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DEVELOPMENT OF COMBUSTION MODELS FOR RANS AND LES APPLICATIONS IN SI ENGINES

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B.Sc.Eng. (Hons.)

Doctoral Thesis

Submitted in partial fulfillment of the requirements for the award of Doctor of Philosophy of Loughborough University

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To My Parents
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Abstract

Prediction of flow and combustion in IC engines remains a challenging task. Traditional Reynolds Averaged Navier Stokes (RANS) methods and emerging Large Eddy Simulation (LES) techniques are being used as reliable mathematical tools for such predictions. However, RANS models have to be further refined to make them more predictive by eliminating or reducing the requirement for application based fine tuning. LES holds a great potential for more accurate predictions in engine related unsteady combustion and associated cycle-to-cycle variations. Accordingly, in the present work, new advanced CFD based flow models were developed and validated for RANS and LES modelling of turbulent premixed combustion in SI engines.

In the research undertaken for RANS modelling, theoretical and experimental based modifications have been investigated, such that the Bray-Moss-Libby (BML) model can be applied to wall-bounded combustion modelling, eliminating its inherent wall flame acceleration problem. Estimation of integral length scale of turbulence has been made dynamic providing allowances for spatial inhomogeneity of turbulence. A new dynamic formulation has been proposed to evaluate the mean flame wrinkling scale based on the Kolmogorov – Pertovskyy – Piskunow (KPP) analysis and fractal geometry. In addition, a novel empirical correlation to quantify the quenching rates in the influenced zone of the quenching region near solid boundaries has been derived based on experimentally estimated flame image data. Moreover, to model the spark ignition and early stage of flame kernel formation, an improved version of the Discrete Particle Ignition Kernel (DPIK) model was developed, accounting for local bulk flow convection effects. These models were first verified against published benchmark test cases. Subsequently, full cycle combustion in a Ricardo E6 engine for different operating conditions was simulated. An experimental programme was conducted to obtain engine data and operating conditions of the Ricardo E6 engine and the formulated model was validated using the obtained experimental data. Results show that, the present improvements have been successful in eliminating the wall flame acceleration problem, while accurately predicting the in-cylinder pressure rise and flame propagation characteristics throughout the combustion period.

In the LES work carried out in this research, the KIVA-4 RANS code was modified to incorporate the LES capability. Various turbulence models were implemented and validated.
in engine applications. The flame surface density approach was implemented to model the combustion process. A new ignition and flame kernel formation model was also developed to simulate the early stage of flame propagation in the context of LES. A dynamic procedure was formulated, where all model coefficients were locally evaluated using the resolved and test filtered flow properties during the fully turbulent phase of combustion. A test filtering technique was adopted to use in wall bounded systems. The developed methodology was then applied to simulate the combustion and associated unsteady effects in Ricardo E6 spark ignition engine at different operating conditions. Results show that, present LES model has been able to resolve the evolution of a large number of in-cylinder flow structures, which are more influential for engine performance. Predicted heat release rates, flame propagation characteristics, in-cylinder pressure rise and their cyclic variations are also in good agreement with measurements.

Key words: RANS, LES, KIVA, BML, DPIK, combustion modelling, spark ignition engines, wall flame quenching, flame surface density
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## ACKNOWLEDGEMENTS

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REST OF THE DOCUMENT IS INSERTED BELOW
Study of flow and combustion characteristics in Internal Combustion (IC) engines has been a topic of greater research interest for many decades. There are a number of reasons behind this motivation. The most influential factors for engine performance are the flow and combustion. Secondly, the physical and chemical processes involved in a reacting flow filed are so complex and some phenomena have not even been exactly understood. Another driving force is the legislative requirements. Increasingly stringent emissions standards and rapidly rising fuel prices make it exceptionally challenging to develop cleaner engines with increased power and efficiency.

The traditional routine of engine optimisation follows repetitive hardware modifications, excessive testing and exhaustive analysis of experimental data. This iterative process is profoundly slow, costly and imparts no way itself in identifying the optimum conditions. Alternatively, the use of Computational Fluid Dynamics (CFD) techniques as a design support tool has become increasingly popular during the last two decades, due to the substantial development in numerical methods and computing technology. CFD is relatively inexpensive compared to experiments, flexible, has a shorter lead-time and avoids or minimise difficult experimental investigations. Moreover, it produces enormous amount of useful data, which might be hardly accessible or virtually impossible to acquire with experimental techniques in a foreseeable future. However, it is important to note that, the actual processes happening in practical combustion systems are highly complicated in nature and CFD provides only approximate solutions, based on a number of simplifications and assumptions bounded by the limits of knowledge and resources. Hence, formulation of a
comprehensive CFD model to capture all the flow and combustion related processes in detail, with a great accuracy, is yet to be devised. Consequently, extensive research is still essential for the progress in CFD modelling techniques.

Present study aims to develop and validate CFD based mathematical models to simulate the combustion process in premixed spark ignited reciprocating piston engines. This chapter provides a brief background of the present study. Some fundamental aspects of turbulent reacting flow simulations related to IC engine modelling are first described. A short summary of the state of the art of computational combustion modelling is also presented. Finally, the objectives, accomplishments and the outline of this research are highlighted. Literature relevant to various aspects of each modelling process is drawn at places, where they are presented and discussed.

Note: The term internal combustion engine has a broad definition. It includes reciprocating piston engines, rotary vane/piston type engines and gas turbines. Study of all these types of engine is equally important; however, the emphasis of the present study is limited to piston engines. More precisely, the spark ignited reciprocating piston engines. Hence, ‘IC engines’ or ‘engine’ herein simply means reciprocating piston engines in general and SI engine means spark ignited reciprocating piston engines, unless otherwise explicitly stated. However, the models developed in this work, may easily be adapted for other types of internal combustion engines as well.

1.1 Some Aspects of Modelling Reacting Flow in IC Engines

The in-cylinder flow is inherently turbulent and, is considered important because of its large influence on the combustion characteristics. Figure 1.1 shows the flame images taken through the piston crown in a spark ignition engine during combustion period. These images depict the complex nature of interactions between flame and turbulent flow. Low and moderate levels of turbulence affect combustion by wrinkling the flame front, whereby its surface area increases. This leads to increased mixing of high temperature burned products with the fresh gas and thus, to an acceleration of the combustion reactions. In that sense, turbulence is advantageous especially in premixed combustion. Nevertheless, very high turbulence levels induce excessive strain and tear apart flame fronts. This may hinder the flame propagation and possibly the flame could be extinguished. Hence, one of the key objectives of CFD modelling should be to precisely estimate the correct level of turbulence throughout the simulation. Turbulence in the engine combustion chamber is characterised with, seemingly chaotic three-dimensional velocity fluctuations. These may occur in a broader range of length and time.
scales. In a typical automotive engine, the length scales can be in the order of bore diameter to sub-millimetre. Corresponding time scale range can be from few microseconds to some milliseconds (Heywood 1988). A perfect simulation must resolve all the eddies, from the smallest to the largest in both space and time.

![Flame images taken through the piston crown in a spark ignition engine](image)

Figure 1.1 Flame images taken through the piston crown in a spark ignition engine (Reproduced from Aleiferis et al. 2000)

Prediction of correct turbulence characteristics in engine configurations remains a challenge. However, the fundamental equations describing thermo-fluid processes are essentially known. Gas motion, for example, may be described by the compressible Navier-Stokes equations (Haworth 1999). The most accurate modelling approach is to solve the Navier-Stokes equations without any form of averaging or approximation, apart from the numerical discretization, whose error can be quantified and controlled. This is obviously the simplest form in the conceptual point of view and called Direct Numerical Simulation (DNS). Unfortunately, for DNS of a realistic IC engine, even with the modern super computers, needs years of computational time. Therefore, the applicability of this approach has been limited to very simple test cases. Alternatively, as a compromise, few other procedures, such as Large Eddy Simulation (LES) and Reynolds Averaged Navier-Stokes equations (RANS) have been
developed, where the turbulent spectrum is partially resolved or entirely modelled using averaging techniques. Potential of these methods applied to IC engine modelling is discussed in detailed in the next section.

Combustion in IC engines is basically described by a set of chemical reactions controlled by the turbulent flow motion. In order to simulate the combustion, the governing fluid flow equations must be harmonized with a chemical reaction mechanism and a reaction rate model. The reaction mechanism prescribes how fuel and oxidant react, what products are formed and in what mutual relations they are combined. The reaction rate model describes how fast the reactions are taken place under the influence of turbulence. Combustion of a substance is associated with a series of chemical reactions. The simplest hydrocarbon - methane, undergoes over 40 elementary reactions during the combustion process (Versteeg & Malalasekera 2007). Models for chemical reaction mechanisms exist in varying degrees of complexity and accuracy. The most complex models use hundreds of different reaction steps and species to describe the reaction mechanism, while the simplest models describe the combustion process only as an instantaneous transition from reactants to products, in the form of a one-step oxidization reaction. The reaction rate may be modelled using an Arrhenius type expression assuming the process is chemically driven. If not, phenomenological models may be derived considering the physical aspects and experimental observations of flame propagation in a turbulent flow field. Accuracy of these types of models is subjective to the application. However, in general, phenomenological models are found to produce better predictions in premixed SI engine simulations.

One of the decisive factors in determining the in-cylinder flow and subsequent combustion characteristics is the geometric configuration. In particular, the intake port, valve assembly, valve lift profile and the combustion chamber. For example, a slight change in port entry angle could result in significant changes in the macro flow structure: i.e. the swirl and tumble motion, consequently, the overall combustion duration (Chen et al. 1998). The discharge gap at valve throat regulates the nature of the micro flow structure; i.e. the turbulent intensity and integral scale, which eventually controls the flame penetration rate (Weclas et al. 1998). Besides, the wave action pertaining to the valve overlap, limits the residual mass fraction, which considerably affects the burning rate. Thus, a complete engine simulation should model not only the in-cylinder processes but also the flow though valves and ports; if possible, the entire intake and exhaust system for better results.
In CFD modelling, the computational domain is represented by a collection of infinitesimal volumes called the *mesh*, on which the discretised governing equations are approximated. The infinitesimal volumes are termed *cells*. To precisely incorporate boundary effects in a simulation, the computational mesh should represent the actual physical boundaries of the computational domain to the closest possible extent. A number of cell types are used in practise to discretise the computational domain. In theory, structured orthogonal hexahedral cell elements are preferred, as the geometric properties, such as surface area and volume can be estimated more accurately. Nevertheless, such elements cannot be used to precisely model complex contoured domains, such as the engine combustion chamber, valves and ports. Thus, in practise, structured non-orthogonal hexahedral elements or untrusted meshes comprises of tetrahedral, hexahedral, prism, pyramid or polyhedral elements are used sacrificing a certain degree of accuracy. Highly stretched, non-convex and skewed cells introduce additional numerical errors. Hence, not only the accuracy of mathematical models, but also maintaining the quality of the computational mesh is equally important in deciding the successfulness of a simulation.

