. The right hand side terms of the kinetic energy transport
equation consists of four parts. The production term refers to the rate at which turbulent kinetic energy is transferred from the mean flow to the turbulence. Dissipation terms can be used to represent the rate at which the turbulent kinetic energy is converted into thermal energy. The diffusion term or the turbulent transport in the kinetic energy equation can be split into two parts in the model according to gradient approach into dilatational pressure and production terms. The last term is the mass transfer which is released by the droplets during evaporation process. Figures (6.23) and (6.24) are demonstrating the variation of turbulent kinetic energy and turbulent dissipation energy with axial distance at different times. At time 0.6 and 1.2 ms only the hydrodynamics are important and evaporation effects are dominated. The turbulence of the gas phase can be affected by the existence of droplets specially if the concentration of droplets is high enough as at nozzle exit. The highest rate of dissipation can be seen at nozzle exit due to high evaporation rate. The influence of turbulent intensity as shown in figures (6.23) and (6.24) decrease as the droplets size decreases as the flow moves downstream. The existence of droplets in flows may generate distortion in the streamlines that leads to modification of the velocity gradient due to shear forces between droplets and the carrier phase. Chemical reactions are involved at time 1.4 and 1.6 ms respectively. It can be seen that the development of the turbulence field in the downstream region is more affected by hydrodynamics effects than chemical reactions. The three terms are decreased due to the increased shear layer thickness (dissipation term). The production term is reduced due to its proportionality to the square of the velocity gradient. While the dilatational term is increased because the molecular transport coefficients are increased with temperature.

On the other hand, a reduction in the drag force takes place because of the generation of wakes behind droplets. Figures (6.25) and (6.26) show the transient radial profile of turbulent kinetic and dissipation energy. At x=15 mm, large droplets almost do not track the turbulent flow field trajectory because of their high inertia. However these droplets are generating low turbulent kinetic energy due to their presence and act as obstacles that create wakes. It is interesting to notice that at x=35 mm where combustion mode is dominating the rate of kinetic energy is increased slightly more than x=25 mm and x=30 mm. While at x=40 mm relatively low turbulence is observed due to the spray flame velocity is moved backwards towards the mixture of gases. While the highest dissipation rate is found at x=35 mm for the same reason as mentioned above. Again the lowest dissipation rate is found at x=40 mm for the same reason as mentioned above also due to the number of droplets reaching this section is very low because of the accumulation of heat at this time due to combustion increase the rate of evaporation of
droplets to the highest extent. The extra source terms for both turbulent transport equation relating to the mass evaporation rate is shown in figures (6.27) and (6.28) respectively. Simply the calculation are repeated with adding this term and without it. The bold symbols are referring to this term added while the light symbols are referring to the case without this term. Unfortunately because the amount of the injected mass is 6 mg the difference is small but in general the turbulent kinetic energy is reduced because there is a reduction in mass due to evaporation process. While the dissipation at 1.2 and 1.4 ms are increased due to adding mass transfer rate as expecting and reduced in 1.6 ms due to development in the reaction rate in which the presence of droplets tend to accommodate the evaporation process.

The relation between turbulent kinetic and turbulent dissipation energy are presented in figures (6.29) and (6.30), with a split of the figure into two in terms of the time. Figure (6.29) show the relation between $k$ and $\epsilon$ at time 0.6 and 1.2 ms, in which there is no chemical reaction effect. The $k$ is proportional to $\epsilon$ where both are increased while the effect of dissipation due to the chemical reactions is clearly shown in figure (6.30). The maximum values of turbulent dissipation energy are found where the turbulent kinetic energy is at approximately lower values.

As mentioned in top lines of this section, a section from the contour of gas temperature at time of 1.1 ms has been taken where Lumped zone is found between 22-25 mm as depicted in figure (6.31). Then the turbulent kinetic energy and turbulent dissipation energy have been calculated at four different radial distances. At $y=0.23$ mm, are recorded the higher values because it is very close to the centreline as explained above. The main radial distances are confined between the upper limit of $y=3.32$ mm and lower limit $y=1.50$ mm which pass through the Lumped zone.

In both figures (6.32) and (6.33), the model can produce a decrease in turbulent kinetic energy due to the rise in temperature at that point but it is only appears clearly shown at $y=1.50$ mm whereas the turbulent dissipation energy is increased in both distances at $y=2.25$ and 3.32 mm and it is decreased at $y=1.50$ mm. Of course there is shifting about 3 mm because the model can produce results for mean field parameters. Therefore in order to complete the task the procedure that have been proposed in section 6.2.1 is applied.