### 1.2 RANS for Engine Simulations

RANS is the today’s standard tool in industry for CFD simulations. This approach is based on ensemble or time averaging the Navier-Stokes equations, in which fluctuations at all scales are dealt with using a turbulence model. RANS modelling techniques are well established. Most of the engine simulation studies conducted at present are based on these procedures. Almost all the modern commercial CFD codes are still being mainly developed for RANS modelling. RANS methods are much popular mainly due to the lower spatial and temporal resolution requirements. Sufficiently accurate solutions of complex industrial flow problems can be obtained with coarser meshes at a reasonable computational time. Due to the frequent use, RANS literature is well documented and numerous benchmarking studies are available for reference. However, this does not mean that RANS methods are flawless. Widespread research is still crucial, in order to extract the full potential and to rectify some known issues as highlighted in the following section.

In RANS, a flow property is decomposed into a time averaged mean value and a fluctuating component. Substitution of these components in the unsteady Navier- Stokes equation results in a number of fluctuating unknown terms. Particularly, these terms in the momentum equation are known as Reynolds stresses. The central problem of RANS modelling is to find an approximation for these Reynolds stresses. A number of different strategies to close
Reynolds stress terms have been suggested. There are ample evidences that, these models have largely contributed to the progress in CFD and related fluid engineering fields. However, universal applicability of these closure models in diverse areas is limited by the fact that, the performances are problem dependent. For example, a particular model will provide excellent results in aerodynamic flows but may produce very poor result in reacting wall bounded systems. RANS techniques are well suited for steady state problems. They can predict the mean flow characteristics at stable engine operation conditions to a reasonable degree of accuracy. Nevertheless, RANS techniques by definition are not capable of predicting unsteady phenomena in detail, due to the averaging and modelling involved (Moureau et al. 2004a).

For example, cycle-to-cycle variations in engines are not accessible from an ensemble-averaged formulation. One of the other drawbacks of RANS modelling is the large dependency of simulation results on to the turbulence model employed. As the entire turbulent spectrum is modelled, the turbulence model drives the modelling of all other physical processes including heat transfer, fuel sprays, mixing, and combustion.

The combustion model plays a vital role in engine simulations. Over the past decades a significant progress has been made in RANS based reacting flow modelling. Diverse conceptual viewpoints have been evolved in relation to flame front description and reaction rate estimation. Standard Arrhenius type models assume the combustion process is completely chemically driven and Eddy-Break-Up (EBU) type models assume the combustion process is turbulence driven (Poinsot & Veynante 2005). Models based on flamelet assumptions consider both chemical and turbulence effects.

However, one of the common weaknesses of the present models is that they are required to empirically tune one or more model coefficients or other input parameters by reference to experimental data to obtain satisfactory quantitative predictions, especially, when dealing with new designs or significantly different operating conditions (Gosman 1999). This may be a consequence associated with the large number of simplifying modelling assumptions or merely due to the poor understanding of the actual phenomenon. For example, the flame surface density (FSD) model proposed by Bray-Moss-Libby (BML) (Bray et al. 1989) involves four model constants, whereas the balance equation proposed by Cant et al. (1990) for FSD contains three model constants (see Zhao et al. 1994a). Case by case tuning of these constants are often required to obtain good predictions, which in practise is a highly time consuming task.
The other main concern of these models is the associated wall flame acceleration problem (i.e. prediction of extremely high unphysical reaction rate near solid boundaries). Consequences of this problem related to the EBU model has been reported in Weller et al. (1994) and related to the BML model, in Watkins et al. (1996). Due to the wall flame acceleration problem, it has become impossible to use these models without modifications in wall bounded reacting flow modelling. These models assume isotropic homogeneous turbulence. Their application in the core region of the flame (where sufficiently homogeneous turbulent can be expected) provides satisfactory results. Conversely, near solid boundaries, the homogeneous assumption is no longer valid, owing to the presence of a sharp gradient of turbulence flow properties. Therefore, to obtain accurate results it is necessary to make sufficient allowances to account for special inhomogeneity in turbulence in the different regions of the problem domain.

Accordingly, various aspects of RANS based combustion models have yet to be thoroughly researched. More importantly, it is interesting to note that, the combustion modelling concepts used in immersing LES modelling are also still based on the ideas developed in RANS. Hence, both the LES and RANS may be equally benefitted from further evaluation and improvements of RANS based flow models.

**1.3 LES for Engine Simulations**

LES, in general is accepted as the next generation tool for turbulence modelling (Rutland 2011). It has been able to bridge the gap between classical RANS modelling and expensive DNS to a certain extent. Instead of time averaging, LES uses a spatial filtering procedure where the large scale motion is exactly calculated and only the effect of sub-filter scale (often called sub-grid-scale (SGS)) motion is modelled. Consequently, the information of larger eddies than a given cut-off filter scale is preserved and only the sub-filter details are lost. The effect of SGS motion on the large scales is expected to be universal. According to the energy cascade concept in Kolmogorov theory of turbulence, energy is transferred from larger anisotropic eddies to smaller eddies, which are in equilibrium. The smaller eddies in the bottom range or the inertial sub range are locally isotropic. Their characteristics are believed to be universal and independent from the flow geometry (Geurts & Schoore 2005). This universality of the small scale turbulence can be advantageous, when the modelled SGS part of LES lies within the inertial sub range. This would lead to a potentially generic simulation and a modelling strategy, where predictions are quite insensitive to the employed SGS model. As a result, the use of LES has become increasingly popular as a more reliable prediction tool.
than RANS for modelling complex flow configurations commonly encountered in engineering applications (Uddin et al. 2006).

The success of a simulation is often related to the empirical tuning of a set of constants, but compared to RANS, LES requires only a low level of empirical input. In fact, there are dynamic LES formulations, where no tuning constants involved at all. Required model parameters are automatically calculated based on the local flow conditions. LES results provide more complete information on the flow structures, as it produces an instantaneous solution without time averaging. As a result, more eddies and vortex structures are resolved, representing a rather realistic flow field. This makes previously inaccessible unsteady phenomena, such as cyclic variability in engines, amenable (Haworth 1999). The knowledge of the mean characteristics alone is not always sufficient for the rapid progress of a field. In particular, the knowledge in every aspect of the three-dimensional turbulence characteristics and effects of combustion instabilities are of utmost importance in engine design. However, these heavily unsteady flow behaviours cannot be adequately predicted with conventional RANS techniques and the only practically possible solution is to use some form of LES. Inherently, the multi-scale modelling approach of LES offers a more complete apprehending of large scale unsteady phenomena and thus, carries good potential for predicting the engine unsteadiness. However, with LES, obtaining a statistically converged mean solution in engine applications requires hundreds of continuous cycle simulations and, is unaffordable at this stage.

Both LES and RANS assume the effect of the modelled part of turbulence on the resolved part to be diffusive. It is taken in to account by introducing an eddy viscosity, which is often called the turbulent viscosity (Ferziger & Peric 2002). The level of importance of the eddy viscosity in a simulation is comparative to the level of modelled portion of the energy spectrum. Hence, the role of eddy viscosity is much persuasive in RANS, where the entire energy spectrum is modelled and, is less important in LES, where the energy spectrum is only partially modelled. However, these features impose additional restrictions on the requirements of LES numerical schemes (Moureau et al. 2004a). The main requirement of RANS methods are to be robust and stable on coarser and distorted meshes and associated numerical dissipation issues are only a second-order aspects. Hence, most of the RANS codes used computationally stable upwind fluxing schemes, where significant level of numerical dissipation presents. In contrast, LES requires much accurate higher order schemes in both space and time as the flow field above the cut-off limit has to be exactly resolved (Moureau et al. 2004a).
Accordingly, LES demands much finer, high quality computational meshes, small time steps and higher order discretisation schemes for better results. Although, this statement is true in general, it seems to overestimate the real situation. It is interesting to note that even with the present RANS mesh resolutions used in engine studies, LES can resolve over 80-90% of the total flow’s kinetic energy (Haworth 1999). Hence, sufficiently accurate LES solution with adequate details is feasible, even with a moderately refined mesh than a typical RANS grid. In fact, the resolution demand can further be reduced by using a well-engineered SGS model than using a simple crude model (Rutland 2011). The poorer the quality of the SGS models, the mesh has to be finer to make sure the bulk of kinetic energy is resolved on the computational mesh, making SGS modelling errors less important. Use of refined grids or higher order numerics is not practical with engine modelling. Typically, second order methods with moderately refined grids are sufficient to obtain good results to meet the engineering accuracy requirements. Ample evidence on this aspect has already been demonstrated by Haworth & Jansen (2000), Sone & Menon (2003) and Liu & Haworth (2010).

LES has already been widely used in cold flow engine studies and fuel spray modelling. However, its use in combustion analysis is fairly limited. In fact, most of the combustion studies have been constrained in simple flow configurations and only very recently, that the modelling of combustion in complex geometries has been experimented. Being a new research area, numerous fundamental questions on combustion modelling in LES context have still to be addressed to comprehend the full predictive potential (Pitsch 2006). Hence, so called best practices are yet to be established (Rutland 2011). Use of LES is not just replacing the RANS turbulence model with a SGS turbulence model and leaving all the other sub models unchanged. Unfortunately, this approach is found to be common among the research community (Rutland 2011). Proper use of LES in engines requires following a substantially different approach than RANS, to be consistent with the LES concepts.

LES has already been tested in relatively a wide range of general combustion problems, including premixed, partially premixed and non-premixed combustion in engines and similar configurations (see Rutland 2011 for more details). However, the literature devoted to engine related premixed combustion modelling with LES has been limited to handful of publications (Naitoh et al. 1992, Colin & Truffin 2011, Enaux et al. 2011 and Franzelli et al. 2012). Premixed combustion modelling in LES presents a particular challenge. In practise, combustion is a sub-grid scale phenomenon. The reaction zone thickness of the flame front is so thin and much smaller than the commonly used LES mesh sizes. As a consequence, the
flame front cannot be resolved on such grids using conventional methods. On the other hand, sub-grid wrinkling effects due to turbulent flame interaction have to be precisely estimated in terms of resolved parameters using a suitable model. Most of the present LES combustion models are essentially similar to RANS combustion modes. Although, this provides a good starting point, it is not certain at this stage, whether these models can extract the full advantage from the resolved field. Hence, there exists a strong requirement to properly re-evaluate present methodologies and make necessary allowances to be consistent with LES concepts.

1.4 The Present Computer Code

The present work is primarily based on the KIVA-4 code. It is a RANS based CFD engine simulation code capable of simulating three-dimensional, multispecies and gaseous flows under steady-state and transient conditions. KIVA was first released for researchers in 1985 by the Los Alamos National Laboratories (LANL), California, USA (Amsden 1989). Since, it has been extensively used by the research community in a wide range of engine and non-engine applications. Being a well-documented open source code, KIVA facilitates integrating custom-made user developments providing full control over the programme. As a result, this code is frequently used for multi-dimensional engine simulations and has been constantly enhanced with advanced features. More importantly, this code has been excessively validated than any other code due to its regular use in combined modelling and experimental studies and, proven to be reliable and accurate by the user community.

KIVA-4: the latest version, consists all the capabilities of earlier versions and some added features. Especially, it can handle unstructured grids with many different cell types including hexahedra, tetrahedra, prisms, and pyramids whereas, previous versions could only use structured or block structured grids with all hexahedral elements. Unstructured grids can largely improve the mesh quality by reducing or completely eliminating the number of distorted elements and easily maintaining the required spatial cell density. Use of unstructured grids is flexible, less time consuming for mesh generation and complex contoured geometries can be more closely represented. Unfortunately, KIVA-4 does not have an unstructured grid generation programme, instead supplies only the old block structured grid generator developed for earlier versions. Mesh generation for complex IC engine geometries with this block structured mesh generator; which was mainly developed for conventionally shaped engines, has long been a tedious task. The mesh structure and indexing constraints make its application in meshing complex geometrical shapes a very time consuming iterative process.
Sometimes it requires months of time to construct a full engine mesh including ports and valves with a sufficient quality. Yet, this procedure does not guarantee a distortion free mesh and often, it is impossible to eliminate non-convex elements (Amsden 1997). Consequently, most of the engine studies conducted using the KIVA code simulate only the valve closed period with an assumed initial in-cylinder flow field, completely ignoring the port flow and valve motion. This approach however, does not account for the correct level of in-cylinder turbulence and bulk flow motion, subsequently leading incorrect estimation of reaction rates. Hence, development of an unstructured mesh generator is certainly beneficial at this stage in taking the full advantage from new KIVA-4 features.

KIVA has been equally used in automotive industry and academic research in developing new engine concepts. Renowned engine manufactures, particularly General Motors, Cummins, Ford and Mercedes-Benz have successfully used it in a variety of investigations, including the analysis of fuel spray, mixing, homogenous charge compression ignition (HCCI), low temperature combustion, turbo charging and emissions formation (Kuo 1992, Stephenson et al. 1996 and Iyer & Yi. 2009). This code has also been an ideal platform for sub model development. A large number of RANS based combustion models have been implemented and tested in both premixed and non-premixed combustion applications. For example, these include eddy dissipation models (Henson & Malalasekera 2000), characteristic time combustion models (Ritz et al. 1992), flame surface density models (Zhao et al. 1993) and G-equation models (Tan et al. 2003). Similarly, various other sub models for fuel spray, wall heat transfer and blow by gases have also been developed and validated. Additionally, several promising attempts have also been made to investigate the potential of higher order turbulence models, such as Reynolds-Stress Model, in engine related turbulence modelling (Yang et al. 2005).

Emphasis of KIVA related developments has also been directed towards implementing LES capability and parallelisation for multi-processor simulations (Sone & Menon 2003 and Torres et al. 2010). A numbers of studies have been carried out on these aspects with encouraging success (Goryntsev et al. 2010 and Huijnen et al. 2005). Fundamental turbulence modelling and validation, fuel-injection, atomisation, sub-grid mixing, cyclic variations, combustion instabilities and related unsteady effects are among some of the interesting issues addressed. Remarkably, the predictions of all these work have shown significant improvements over traditional RANS results. However, as already mentioned in section 1.3 the bulk of these simulations are devoted for cold flow and spray modelling. Only a very few of them have attempted to model combustion and related phenomena. Some of the promising
efforts in non-premixed and HCCI combustion modelling applied to realistic engine configurations can be found in Vressner et al. (2008) and Goryntsev et al. (2012). Surprisingly, the work of Naitoh et al. (1992) remains as the first and only LES premixed combustion study performed using the present code to date.

1.5 Objectives and Accomplishments

Although, considerable research efforts have been directed towards developing accurate mathematical models for CFD simulations of IC engines, there is still a convincing need for further developments and improvements of current modelling techniques. RANS models have to be further refined to make them more predictive by eliminating or reducing the requirement for application based fine tuning. Some of the fundamental turbulent and flame related assumptions, conventionally made during model derivations, are not valid in general for complex engine flows. Therefore, the existing models have to be revisited and necessary allowances have to be made to suite engine environment. On the other hand, LES holds a great potential for more realistic and accurate predictions in engine related problems. The informative results of LES simulations can effectively be used in understanding unsteady effects and combustion instabilities. Nevertheless, as LES combustion modelling is still in the early stage of research, there are many unresolved LES related issues. Hence, in order to gain the confidence, present LES model formulations have to be thoroughly validated in various types of applications, while exploring new possibilities for perfections.

The work presented in this thesis aims to develop multidimensional computational models for simulating turbulent flow and premixed gaseous combustion in spark ignited reciprocating engines. It is intended to address the issues highlighted in previous sections of this chapter, related to the present perspective in both RANS and LES techniques. The RANS based KIVA-4 engine simulation code serves as the base platform for code implementation and development. Specifically, the following objectives were set as a guide line for the study. An introductory overview for the approach taken to accomplish each of the objectives is also given for completeness.

- Development of a mesh generation methodology

At the time of start of this research in early 2010, neither KIVA-4 itself nor any established commercial grid generation package provided the facility to construct unstructured grids to be used with the present solver. Aiming to take the maximum benefit from new unstructured mesh feature, it was decided to develop a new unstructured mesh generation methodology in
place of the old block structured grid generator. Hence, the initial work concentrate on developing an efficient grid generation tool for constructing high quality meshes of complex geometries for both engine and non-engine applications. GAMBIT is a widely used industry standard general purpose grid generation software package that has more advanced grid generating features. Therefore, using GAMBIT as the base software, an interface programme was designed and developed for exporting GAMBIT generated meshes to KIVA-4 format. A number of grids with a range of complexity, including full engine geometries with ports and valves, were generated and successfully tested for the compatibility with KIVA-4.

- Development and validation of an extended model for simulating premixed combustion in spark ignited engines in the RANS context

Traditionally, RANS combustion models involve several model constants, which need application based adjustments. It is expected here to investigate the possibilities of eliminating or reducing the effect of these constants with respect to engine applications by dynamically evaluating required model parameters, based on local flow properties. On the other hand, most of the existing combustion models are based on underlying simplified assumptions valid only for simple open stagnation flames. Consequently, the application of such models in highly turbulent wall bounded engine combustion calculations are no longer justified and additional corrective measures are required; particularly, for accounting spatial anisotropy of turbulence and wall quenching effects. Accordingly, the well-known Bray-Moss-Libby (BML) (Bray et al. 1989) combustion model is revisited and theoretical and experimental based modifications have been investigated, such that the BML model can be applied to wall-bounded combustion modelling, eliminating the wall flame acceleration problem. Estimation of the integral length scale of turbulence has been made dynamic, so that allowance for spatial inhomogeneity of turbulence is made. A new dynamic formulation was proposed based on the Kolmogorov-Petrovski-Piskunov (KPP) analysis and fractal geometry to evaluate the mean flame wrinkling scale. In addition, a novel empirical correlation to quantify the quenching rates in the influenced zone of the quenching region near solid boundaries was also derived, based on experimental flame image data.

The proposed models were then applied to simulate the premixed combustion in spark ignition engines. The model was first validated against experimental data on SI engine combustion in the public literature. Subsequently, the full cycle combustions in a Ricardo E6 research engine for different operating conditions were simulated. The work was comprehensively validated against experimentally measured engine data of the same engine.
Hence, a dedicated engine testing programme was also conducted to measure the important combustion parameters required in the validation process.

- **Development of an ignition and flame kernel model for simulating early stage of the flame propagation in SI engines**

  Onset of a flame kernel due to the deposition of spark energy and the early stage of flame propagation show fundamental differences compared to a fully developed flame. Consequently, the flame kernel formation cannot be accurately simulated using conventional combustion models developed for fully developed turbulent combustion simulations. Therefore, an improved model based on Discrete Particle Ignition Kernel (DPIK) (Tan et al. 2003) model is developed and validated against published experimental data in an engine like environment. Special emphasis was made to incorporate bulk flow convection effects on the growing flame kernel, which is often neglected in many studies without a proper justification. However, particularly in engines, where strong convection fields present in the vicinity of the spark location, it is of vital importance to estimate the true flame behaviour as revealed by numerous experimental investigations. The model is then used to simulate the flame kernel formation in Ricardo E6 engine and the importance of accounting for bulk flow effects in engine modelling is comprehensively demonstrated.

- **Implementation of LES capability and its validation in non-reacting flows**

  Large Eddy Simulation technique is a better and more accurate modelling technique compared to RANS based techniques. Therefore, aiming to investigate the potential of LES in engine related problems, work was undertaken to extend the capability of the present code to perform LES calculations. Present RANS code was extensively modified to replace time averaged RANS equations with filtered LES equations. An eddy viscosity base sub-grid scale turbulence model was implemented, where a separate transport equation is solved for the sub-grid scale kinetic energy. The implementation was comprehensively validated against published experimental data in a backward facing step geometry and an axisymmetric research engine. In addition, results were compared with RANS predictions to assess the present improvements. The model sensitivity was further investigated in different mesh configurations with unstructured hexahedron elements. The validated code was then applied to simulate the full cycle motored flow in a Ricardo E6 engine and to visualize unsteady variations of in-cylinder flow structures during intake and compression strokes.
• **Development of LES based dynamic combustion models for simulating ignition and premixed combustion process in SI engines**

Conventional RANS combustion models cannot be used in their exact forms for combustion simulations in the LES context due to the fundamental differences in modelling principles. RANS models must be appropriately adopted, to be in-line with LES concepts. Accordingly, a dynamic flame surface density (FSD) model was developed for premixed combustion modelling with necessary allowances for SGS and resolved scale contributions. A procedure for test filtering in wall bounded reacting flows was also developed and employed to dynamically estimate the model constants in both space and time, using resolved information of local flow properties. As already discussed in RANS combustion modelling, the characteristic differences in the early stage of flame kernel development restrict the use of common LES combustion models usually derived under equilibrium assumptions. Hence, an improved ignition and flame kernel model was developed during this study to calculate the reaction rate and SGS flame wrinkling, until the flame kernel is fully developed. The model is validated against experimental measurements and subsequently, combined with the dynamic FSD formulation, the combustion process in the Ricardo E6 engine was simulated. Quality of the predictions was assessed with respect to experimentally measured mass burn data and the pressure history in a range of operating conditions. The study was further successfully extended to investigate the cyclic variation characteristics of the same engine.

### 1.6 Outline of the Thesis

**Chapter 2:** This chapter explains the methodology used to develop an unstructured grid generation for KIVA-4 code. Limitations, challenges and opportunities of currently available meshing techniques are also assessed with regard to IC engine simulations. Underlying logical and mathematical concepts adopted in the present development are highlighted with a number of examples. A comprehensive user guide to the present meshing tool has also been provided for reference.