### 6.10.8 Grid analysis

Three different computational grids of different grid resolution are made to show the effects of grid refinement. Table (6.1) shows the grid specifications. In order to get an optimum spray combustion calculation with a grid refinement, in all cases the nozzle orifice and the area of
the nozzle vicinity are discretized into fine grids with four cells at the injector. According to Abraham [1997], the refinement of the grid works to resolve the flow emerging from the injector which allows to capture the transient behaviour of the flow. The reason behind using fine grids in this study is also because the Lumped model is used to capture the smallest length scale. However if the grid size is too small, the calculations in the cell are enough to ensure that the unmixed zone can be captured and meets the numerical accuracies and stabilities for the modelling which is the aim for this model.

### Table 6.1: Grid specifications

<table>
<thead>
<tr>
<th>case</th>
<th>No. volumes</th>
<th>No. faces</th>
<th>No. vertices</th>
<th>No. injection cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>6490</td>
<td>13128</td>
<td>6639</td>
<td>4</td>
</tr>
<tr>
<td>B</td>
<td>8597</td>
<td>17357</td>
<td>8761</td>
<td>4</td>
</tr>
<tr>
<td>C</td>
<td>10738</td>
<td>21656</td>
<td>10919</td>
<td>4</td>
</tr>
</tbody>
</table>

The computational grids have the same compression ratio to show the effects of the grid on the solution as show in figure (6.34). The coarse grid (case A) as shown in figure (6.34) (a) is not capturing both spray penetration and the auto-ignition point delay time and location. Figure (6.35)(a) shows the auto-ignition point at axial distance of 17 mm away from the injector at a delay time of 2.00 ms. The spray is ignited more slowly than the experimental auto-ignition delay time as shown in table (6.2). That leads to more evaporation for the droplets due to high air temperature of 823 K which tends to reduce the penetration to 41 mm at 2.00 ms compared with experimental data of 52 mm. With the increase of grid refinement for case B as shown in figure (6.34)(b), the auto-ignition delay time is close to the experimental point as shown in figure (6.35)(b) but the penetration is over-predicted. However a further refinement for the grid has been made for case C as shown in figure (6.34)(c), in order to reduce the spray penetration. The increase of the control volumes means more air is entrained in the spray which enhances the drag effect as shown in figure (6.36). The auto-ignition delay time of 1.28 ms at axial distance of 38 mm away from the injector as shown in figure (6.35)(c) are reasonable compared with experimental data in table (6.2).
Table 6.2: Grid test

<table>
<thead>
<tr>
<th>Exp.</th>
<th>Auto-ignition (sec)</th>
<th>Axial position (mm)</th>
<th>Penetration (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>case A</td>
<td>2.00</td>
<td>17</td>
<td>41</td>
</tr>
<tr>
<td>case B</td>
<td>1.25</td>
<td>34</td>
<td>58</td>
</tr>
<tr>
<td>case C</td>
<td>1.28</td>
<td>38</td>
<td>49</td>
</tr>
</tbody>
</table>

6.11 Conclusions

In many practical combustion applications like gas turbine and diesel engine, the combustion takes place in turbulent flow field. Therefore it is important to model the effects of turbulence and mixing interactions including all related processes either physical or chemical. In the present model the emphasis is on how the turbulence leads to increased mixing in order to be used to compensate for the inaccurate prediction for the chemical reaction rate. However this has to be treated numerically and physically. Both ways are referring to the incomplete mixing process that may lead to ignite the fuel vapour before the auto-ignition delay time or out of the main reaction zone. Physically, the mixing process tends to speed up the overall reaction rate by stretching and wrinkling of the preheating zone. In addition the simulation of turbulent spray combustion remains quite a hard task because many problems may occur due to strong coupling that exists between predicted vapour mass fraction and the chemical reaction. Numerically, in order to distribute the evaporation zone and consequently the diffusion of the spray flame, the new technique based on combination of a new micro-mixing model incorporated with a proposed ratio related to the Kolmogorov length scale (diffusion flame thickness) at the separated flame zone to the reaction flame thickness if the mentioned parameters are not captured within a certain procedure. After applying CCM to simulate solid cone spray combustion inside chemical reactor, observations had been made to these small regions through the simulation of spray combustion but unfortunately it is not possible to know that this phenomena is caused by nature to be considered as extinction regimes or generated due to the numerical simulations. For both cases, all the investigations and the calculations are based on treating this regimes as reaction zone i.e., that means the model is used to identify the combustion zones inside the chamber and the ratio is used only when the reaction flame thickness is too small so the ratio gives large value (trivial value). It is found that the simulated results accelerated the auto-ignition delay more than CCM model which is there are many treatments have been done. This ratio allows a description of the transient flamelet regime and attempts not to distribute it.
Figure 6.1: Computational domain.