**Chapter 3:** A detailed description of the adopted modelling strategy during the present research is provided in this chapter. Adaptation of the governing fluid flow equations to suite engine combustion modelling are described, related to the present RANS implantation. Turbulence closure models, boundary conditions and boundary layer modelling, discretisation procedure and solution algorithms are also briefly summarised.
Chapter 4: Emphasis of this chapter is placed on the development of an improved ignition and flame kernel formation model to simulate the early stage of spark ignited flame propagation. Having explained the fundamental characteristics of the spark ignition process in engine related applications, a detailed mathematical model is developed to compute the correct species consumption rate and flame propagation behaviour.

Chapter 5: In this chapter, a mathematical model for simulating the fully developed stage of turbulent premixed combustion is formulated. State of the art combustion modelling techniques are also appropriately reviewed. Important aspects, particularly in engine combustion are highlighted, while necessary corrective measures are suggested to overcome some inherent deficiencies in existing modelling approaches.

Chapter 6: A brief description is provided on the present experimental programme, conducted to acquire a validation data set for a range of engine operating conditions of the E6 engine. A description of the test engine, instrumentation and the data acquisition procedure is presented. Followed data analysing techniques and quality assessment methods are also summarised.

Chapter 7: The validation and verification procedure of the developed RANS simulation models are detailed in this chapter. The verification of ignition model and the combustion model against published literature are discussed. Subsequently, the success of the both models applied to predict the combustion characteristics in the Ricardo E6 engine is comprehensively evaluated with respect to experimental observations and the published literature.

Chapter 8: The relevant theoretical and practical concerns in modifying the present RANS computer code for implementing LES filtered governing equations and SGS turbulence models are presented. Present simplifying assumptions and their influence on the predictions are outlined together with possible remedies.

Chapter 9: Challenges of premixed combustion modelling in LES context and current modelling strategies are elaborated herein. Development of a new ignition model and a dynamic flame surface density combustion model is presented. Special modifications needed in LES filtering procedure to implement FSD based combustion models and the test filtering techniques adopted for dynamic combustion modelling in wall bounded systems are also discussed.

Chapter 10: The validation of the present LES models and combustion sub models in both reacting and non-reacting cases are presented in this chapter. The predictions are critically evaluated compared to experimental findings. Achievements of the present LES
implementation with respect to RANS capabilities are qualitatively assessed. Applicability, of the present combustion model in examining unsteady cycle-to-cycle variations in engine combustion is also investigated.

**Chapter 11:** This chapter provides concluding remarks from the present research. Important findings, notable achievements, limitations and suggestions for future improvements are discussed.
In CFD, the accuracy of a computed solution is directly dependent on the quality of the computational mesh. The mesh quality can significantly be improved in complex shaped geometries, with relatively a little effort, by using unstructured grids. Therefore, aiming to exploit the benefits from unstructured grid capability of the KIVA-4 code, a mesh generation strategy is designed and implemented during the present work. It is expected to extract mesh data from a commercial grid generator and further process to suite the meshing requirements of KIVA-4 code.

The discussion in this chapter starts with highlighting the requirement of a robust grid generation methodology for the present solver. It is proposed to develop a mesh conversion process, as the most viable solution. It also explains the primary challenges to be accomplished during such a task. From section 2.3 to 2.5, logical and mathematical concepts adopted to perform the required mapping operations are demonstrated. In section 2.5, the attention is particularly given to describe the conversion procedure of degenerated cell elements. A brief introduction to the developed computer programme: $N2K$, is presented in section 2.6. Use of $N2K$ requires following some specifically predefined meshing procedures. Hence, a comprehensive user guide has been provided in section 2.7, on using the $N2K$ programme with commercial grid generation tools for generating complex meshes for both engine and non-engine applications. Some of the example grids constructed using the present strategy have been illustrated in section 2.8.
2.1 Mesh Generation for KIVA-4

Governing transport equations are numerically approximated over each of the computational cell to determine the spatial and temporal distribution of flow properties. The computational mesh approximately represents the physical shape of the problem domain. It is crucial to create a mesh well adapted to the physical properties of problem under consideration. In particular, the study of the flow field in spark ignition engines requires meshing tools with the capability of representing highly contoured interior surfaces of the manifolds and combustion chambers (Henson 1998). These tools should efficiently control the vertex placement avoiding mesh distortions and preserving the innate profile of the geometry.

The block-structured grid generation programme: K3PREP, provided with KIVA-4 has the capability of producing all hexahedral cells. However, the fixed-formatted input data file for the K3PREP has to be created manually by the user, including all the information of geometric dimensions, surface curvature coordinates, block-patching and valve profiling instructions and boundary definitions (see Amsden 1993 & Amsden 1997 for more details). Therefore, the mesh generation process for KIVA has always been a tedious task that demands extensive effort. If the engine geometry is of high complexity, such as irregularly shaped non-conventional manifolds and combustion chambers, the task becomes painstakingly slow, as it requires manual specification of boundary-profiling coordinates. Besides, it is rather difficult or practically impossible to use localized mesh refinement techniques with the block-structured approach. Hence, this meshing approach largely discouraged the users from modelling flow through complex ports and valves; consequently, the bulk of the KIVA simulations have been limited to valve closed period of the engine cycle, with approximated engine geometries. The other known problem associated with the K3PREP generated grids is that, it results in relatively a high percentage of skewed and concave cells (Amsden 1997), which leads to problems in numerical convergence. As the user has no facility to oversee the mesh beforehand and has no mechanism to examine the mesh generation process systematically, meshing with K3PREP is always a slow and iterative process. The latest of the KIVA family of codes: KIVA-4, is capable of handling unstructured meshes. However, it does not provide any facility for unstructured grid generation. As a result, users have to employ their own meshing tools to generate unstructured grid.

At the time of the start of this research in early 2010, there was no any commercial meshing tool which supported KIVA-4, other than TrueGrid® (Torres 2007). In fact, TrueGrid®-KIVA module was in its early stage of development and the reliability in complex geometries had
not been thoroughly assessed. In addition, TrueGrid® was found to be largely command driven and less user-friendly. Development of a completely new meshing tool was obviously an impractical solution. Therefore, in this work, as a remedy for this problem, using GAMBIT as the base meshing tool, a grid generation methodology and an interface programme for converting GAMBIT generated meshes to KIVA-4 format was developed. Several commercial mesh generation programmes now support exporting grids for KIVA-4. However, being a low cost alternative with greater flexibility, the present formulation is still very much superior to such black-box type tools. On the other hand, procedures developed in this study can easily be modified to use with any other mesh generation programme.

GAMBIT is a commercial grid generation package, which has advanced features for automatic grid generation. Most of all, it has a user friendly graphical 3D environment, in which the user can construct a 3D geometry part by part. As the quality of both the mesh and the geometry can be examined during the modelling and meshing phase, concave and distorted cells can be easily repaired or eliminated. GAMBIT has special facilities for mesh modifications and refinements, so that it provides a better platform for accurate meshing of complex shapes. For example, both mapping and cooper meshing techniques are available for hexahedral grid generation. Mesh quality could be improved by using Laplacian or equipotential smoothing. It also supports importing geometries from various computer aided drawing (CAD) packages in IGES or STEP file formats. Thus, it could be easily used to model complex manifolds and combustion chambers in engine geometries.

The developed mesh conversion programme during the present work, uses the GAMBIT mesh connectivity database exported in the form of a neutral file (.neu file format), and produces the required input mesh data file kiva4grid for KIVA-4. A comprehensive description of this methodology is given in the following sections. Sample formats of the neutral file and the kiva4grid are provided in the Appendix A of this thesis. In addition, further details and explanations on meshing requirements are available in the GAMBIT user manual on neutral file format and the KIVA-4 user manual (Torres 2007).

2.2 GAMBIT and KIVA-4 Indexing Conventions

Four major points have to be considered in the process of GAMBIT to KIVA-4 mesh conversion: cell indexing, node indexing, cell orientation and boundary face mapping. Assigning a unique number (cell address) for each of the computational cells is meant by the term cell indexing. Similarly, in node indexing a unique number known as the node address is assigned to each of the cell vertices. Each vertex has its own unique location in space and
therefore, associated with a unique set of coordinates. In structured grids, often a particular order is maintained in both node and cell indexing in order to construct a global connectivity database. However, as KIVA-4 is an unstructured code, it does not have a specific cell indexing convention and it maintains a local connectivity structure. Therefore, no effort has been taken herein to orderly arrange the cell numbers generated by GAMBIT. Instead, the default addresses are retained. In addition, there is no necessity to change the node addresses assigned to a certain vertex. Therefore, GAMBIT generated spatial coordinates and corresponding node addresses are used with associated unchanged cell addresses.

For calculation purposes, it is necessary to identify the relative position of a vertex with respect to the other vertices of the same cell. This task is usually accomplished by specifying the cell addresses and the associated vertex addresses following a predefined order (convention) in the input mesh data file. Different conventions may be followed by different CFD codes. In the present case, the order of the node addresses written in the neutral file by GAMBIT describing a given cell, is different from the order expected by the KIVA-4 format in \textit{kiva4grid} file.

Figure 2.1: (a) An arbitrary hexahedral cell whose cell address is 105. Corresponding node addresses are marked at the relevant vertex
(b) The cell indexing convention-I of the GAMBIT neutral file
(c) The cell indexing convention-II of the GAMBIT neutral file

GAMBIT uses two node indexing conventions, which are slightly different from each other. For example, the arbitrary hexahedron in Figure 2.1(a) may be defined in GAMBIT \textit{neutral} file as follows using the convention-I in Figure 2.1(b):

\begin{verbatim}
<table>
<thead>
<tr>
<th>Cell No</th>
<th>Node 1</th>
<th>Node 2</th>
<th>Node 3</th>
<th>Node 4</th>
<th>Node 5</th>
<th>Node 6</th>
<th>Node 7</th>
<th>Node 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>105</td>
<td>55</td>
<td>79</td>
<td>46</td>
<td>85</td>
<td>41</td>
<td>34</td>
<td>12</td>
<td>47</td>
</tr>
</tbody>
</table>
\end{verbatim}
Chapter 2: Development of a Mesh Generation Strategy for KIVA-4

It can also be denoted by using the convention-II in Figure 2.1(c) as:

<table>
<thead>
<tr>
<th>Cell No</th>
<th>Node 1</th>
<th>Node 2</th>
<th>Node 3</th>
<th>Node 4</th>
<th>Node 5</th>
<th>Node 6</th>
<th>Node 7</th>
<th>Node 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>105</td>
<td>55</td>
<td>46</td>
<td>79</td>
<td>85</td>
<td>41</td>
<td>12</td>
<td>34</td>
<td>47</td>
</tr>
</tbody>
</table>

It is important to note that, the values shown on the vertices of the cell in Figure 2.1(a) are the node addresses and shown in Figure 2.1(b) and Figure 2.1(c) are the order of the node addresses that appear in the GAMBIT neutral file.