Figure 6.2: Comparison of predicted spray penetration with experimental data.
Figure 6.3: Comparisons of predicted auto-ignition point with experimental data.

Figure 6.4: Evolution of vapour mass fraction with time.
Figure 6.5: Evolution of gas temperature with time.

Figure 6.6: Radial profile of gas temperature at different axial cross sections.
Figure 6.7: Comparisons of gas temperature contour plots at time 1.2, 1.42 and 1.52 ms.
Figure 6.8: Prediction of reaction zone and gas temperature with mixture fraction at different times.

Figure 6.9: Prediction of reaction zone and gas temperature with axial distance at different times.
Figure 6.10: Axial profile of mixture fraction at different times.

Figure 6.11: Radial profile of mixture fraction at different times.
Figure 6.12: Scalar dissipation rate contour plots at time 1.2, 1.52 and 1.95 ms.

Figure 6.13: Prediction of scalar dissipation rate with axial distance at different times.
Figure 6.14: Axial profile of scalar dissipation rate at time=1.8 ms.

Figure 6.15: Radial profile of scalar dissipation rate at time=1.8 ms.
Figure 6.16: Axial profile of axial gas velocity at different times.

Figure 6.17: Radial profile of axial gas velocity at different times.
Figure 6.18: Axial profile of radial gas velocity at different times.

Figure 6.19: Radial profile of radial gas velocity at different times.
Figure 6.20: Comparisons of axial and radial gas velocity at time 1.2, 1.42 and 1.52 ms.
Figure 6.21: Regimes of turbulent diffusion flames proposed by Borghi, 1988.

Figure 6.22: Structure of spray combustion with lumped zone compared with schematic spray diffusion flame suggested by Faeth, 1977.
Figure 6.23: Temporal profile of turbulent kinetic energy with axial distance.

Figure 6.24: Temporal profile of turbulent dissipation energy with axial distance.
Figure 6.25: Radial profile of turbulent kinetic energy at different axial cross section at 1.8 ms.

Figure 6.26: Radial profile of turbulent dissipation energy at different axial cross section at 1.8 ms.
Figure 6.27: Transient of adding mass transfer effect to the turbulent kinetic energy transport equation.

Figure 6.28: Transient of adding mass transfer effect to the turbulent dissipation energy transport equation.
Figure 6.29: Transient relation between turbulent kinetic and dissipation energy at 0.6 and 1.2 ms.

Figure 6.30: Transient relation between turbulent kinetic and dissipation energy at 1.4 and 1.6 ms.
Figure 6.31: Sector from gas temperature contour at time 1.1 ms.

Figure 6.32: Prediction of turbulent kinetic energy with axial distance at time 1.1 ms.
Figure 6.33: Prediction of turbulent dissipation energy with axial distance at time 1.1 ms.
Figure 6.34: Computational grid.

(a) Case A

(b) Case B

(c) Case C
Figure 6.35: Location of the auto-ignition point.
Figure 6.36: Penetration of spray with variation of number of control volumes.
Chapter 7

Outlook

This chapter attempts to give a more global view of the models that have been developed and on general directions that may be followed in further work. The work presented in this thesis can be related into three different objectives. In addition topics to be addressed which are outside the aims of the study are also presented as additional areas for further work.

7.1 Conclusions

This research work has been concerned with implementation and validation of computational fluid dynamic methodology for simulation of spray droplets based on the drop size distribution moments method proposed by Beck and Watkins [2002] at different ambient conditions. The conclusions are placed at the end of each chapter containing results and are summarized here.

1. A higher order convection scheme has been constructed to deal with interfacial flow in two-phase systems. The scheme is based on the finite volume method and is implemented with unstructured grids of arbitrary shape. In addition the scheme has been employed in the moments and momentum transport equations in order to have the highest level of accuracy. The hollow cone spray has been successfully simulated producing good penetration and sheet thickness results. The edges of the spray are also captured and evident in the simulation.

2. The prediction of the thermo-physical properties in the gas around a droplet is a problem all evaporation models. Two well known relation were found in the literature, either one-third rule or half-rule equations are used in order to predict the properties under evaporation conditions. The author used the heat conduction equation for a sphere to derive
an equation for the temperature distribution in the vapour generated around the droplet during the evaporation process. It was found the new equation is based on half rule first plus a ratio of the vapour film thickness over droplet diameter. In order to implement the new equation in spray evaporation case study, the ratio is approximated in terms of fuel vapour mass fraction. The vapour mass fraction is considered as a dynamic factor related mainly to the mass transfer rate which can give an indication about the droplets evaporation according to their spatial and temporal status. Thus the film equation can provide a better prediction for the thermo-physical properties rather than two previous approaches mentioning above. A hollow cone spray case has been simulated under evaporation conditions to validate the new equation.