According to the indexing convention of GAMBIT, any of the vertices may be chosen as the first node (here address 55), but the rest of the node addresses have to be orderly presented following either of the two conventions. The difference in the two indexing methods is associated with the direction of node ordering. Starting direction of the convention-I is in the anti-clockwise direction whilst, the convention-II is in the clockwise direction as seen by an observer at 5th node. Note that, there is no any restriction, which controls the choice of the indexing convention in exporting the neutral file. It is completely arbitrary and may depend on the mesh generation algorithms used, which is beyond the control of the user.

![Node indexing convention of a KIVA-4 cell](image)

**Figure 2.2:** Node indexing convention of a KIVA-4 cell

In contrast, the node indexing convention of KIVA-4 is unique as shown in Figure 2.2. The above cell in Figure 2.1(a) may be specified in the kiva4grid files as follows.

<table>
<thead>
<tr>
<th>Cell No</th>
<th>Node 1</th>
<th>Node 2</th>
<th>Node 3</th>
<th>Node 4</th>
<th>Node 5</th>
<th>Node 6</th>
<th>Node 7</th>
<th>Node 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>105</td>
<td>55</td>
<td>79</td>
<td>85</td>
<td>46</td>
<td>41</td>
<td>34</td>
<td>47</td>
<td>12</td>
</tr>
</tbody>
</table>

KIVA-4 indexing convention expects the node addresses to be ordered in anticlockwise direction such that the first four nodes create the bottom face and the rest of the four nodes form the top face of the cell. Accordingly, the functionality of the conversion programme
should be to read the input data stream of node addresses from the \textit{neutral} file, identify its indexing convention and appropriately rearrange the order of the node addresses before writing it to the \textit{kiva4grid} file. However, this rearrangement process is not that straightforward as it appears. This difficulty is mainly due to the use of two node indexing schemes in GAMBIT. Hence, special techniques are needed to identify the actual node indexing order prior to format conversion.

2.3 Node Conversion

Indicated below on the left hand side of Figure 2.3 are the two indexing conventions of node numbering in the GAMBIT \textit{neutral} file. The KIVA-4 indexing convention is depicted in the right side of the same figure. It is important to stress here that the numbers indicated at vertices represent the order of the node indexing of the corresponding mesh data files and they are different from the actual node addresses.

![Diagram showing two indexing conventions of node numbering in GAMBIT](image)

Figure 2.3: Shown on the left is the possible node indexing orders of a GAMBIT cell in the \textit{neutral} file. The expected node indexing order by KIVA-4 is shown on the right.

The two indexing conventions of GAMBIT may be distinguished by identifying the location of the vertex 1, 2 and 4 with respect to the position of vertex 5. The direction order of vertices 1-2-4 is anticlockwise in the cell (a) in Figure 2.3, whereas it is clockwise in the cell (b). This
order has to be identified and the order of the node addresses must be appropriately modified before writing into the *kiva4grid*. The KIVA-4 cell must be always anti-clockwise notated. It appears to be possible to identify whether the nodes 1-2-4 are clockwise or anti-clockwise notated by evaluating the sign of the vector product of vectors connecting vertices 1-2 and 2-4. Nevertheless, this method is valid only if the vertices 5, 6, 7 and 8 are located vertically above the vertices 1, 2, 3 and 4; yet in practice, a GAMBIT cell can pose any orientation, irrespective of the spatial location. Therefore, alternative tests are needed to correctly identify the node indexing order.

There are two possibilities for node conversion. One is to identify the node order of the GAMBIT cell and subsequently perform the appropriate vertex mapping operation. Alternatively, it is possible to perform the mapping operation following a prescribed mapping order first and then, test for the node indexing order of the resultant cell. The latter was found to be less complex in implementing and is retained in this study. Consequently, a procedure is prescribed for mapping GAMBIT vertex indexes to KIVA-4 format, where the 1\textsuperscript{st} node index of the GAMBIT cell is mapped to the 5\textsuperscript{th} node of the KIVA cell, while the 2\textsuperscript{nd} node index is mapped to the 8\textsuperscript{th} node of the KIVA cell. The complete mapping procedure is given in Table 2.1.

<table>
<thead>
<tr>
<th>GAMBIT node index</th>
<th>Mapped KIVA-4 node index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>7</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>4</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>3</td>
</tr>
</tbody>
</table>

It should be noted here that, this procedure is not the only possible way of mapping and an appropriate order may be used as long as the KIVA’s anticlockwise indexation is preserved. The order presented here is based on the results of number of computing experiments and is found to largely reduce subsequent computational time.
Figure 2.4: Two types of cells would be possible after mapping the GAMBIT cells using the order given in Table 2.1. Shown in left are the GAMBIT cells and shown in right are the resultant cells after performing the node mapping operation.

As illustrated in Figure 2.4, only two types of cells can be resulted after following the defined mapping procedure in Table 2.1. The second type of the resultant cell, shown on the right side of Figure 2.4 (b) is compliance with the KIVA-4 indexing convention, as it is anticlockwise notated as observed from the 5th node. However, the first resultant cell shown in Figure 2.4 (a) is clockwise notated and needs further modifications prior to writing into the kiva4grid file.

The measures taken to rectify this issue mainly use mathematical concepts in vector algebra and are elaborated further in the next section.

### 2.3.1 A Generic Test for Identifying Node Indexing Order

The method formulated in this section allows the identification of the exact node indexing order of a given hexahedral cell by comparing the relative location of each of the cell nodes. Figure 2.5 shows a typical convex cell with correct KIVA-4 node indexing. Assuming vertex A is to be node 1 and vertex B is to be node 2 etc..., the spatial coordinates of each vertex is subscripted with the corresponding node index. \( G \) is the centroid of face \( A - B - C - D \). The unit normal vector to the face \( A - B - C - D \) is \( \eta \) and \( \theta \) is the angle between \( \eta \) and \( \overrightarrow{GQ} \).
Figure 2.5: KIVA-4 hexahedral cell and coordinate indices. Unit normal vector to face $A - B - C - D$ creates a $\theta$ angle with $\vec{GQ}$.

If nodes $A, B, C$ and $D$ always lie in the opposite side of nodes $P, Q, R$ and $S$ the following relation can be established.

*If $A - B - C$ is ANTICLOCKWISE as seen from $D$ then $0^\circ < \theta < 90^\circ$ & $1.0 > \cos \theta > 0.0$*

*If $A - B - C$ is CLOCKWISE as seen from $D$ then $90^\circ < \theta < 180^\circ$ & $-1.0 < \cos \theta < 0.0$*

This implies that for any position of $Q$ in any plane other than $ABCD$ the angle $\theta$ is acute as long as $A - B - C$ is located anticlockwise as seen from the vertex $D$.

The value of $\cos \theta$ is evaluated as shown below.

Let, the vectors $\vec{AB}$ and $\vec{BC}$ in usual notation as:

$$\vec{AB} = (x_2 - x_1)i + (y_2 - y_1)j + (z_2 - z_1)k$$
$$\vec{BC} = (x_3 - x_2)i + (y_3 - y_2)j + (z_3 - z_2)k$$

If the vertices $ABCD$ are coplanar, an expression for $\eta$ can be derived in terms of vector product of $\vec{AB}$ and $\vec{BC}$:

$$\eta = \frac{\vec{AB} \times \vec{BC}}{|\vec{AB} \times \vec{BC}|} = ai + bj + ck$$

where, $a^2 + b^2 + c^2 = 1$.

The coordinates of $G$ can be approximated by averaging the coordinates of corner vertices.
\[ G(x_g, y_g, z_g) = G \left[ \frac{x_1 + x_2 + x_3 + x_4}{4}, \frac{y_1 + y_2 + y_3 + y_4}{4}, \frac{z_1 + z_2 + z_3 + z_4}{4} \right] \] (2.4)

Then, the vector \( \overrightarrow{GQ} \) can be estimated as
\[ \overrightarrow{GQ} = (x_6 - x_g)i + (y_6 - y_g)j + (z_6 - z_g)k \] (2.5)

Scalar product of \( \eta \) and \( \overrightarrow{GQ} \) yields:
\[ \overrightarrow{GQ} \cdot \eta = |\overrightarrow{GQ}| \cos \theta = a(x_6 - x_g) + b(y_6 - y_g) + c(z_6 - z_g) \] (2.6)
\[ \cos \theta = \left[ \frac{a(x_6 - x_g) + b(y_6 - y_g) + c(z_6 - z_g)}{|\overrightarrow{GQ}|} \right] \] (2.7)

Hence, by comparing the sign of the \( \cos \theta \) value, it is determined whether the resultant cell after mapping is clockwise or anticlockwise. If the cell is anticlockwise notated, it automatically adheres to the KIVA-4 node indexing and if it is clockwise notated, node addresses are rearranged accordingly.

### 2.3.2 Mapping Cell Face Boundary Conditions

The interested physical calculation domain is often surrounded by several types of boundaries. These may include solid walls, moving faces and openings to the surrounding. Each of these boundaries is represented in a computational mesh by a unique identification index assigned to each of the cell faces, which lies on a particular boundary. Hence, during the mesh conversion process, it is required to appropriately interchange face boundary indexes to suit the KIVA-4 face index convention. GAMBIT and KIVA have two different face indexing convention and they are briefly summarized in Table 2.2.

<table>
<thead>
<tr>
<th>Face ID</th>
<th>GAMBIT cell</th>
<th>Corresponding node indexes</th>
<th>KIVA-4 Cell</th>
<th>Corresponding node indexes</th>
</tr>
</thead>
<tbody>
<tr>
<td>face 1</td>
<td>1-2-6-5</td>
<td></td>
<td>face 1 (left)</td>
<td>4-3-7-8</td>
</tr>
<tr>
<td>face 2</td>
<td>4-2-6-8</td>
<td></td>
<td>face 2 (front)</td>
<td>1-5-8-4</td>
</tr>
<tr>
<td>face 3</td>
<td>4-8-3-7</td>
<td></td>
<td>face 3 (bottom)</td>
<td>1-2-3-4</td>
</tr>
<tr>
<td>face 4</td>
<td>1-3-7-5</td>
<td></td>
<td>face 4 (right)</td>
<td>1-2-6-5</td>
</tr>
<tr>
<td>face 5</td>
<td>1-2-4-3</td>
<td></td>
<td>face 5 (derriere)</td>
<td>2-3-7-6</td>
</tr>
<tr>
<td>face 6</td>
<td>5-6-8-7</td>
<td></td>
<td>face 6 (top)</td>
<td>5-6-7-8</td>
</tr>
</tbody>
</table>
Even though GAMBIT has two node indexing conventions, the face indexing convention is always the same, irrespective of the node indexing method. For example, the face bounded by the vertices 1, 2, 6 and 5 is always taken to be the first face as shown in the above table. Whereas, in KIVA-4, the first face is made of vertices 4, 3, 7 and 8 and called the left face.