3. A combustion region has been observed during the simulation of the spray combustion for the diesel engine. The phenomenon occurs before the auto-ignition delay time and outside the reaction zone. A new model has been proposed by the author in order to capture this phenomenon. The proposed model contains two possibilities which are suggested to explain this observation. Firstly, physical justification is used to understand why and where this region has occurred. During the injection period different droplet sizes are generated through the atomisation process. Differences in droplets sizes mean differences in momentum that lead to small droplets evaporated and combusted near the outer edge of the spray before the auto-ignition delay time. In this regime mainly two physical effects are found. The first is that, droplets are subjected to a higher heat flux due to the higher gas temperature than other parts of the spray. The second is that, there is a weak effect of mixing process due to the small gas velocity. Secondly, numerical error analysis has also been used in case this phenomenon appears due to modelling errors. The incompatibility between the chemical reaction rate and the mass transfer rate can cause such a region. The Lumped strategy has been implemented to eliminate such an error in this zone, after it has been captured. The Lumped strategy identified this error by modifying two parameters, Arrhenius parameter and diffusion coefficient to correct the modelling without any modification of the flow field.

7.2 Further topics

It is hoped that this work will provide an initial foundation for future progress in each area.
1. For non-reactive flow, a new family of high order finite volume convection schemes is built up from the combination of two schemes to resolve the interfacial flow in two-phase flows system. It is more challenging to deal with phase transition like evaporation where the flux limiter should be updated in each time step according to the reduction in fuel amount and consequently the blending factor is purely calculated from flow information without using mesh lines.

With the capability of the designed code Jones [2009], the spray moment theory could be improved by extension to be applied to complex three dimensional models in real space like gas turbine combustor or combustion chamber of diesel engine. In addition an important issue mentioned in Jones [2009] is droplet velocity profile. Here the starting point is specified by extending the existing model to third or fourth order model for velocity distribution to yield the lower moments to be transported properly. Finally a still quite difficult task for the researchers is to refine physical sub-models, for example using Kolmogorov length scale in droplet breakup model.

2. In order to assess the film temperature theory to successfully predict the mass and heat transferred and vapour distribution, in any combustion process the rise in temperature is not linear as presented by the one-third rule, due to accumulation of heat. But this is not the only reason, in case of spray combustion modelling through using such as Burke-Schumann and Asymptotic Steady State Flamelet models, both models need accurate prediction for the fuel vapour mass fraction and temperature. However in further work both models will be implemented by using the new film and one third rule to prove that.

On the other hand, in order to characterise the turbulence effects on evaporation interaction regimes, a parameter like Damkohlar number or similar has to be introduced. Also the most important effect of droplets dispersion must be modelled or added as an extra term to represent the drift correction in terms of the relative velocity between the phases to achieve a comprehensive evaporation model.

3. The subject of sprays combustion work in this thesis has been directed towards inserting the fractal parameter of premixed wrinkled flames in a procedure to determine whether the viscous cutoff time scale is able to predict the dissipation length scale. The complexity of spray combustion can be reflected on the fractal dimension that covers a wide range of turbulence scale according to equation (6.18). RANS calculations of the turbulent field
can provide evidence supporting the central hypothesis of the model where the lumped reaction zone is said to exist when Kolmogorov scale is larger than the turbulent flame thickness. Based on the observation in the present model, the sensitivity of the turbulence closure is highly recommended to be investigated. Although the impact of the underlying turbulence model on the predictions of diffusion flame thickness also needs to be revisited. It may be helpful to use Bradley et al. [1994] calculations where they used the stretch rate based on flamelet modelling. It can be understand from the proposed approach in Bradley et al. [1994] that the heat release is strongly affected by turbulence. That is modelled as a transport equation for Reynolds stress where the effect of temperature fluctuation is added to the total diffusive transport term. It is more accurate to link this to the heat release. Heat release during combustion causes fluctuation in density and leads to an increase in temperature which in turn accelerates the chemistry in some critical regions. Therefore the mean volumetric heat release rate can be expressed in terms of the heat release versus temperature profile. This will be performed by using a joint probability density function. This will be more accurate because it will be implemented at every point of JPDF instead of just one cell for the entire domain.

An alternative is to follow Truffin and Benkenida [2008] by modelling temperature fluctuations by constructing a transport equation for the sensible enthalpy variances. Where the destruction term for the scalar dissipation rate incorporates with the effect of turbulent Reynolds number associated to the Taylor microscale that is called a dynamic model.
References