Accordingly, during the conversion, face 1 of every GAMBIT cell is assigned to the front face of the corresponding KIVA cell (assuming node 5 of the GAMBIT cell has been mapped to node 1 of the KIVA cell). Hence, the rest of the assignments are; face 2 to left, face 3 to derriere, face 4 to right, face 5 to top and the face 6 to bottom. It is important to note that, this face mapping order is valid only if it is performed just after the vertex mapping and before rectifying the clockwise notated cells. During the correction step of clockwise cells, face boundary indexes also have to be interchanged appropriately.

2.4 Re-Orientation of Squish and Valve Cells

In addition to the vertex convention, there are some additional restrictions imposed on the cell elements in squish and valve region of an engine mesh by KIVA-4. Valve and piston snapping algorithms assume that, the mesh is vertically aligned, so that the z coordinates of the top face vertices 5, 6, 7 and 8 are always located above that of the bottom face vertices 1, 2, 3 and 4. If these criterions are not satisfied, KIVA aborts the run due to the formation of inverted cells. As a result, additional tests are required to verify whether this criterion is satisfied by the squish and valve cells and relevant corrective steps must be taken to reorient the cell indexing. However, comparison of the Z coordinate of individual vertex alone is not sufficient to identify incorrectly oriented cells. The approach taken here evaluates relative position and direction of each vertex, with respect to the neighbour vertices of the same cell. Thereby, establishing a unique property, which is satisfied only by the face located in top most position in the Z direction.

![Figure 2.6: A – B – C: three coplanar points clockwise indexed as seen by the reader](image-url)
Three points: $A$, $B$ and $C$ on $XY$ plane are considered as depicted in Figure 2.6. Respective spatial coordinates are as shown in brackets. The direction of $A - B - C$ indexation with respect to point $A$ is clockwise as observed by the reader.

The position vectors of point $A, B$ and $C$ are defined as $\vec{a} = (x_a i + y_a j)$, $\vec{b} = (x_b i + y_b j)$ and $\vec{c} = (x_c i + y_c j)$ respectively in usual notation. For any three points on a given plane, which are located in clockwise direction, the following property $P_{abc}$: the vector product of $\vec{BA}$ and $\vec{CB}$, exists.

$$\overrightarrow{P_{abc}} = \overrightarrow{BA} \times \overrightarrow{CB} < 0 \quad (2.8)$$

$$\overrightarrow{P_{abc}} = [(x_b - x_a)(y_c - y_b) - (y_b - y_a)(x_c - x_b)] k < 0 \quad (2.9)$$

where, $k$ is the unit vector in positive $Z$ direction. Thus, the following relation is obtained.

$$P_{abc} = [(x_b - x_a)(y_c - y_b) - (y_b - y_a)(x_c - x_b)] < 0 \quad (2.10)$$

Hence, the property $P_{abc} < 0$, if the points $A - B - C$ are clockwise notated, whilst $P_{abc} > 0$, if the points $A - B - C$ are anticlockwise notated. These relations can effectively be used to identify the top face of a cell as demonstrated in the following section.

### 2.4.1 Identification of the Top Face of a Cell

According to Figure 2.7(a), the face bounded by nodes 5, 6, 7 and 8 is in topmost position in space facing upward direction. It should be noted that, this cell adheres to the KIVA-4 notational conventions and thus, in this case, the topmost located face and the top face of the KIVA cell are the same. In order to identify this face, it is possible to use the following logic, comparing the $Z$ coordinates of vertices.

“If: $(z_5 > z_1)$ and $(z_6 > z_2)$ and $(z_7 > z_3)$ and $(z_8 > z_4)$ Then: face bounded by vertices 5, 6, 7 and 8 is the top face.”

However, further examination on in Figure 2.7(b) reveals that, this condition alone cannot establish the required relation. In this figure also, nodes 5, 6, 7 and 8 are located above that of 1, 2, 3 and 4 in the $Z$ plane, though the pane bounded by nodes 5, 6, 7 and 8 is not located at the topmost $Z$ level. Because of this reason, the above statement was further expanded as shown below, using the directional property stated in the Eq. (2.10).
Figure 2.7: Some of the special cell orientations need to be considered when identifying the top face of a cell

The coordinates of node 1 in space is taken to be \((x_1, y_1, z_1)\), and node 2 to be \((x_2, y_2, z_2)\) etc... If 1’, 2’, 3’, 4’, 5’, 6’, 7’ and 8’ are the projected points of nodes 1, 2, 3, 4, 5, 6, 7 and 8 on XY plane, then the coordinates of 1’ is given by \((x_1, y_1)\) and coordinates of 2’ is \((x_2, y_2)\) etc... Thus, the following relations may be established for the hexahedral cell shown in Figure 2.7(a).

\[
\begin{align*}
& (z_5 > z_1) \text{ and } (z_6 > z_2) \text{ and } (z_7 > z_3) \text{ and } (z_8 > z_4) \text{ and } \\
& \text{P5’6’4’} = [(x_6 - x_5)(y_4 - y_6) - (y_6 - y_5)(x_4 - x_6)] > 0 \text{ and } \\
& \text{P6’7’1’} = [(x_7 - x_6)(y_1 - y_7) - (y_7 - y_6)(x_1 - x_7)] > 0 \text{ and } \\
& \text{P7’8’2’} = [(x_8 - x_7)(y_2 - y_8) - (y_8 - y_7)(x_2 - x_8)] > 0 \text{ and } \\
& \text{P8’5’3’} = [(x_5 - x_8)(y_3 - y_5) - (y_5 - y_8)(x_3 - x_5)] > 0
\end{align*}
\]

Then: face bounded by vertices 5, 6, 7 and 8 is the top face.”

This indicates that, if nodes 5, 6, 7 and 8 are located above that of nodes 1, 2, 3 and 4 respectively and the relative direction of vertices 5’-6’-7’-8’, 6’-7’-1’-7’-8’-2’ and 8’-5’-3’ are anticlockwise on XY plane, then the face bounded by the vertices 5, 6, 7 and 8 is the top face.

As a verification measure, the same set of equations is now applied to the cell shown in Figure 2.7(b) and results are as follows:

\[
\begin{align*}
& (z_5 > z_1) - True \\
& (z_6 > z_2) - True
\end{align*}
\]
\[(z_7 > z_3) - True \tag{2.18}\]
\[(z_8 > z_4) - True \tag{2.19}\]
\[P5'6'4' = [(x_6 - x_5)(y_4 - y_6) - (y_6 - y_5)(x_4 - x_6)] > 0 - True \tag{2.20}\]
\[P5'6'4' = [(x_6 - x_5)(y_4 - y_6) - (y_6 - y_5)(x_4 - x_6)] > 0 - True \tag{2.21}\]
\[P6'7'1' = [(x_7 - x_6)(y_1 - y_7) - (y_7 - y_6)(x_1 - x_7)] > 0 - Can be True or False \tag{2.22}\]
\[P7'8'2' = [(x_8 - x_7)(y_2 - y_8) - (y_8 - y_7)(x_2 - x_8)] > 0 - False \tag{2.23}\]
\[P8'5'3' = [(x_5 - x_8)(y_3 - y_5) - (y_5 - y_8)(x_3 - x_8)] > 0 - Can be True or False \tag{2.24}\]

The location of 7’ and 6’ cannot be exactly determined with given data. Hence, \(P6'7'1'\) can be either negative or positive. The same logic can be applied for \(P8'5'3'\) as well. However, it is clear that, \(P7'8'2'\) is always positive as node 7 and 8 form an edge of the top face. Therefore, the cells in Figure 2.7(a) and (b) can be distinguished from each other by checking the above conditions.

The cell element shown in Figure 2.7(c) is now considered. The cell vertex indexation is same as in Figure 2.7(a), except the bottom face is displaced to the right such that \(P6'7'1' < 0\). This indicates that, the relation derived above does not hold for Figure 2.7(c). This is indeed true mathematically, but in KIVA-4, there is a restriction imposed on user to maintain the grid lines 1-5, 2-6, 3-7, and 4-8 of each squish cell nearly vertical in vertical valve engine configurations, due to the assumptions made in the valve and piston snapping routines (Amsden 1997). It is the responsibility of the user to ensure that the mesh is vertically aligned. Therefore, in general, the relation derived above holds for all KIVA-4 cells in the squish region and is used in the conversion code to identify inverted cells. There are plenty of meshing techniques, such as cooper meshing technique (Blacker 1996) in GAMBIT to easily obtain a vertically aligned mesh. Therefore, the first version of the N2K code was developed with this restriction and all the grids shown in this thesis are constructed using this version. However, non-vertically aligned meshes are unavoidable; for example, in pent-roof engines and canted valve engine. Thus, a generic test to identify the cell orientation, which can be universally applied for any mesh arrangement, is needed. It is mandatory in KIVA that, the cylinder region of the computational mesh has to be composed of vertically layered cell arrays; i.e, the two dimensional mesh arrangement in the \(XY\) plane across a given cross...
section should be nearly the same for the entire cylinder region. Using this constraint the following logic test is formulated.

The cell layer and associated cell faces attached to the piston face may be identified by a unique cell face index. Thus, they may be easily reoriented to comply with KIVA-4 constraints. Similarly, a cell located just above this piston face cell layer can be identified by searching for cells, which has a similar set of vertices as the top face of the piston face cell. It is clear that, this face should be the bottom face of the cell. Hence, the vertex indices and cell face boundary indices may be altered accordingly. This procedure can be carried out for all the cell layers in the cylinder region, until the cylinder head cell layer is reached. This method is currently being tested in the second version of the N2K code. However, it requires relatively a large computational time for search operations. Hence, the code was parallelised using OpenMP directives for multi-processor operation in the present study. The other possibility of reducing the associated computational overhead is to construct a connectivity database using the node, face, and cell data in the neutral file. The time spent on searching for neighbouring cells should largely be reduced in this method. However, this procedure has not yet been implemented.

2.5 Conversion of Degenerated Mesh Elements

KIVA-4 is capable of handling unstructured mesh elements, such as tetrahedrons, prisms and pyramids to a limited extent. These elements may be used in a hybrid mesh, in regions such as ports or piston bowl, where the mesh structure is not affected by the piston or valve motion. KIVA-4 rezoning and snapping algorithms are not yet advanced enough to accommodate such element types in snapping regions. KIVA-4 needs these element types to be constructed by degenerating hexahedral cells as shown in Figure 2.8.

A pyramid cell can be created by degenerating a face of a hexahedral cell, while a tetrahedron cell may be created by degenerating an edge of the square surface of a pyramidal element. Prism cells are created by degenerating two edges in the opposite faces of a hexahedral cell. Thus, theoretically in KIVA-4, all the cell types are made of eight vertex nodes. The present conversion code has also been improved to convert GAMBIT generated tetra, pyramid and prisms cells into KIVA-4 degenerated elements. However, GAMBIT has different number of nodes for each cell type, which in general, is equal to the number of vertices of the element. Thus, care must be taken to appropriately define the degenerated nodes and faces to match with KIVA-4 indexing convention. For example, the node address of the fifth node has to be
repeated as the sixth, seventh and eighth node addresses for the pyramid cell in Figure 2.8 (a). Node addresses for the other cell types are also stated in a similar way.

![Figure 2.8](image-url)

Figure 2.8: (a) A pyramid cell is created by degenerating face vertices 5,6,7 and 8 (b) A tetrahedron cell can be created by degenerating an edge of the pyramid (c) A prism cell is created by degenerating two edges of opposite faces

It is mandatory, even for the degenerated elements to maintain the KIVA-4 anticlockwise indexing convention. As in the case of hexahedral elements, both anticlockwise and clockwise noted cells are resulted after node index mapping operation. Thus, for identifying the indexing convention, a similar strategy may be used as in the previous section. The procedures are described below, related to the tetrahedral cell shown in Figure 2.9 as an example.

![Figure 2.9](image-url)

Figure 2.9: Indexing convention of a degenerated element can be identified by valuating the angle $\theta$. The centroid of the face $ABC$ is $G$ and $\eta$ is the unit normal to that face
If \( A - B - C \) is ANTI_CLOCKWISE as seen from \( D \rightarrow 0^\circ < \theta < 90^\circ \rightarrow 1.0 > \cos \theta > 0.0 \)

If \( A - B - C \) is CLOCKWISE as seen from \( D \rightarrow 90^\circ < \theta < 180^\circ \rightarrow -1.0 < \cos \theta < 0.0 \)

The unit normal vector \( \vec{n} \) is calculated using the cross product of \( \vec{AB} \) and \( \vec{BC} \). The angle \( \theta \) may be evaluated using the dot product between \( \vec{n} \) and the \( \vec{GD} \). Similar logics can be defined for pyramid and prism cells appropriately and used in the correction of node indexing.

### 2.6 N2K: The Computer Programme

The conversion programme developed in this work, has been named as \( N2K \). The programme was coded using FORTRAN 90 standards, so that FORTRAN 90 or a later version of a compiler may be used. Currently, the code has been tested only with Intel Fortran11.1 compiler in 64 bit Fedora 10 and Fedora 12 Linux systems. ‘Convert’ is the main drive of the programme. The code consists of one module and several other subroutines and functions. Module CELDAT defines global variables, which may be shared among subroutines. Function of each subroutine and the procedures used have been explained within the subroutine itself. The executable file obtained after compilation is named as \( N2K \). The input neutral file to the programme should be named as ‘e6grid.neu’. After the execution, following files are created

- \( kiva4grid \) – input file to the KIVA-4 code.
- \( kiva4griddummy \) – a duplicate of \( kiva4grid \) with additional information for error tracing.
- \( invcell.dat \) – information on repaired inverted cells.

In order to use the \( N2K \) converter, specific procedures have to be followed by the user during the mesh generation process in GAMBIT. The following sections present a guide line, which has to be strictly followed by the user.

### 2.7 Mesh Generation for KIVA-4 Using GAMBIT

\( N2K \) converter has been developed to convert GAMBIT 2.4.6 neutral files. If it is used with other versions, code may be accordingly modified to cater for any change in the neutral file format. No restrictions are made on the mesh generation methodology using GAMBIT. Thus all the meshing tools and techniques available can be used appropriately. However, a number of restrictions have been imposed on naming boundary faces and regions of the mesh. Since \( N2K \) identifies regions and boundaries by their names, they should be labelled exactly as mentioned later in this section. Currently, the provision is only to use hexahedral, tetrahedral and pyramid cells. No routines have been included to convert prism cells. Apart from that
users have to strictly follow the rules imposed by KIVA-4 on mesh construction. Some of those will be discussed later in this chapter for completeness.

### 2.7.1 Definition of Mesh Regions

It is required to split the model into several regions before meshing the geometry as shown in Figure 2.10. They may be labelled as shown, specifying appropriate *continuum* type using the *zone* option in GAMBIT. User may split the cylinder region into four main regions: *dome*, *squish_upper*, *squish_middle* and *squish_lower*. This is only for the ease of meshing and if necessary, all three regions may be merged and labelled using any of the three names. It is required to include the entire region affected by the valve movement into the squish region. There are no restrictions on labelling any other region and user may consider the region names with the usual meaning indicated by the label. Currently, the conversion programme can facilitate maximum of four valves and four ports. The number associated in port and valve naming has to be suitably modified if there are more of them. The continuum type of valves is to be selected as *solid* and for all the other regions as *fluid*. Any additional geometry attached to the model may be included to any of the region appropriately. *N2K* identifies individual region by their names and assigns a unique region index for each of the cell in a particular region. Subsequently, this index is written in the *kiva4grid* file, so that KIVA-4 can distinguish between different mesh regions.

![Diagram](image)

**Figure 2.10:** Region types of a GAMBIT generated engine mesh for *N2K*
KIVA-4 uses the following regions identification indices.

- **Inactive**: 0 used for valves, valve stems and other inactive solid regions
- **Squish**: 10 for the region between the cylinder head and the piston
- **Bowl**: 11 used in piston bowl region
- **Dome**: 14 for the dome region
- **Port 1**: 20
- **Port 2**: 30
- **Port 3**: 40
- **Port 4**: 50

Region labels defined during the GAMBIT meshing are appropriately converted to these region indices within the \textit{N2K} code, without any intervention form the user.

### 2.7.2 Definition of Mesh Faces

GAMBIT creates neutral files, only if the \textit{Generic} solver is chosen. It is recommended to select the \textit{Generic solver} option, before meshing the model. The use of non-hexahedral cells to model a squish region with valves is not allowed at the moment in KIVA-4. If valve motion is to be simulated, it is recommended to mesh the model using all hexahedral cells.

![Face types of a GAMBIT generated engine mesh. Face names must be exactly assigned as indicated. Note that entire piston crown is assigned a single label](image)

Figure 2.11: Face types of a GAMBIT generated engine mesh. Face names must be exactly assigned as indicated. Note that entire piston crown is assigned a single label.
Figure 2.11 shows the labels assigned to the face boundaries of the ports and engine cylinder. Figure 2.12 shows the labels given to valve surfaces. These labels should be exactly used to name the meshed faces and no other label is allowed. Note that, *ioprt1_in* and *eport1_out* are pressure boundaries. They are often used in engines. If velocity boundaries are required, *vel_in* and *vel_out* may be used. Typically, these boundaries are used only with non-engine applications.

![Valve Faces](image)

Figure 2.12: Face labels of valves. Note that both the valve skirt and valve seat faces are assigned a single label. The number associated with the face label may be suitably modified depending on the number of valves.

During the mesh conversion process, the *N2K* code converts these boundary labels into the following face indices used by the KIVA-4 programme. Later, each of the cell faces is appropriately assigned the relevant boundary index given below.

<table>
<thead>
<tr>
<th>Index</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>used only with the piston face</td>
</tr>
<tr>
<td>11</td>
<td>bottom face of the first valve</td>
</tr>
<tr>
<td>12</td>
<td>top face of the first valve</td>
</tr>
<tr>
<td>13</td>
<td>bottom face of the second valve</td>
</tr>
<tr>
<td>14</td>
<td>top face of the second valve</td>
</tr>
<tr>
<td>15</td>
<td>bottom face of the third valve</td>
</tr>
<tr>
<td>16</td>
<td>top face of the third valve</td>
</tr>
<tr>
<td>17</td>
<td>bottom face of the fourth valve</td>
</tr>
<tr>
<td>18</td>
<td>top face of the fourth valve</td>
</tr>
</tbody>
</table>
20 : other solid faces
21 : should be used with the cylinder head instead of 20
30 : axis
40 : fluid faces
50 : front periodic face
60 : derriere periodic face
70 : velocity inflow boundary
80 : continuative outflow boundary
90 : pressure inflow boundary
100 : pressure outflow boundary

It is worth mentioning here that, the present N2K code does not support the conversion of periodic and axis boundary conditions.

2.7.3 Region and Face Definitions for Non-Engine Applications

The conversion programme can be used in mesh generation for non-engine applications as well. However, the approach to be followed is largely problem dependent. It is assumed here that, no valve or piston snapping routines are used during KIVA-4 simulations. If the calculation domain is fully enclosed by boundaries, the top and bottom faces may be assumed as cylinder head and the piston face. The side faces can be taken as the cylinder wall, while engine speed is set to zero during the simulation to prevent the piston face from moving. In case of a problem with open boundaries, such as in backward facing step problem, the domain may be split into three regions as illustrated in Figure 2.13. Faces and boundaries are named appropriately as shown. It is important to note that, shown in this figure is only one of the possible methods of region and face naming. There can be several possibilities for splitting into regions and naming faces for a given problem domain.

Figure 2.13: Region definition for a backward facing step geometry
Figure 2.14 depicts a possible way of face labelling for a backward facing step geometry. Flow inlet is defined as a *velocity_in* boundary, where the face normal velocity has to be prescribed in the KIVA-4 *itape5* input file. Rest of the outside walls in the *intake_port1* region may be named as *iport1_wall* boundaries. Similarly, in the *squish_lower* region, the bottom face is named as the *piston_top*, while all the others as *cyl_wall*. Outlet is assigned a pressure boundary under the name *eport1_out* and all the other walls in the *exhaust_port1* region is named as *eport1_wall*.

![Face definitions at boundaries for the backward facing step geometry](image)

**2.7.4 Meshing the Ricardo E6 Engine**

Bulk of the engine simulations carried out during the present investigation is based on the Ricardo E6 engine. It has a pancake combustion chamber with vertical valves. Given below in Figure 2.15 is the block structure used in constructing the engine mesh. Splitting the engine geometry into number of simpler regions makes meshing easier, providing enhanced flexibility of maintaining adequate level of local mesh refinement. According to the requirements of KIVA-4, vertical valve engines have to be meshed at maximum valve lift positions of both valves. In addition, the mesh in valve traverse region should follow the valve surface profile. Therefore, the region above the valve is split into number of regions, in order to make sure that meshing requirements are satisfied.

Shown in Figure 2.16 is the Ricardo E6 engine mesh constructed during the present study. The mesh contains nearly around 400,000 unstructured hexahedral cells and used for RANS simulations. The engine geometry and mesh were originally created in GAMBIT and later converted to KIVA-4 format by using the *N2K* mesh conversion code.
Figure 2.15: Block structure of the Ricardo E6 engine mesh. (a) A view across the intake valve plane. (b) Plane view across the plane XY. (c) Enlarged view of the block structure around the intake valve region

Some of the key restrictions imposed by KIVA-4 are reported here for the benefit of other users. The number of cell layers on the valve_ side faces in vertical direction has to be limited to a maximum of two as illustrated in Figure 2.17. The volume directly above the valve skirt, affected by valve motion, needs to be uniformly meshed, such that the valve skirt profile propagates upward. The reasons for splitting the valve regions into number of sub regions as already noted in Figure 2.15, is primary due to this constraint. The boundary face between the squish and the port regions has to be chosen, such that the entire volume swept by the valve motion lies within the squish region. It is also visible from Figure 2.18 that, the mesh structure on XY plane propagates from the cylinder head to the piston crown surface.
Figure 2.16: Computational mesh for the Ricardo E6 engine. Mesh was originally constructed in GAMBIT and later converted to KIVA-4 format by using N2K
Figure 2.17: Mesh structure of the Ricardo E6 engine mesh across the intake and exhaust valve planes during the intake stroke

Figure 2.18: Internal mesh structure of the Ricardo E6 engine mesh. Only the mesh lines on solid surfaces are shown
2.8 Some of other Meshes Created Using N2K

Shown below are some of the other engine and non-engine geometries constructed using the present approach. These grids confirm the flexibility of the current mythology and its capability to create high quality grids of complex geometries with relatively a less effort. Some of these meshes will be used later in other chapters of this thesis for simulations.

![Meshes Created Using N2K](image)

Figure 2.19: Pent roof combustion chamber (a) Meshed using mapping algorithms (b) Unstructured hexahedral mesh created using paving algorithms

![Computational mesh of an engine cylinder](image)

Figure 2.20: (a) Computational mesh of an engine cylinder with a piston bowl constructed using unstructured hexahedral elements
(b) Pancake engine cylinder meshed with tetrahedral elements
Both grids were converted to KIVA-4 format by using the N2K programme
Figure 2.21: Hexahedral mesh of a backward facing step geometry

Figure 2.19 depicts the mesh of a pent roof combustion chamber. Note that, highly skewed cells on the four corners of the grid created using mapping techniques can be eliminated by using an unstructured grid with cell paving methods. Sample grids of a piston bowl, tetrahedral engine cylinder and a backward facing step geometry are shown in Figure 2.20 and Figure 2.21.

2.9 Summary

- Development and implementation of a methodology to convert GAMBIT generated computational meshes to suite KIVA-4 format was described in this chapter.
- Unavailability of a suitable grid generation tool and the limited capability of the existing methods were found to be the main reasons for the requirement of such a mesh conversion strategy.
- Conversion of the cell indexing order, adjustments in cell orientation, region and boundary condition mapping were the main challenges to be overcome during the conversation process.
- The developed methodology was mainly based on identifying the location of each of the vertices relative to the neighbouring vertices of the same computational cell and also relative to the global coordinate system.
- Mathematical concepts in vector algebra were extensively used for these purposes together with general logic test formulations.
• A mesh generation guideline to be used during the meshing phase in GAMBIT was designed, so that the exported *neutral* file containing mesh and connectivity data can be used to convert to *kiva4grid* format by using the developed interface programme *N2K*.

• Number of sample meshes comprising both engine and non-engine geometries with varying degree of complexity have been constructed using the present mesh generation strategy and successfully tested in the KIVA-4 simulations.
Until most recently, RANS has been the standard computational modelling technique for simulating reactive flows. Initial phase of the present study is focused on developing turbulent combustion models coupled with RANS techniques to simulate premixed combustion in SI engines. RANS approach is based on finding time averaged solutions of a set of largely simplified governing equations. The simplification process involves numerous approximations, assumptions and a large proportion of mathematical modelling, which are often application specific. The computer programme used in this research, is capable of solving the Reynolds averaged governing equations with spray dynamics and chemical reactions. The code has been extensively modified during this work, particularly for combustion model implementations and for LES calculations as described in a later chapter. In order to facilitate forthcoming discussions, the governing equations of reacting fluid flows are described in this chapter, mostly in relation to the engine combustion as employed in the present code.

The fundamental conservation equations and their progression to reactive turbulent flows are presented in section 3.1. Turbulent closure approach and the integration of boundary effects are discussed in sections 3.2 and 3.3 respectively. A justification of the turbulent model selection for the present study has also been included in section 3.2. Refinements made for the standard governing equations to make them solvable in practice have also been demonstrated. Discretisation of governing equations and their solution procedures are briefly stated in sections 3.4 and 3.5. Section 3.6 provides a concluding summary of the present chapter.
3.1 Governing Equations of Reacting Flows

The state of a turbulent reacting flow field is fully defined, once its pressure $p$, temperature $T$, density $\rho$, velocity $U$ and the mass fractions $Y_m$ of each species $m$ are known in both space and time $t$ for all points. Temporal and spatial variations of these properties can be mathematically computed using conservation laws of mass, momentum and energy. Application of conservation laws into a system, considering physical phenomena: for instance advection, conduction, molecular transport and chemical reactions results in a coupled set of partial differential equations, often named as governing equations. The instantaneous governing equations for a gaseous reactive flow field can be written in usual vector notations in Cartesian form as shown in Eq. (3.1) – (3.4). Detailed derivations of these equations can be found in Versteeg & Malalasekera (2007), Turns (1996), Warnatz et al. (1996) and Kuo (2005).

Species mass conservation  
\[
\frac{\partial}{\partial t} \left( \rho Y_m \right) + \nabla \cdot (\rho Y_m U) + \nabla \cdot (\rho Y_m V_m) = \dot{\omega}_{m,s} \tag{3.1}
\]

Global mass conservation  
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = \dot{\rho}_S \tag{3.2}
\]

Momentum conservation in $x$ direction  
\[
\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho U) + \frac{\partial p}{\partial x} - \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{yx}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} = \dot{F}_x \tag{3.3}
\]

Internal energy conservation  
\[
\frac{\partial}{\partial t} (\rho I) - \rho (\nabla \cdot U) + \nabla \cdot \rho I U + \nabla \cdot q + (\nabla \otimes U)^T : \tau = \dot{Q}_{I,S} \tag{3.4}
\]
The symbol $\nabla$ denotes the gradient operator in three dimensional Cartesian coordinate system and, has the usual definition as given in Eq.(3.5). $i, j$ and $k$ represent the unit vectors in $x, y$ and $z$ directions respectively.

$$\nabla = \frac{\partial}{\partial x} i + \frac{\partial}{\partial y} j + \frac{\partial}{\partial z} k \tag{3.5}$$

The velocity vector $U$ comprises of the three directional components $u, v$ and $w$ in the coordinate directions. Transport of species mass in and out from the system is attributable to the convective and diffusive fluxes. $V_m$ is the resultant diffusion velocity of species $m$ due to molecular transport. The source (or sink) term $\dot{\omega}_{m,s}$, accounts for the possible consumption or production of species $m$ as a result of chemical reactions. This may also include any species addition by an external mean, such as fuel injection. A relation for the global mass conservation can be obtained by summing up all the species equations. The chemical source terms of the species equations are naturally cancelled out with each other, as no net generation or destruction of total mass occurs in chemical reactions. Thus, only the externally added (or removed) mass source is left.

$$\tau = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} \tag{3.6}$$

$$(\nabla \otimes U) = \left( \frac{\partial}{\partial x} i + \frac{\partial}{\partial y} j + \frac{\partial}{\partial z} k \right) \otimes (ui + vj + wk) = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial v}{\partial x} & \frac{\partial w}{\partial x} \\ \frac{\partial u}{\partial y} & \frac{\partial v}{\partial y} & \frac{\partial w}{\partial y} \\ \frac{\partial u}{\partial z} & \frac{\partial v}{\partial z} & \frac{\partial w}{\partial z} \end{bmatrix} \tag{3.7}$$

$$(\nabla \otimes U)^\tau: \tau = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{bmatrix} : \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} = \tau_{xx} \frac{\partial u}{\partial x} + \tau_{xy} \frac{\partial u}{\partial y} + \tau_{xz} \frac{\partial u}{\partial z} + \tau_{yx} \frac{\partial v}{\partial x} + \tau_{yy} \frac{\partial v}{\partial y} + \tau_{yz} \frac{\partial v}{\partial z} + \tau_{zx} \frac{\partial w}{\partial x} + \tau_{zy} \frac{\partial w}{\partial y} + \tau_{zz} \frac{\partial w}{\partial z} \tag{3.8}$$
The momentum equation shown in Eq. (3.3) has been applied in the $x$ direction. Similar equations can also be derived for $y$ and $z$ directions. $\tau$ is the viscous stress tensor, usually written in the form given in Eq. (3.6) – (3.8). It represents all the nine components of possible shear and normal stresses that might act upon an infinitesimal fluid volume. It is noteworthy to highlight the order of the subscript notation of $\tau_{xy}$ term. The second subscript index $y$ represents the direction of the stress component, while the first subscript: $x$ in this case, shows the normal direction to the plane, upon which the stress acts. $\hat{F}_x$ is the $x$ component of momentum source term.

The balance equation for the specific internal energy is given in Eq. (3.4), where $q$ is the heat flux vector and $\dot{Q}_{I,s}$ is the specific internal energy source term. This source may either be a result of enthalpy change due to chemical reactions, fuel addition or by wall heat losses. Detailed expressions for these terms will follow in later sections in this thesis. The operator $\otimes$ represents dyadic tensor product and $\mathbb{T}$ is the transpose of the tensor. Also, note that the operator colon ($:$) in Eq. (3.7) and (3.8) is the tensor double dot product.

### 3.1.1 Navier–Stokes Equations

The above set of governing equations is yet unclosed as they contain several unknown terms, such as the viscous stress tensor, diffusion velocity and the source terms of each equation. Closure of these equations requires incorporation of suitable mathematical models: usually based on physical arguments. In most isotropic Newtonian flows, viscous stresses can be modelled as proportional to the local strain rate. In three-dimensional flows, the local rate of deformation is composed of linear deformation and the volumetric deformation (Versteeg & Malalsekera 2007). Accordingly, a general expression for the viscous stress terms may be written in the following form (Kuo 2005):

$$\tau_{xy} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \lambda (\nabla \cdot U) \delta_{xy} + \mu' (\nabla \cdot U) \delta_{xy}$$  \hspace{1cm} (3.9)

where, $\mu$ is usually called the dynamic molecular viscosity or the first viscosity. $\mu'$ is called the bulk viscosity and of which, only a very little is known up to now. $\lambda$: often named as the second viscosity, is also occasionally called the bulk viscosity by some authors as it is associated with the volumetric expansions (Kuo 2005). $\delta_{xy}$ is the Kronecker delta symbol defined to have the following properties.
The usual practice is to employ the Stokes hypothesis, to arrive at an expression for the second viscosity $\lambda$. The effect of $\mu'$ in combusting flows is negligible, but could be important in shock waves or in the absorption and attenuation of acoustic waves. Therefore, in this work, the relation between the first and the second viscosities is postulated by:

$$\lambda + \frac{2}{3}\mu = 0, \quad \mu' = 0$$

The assembled stress tensor is then written in compact vector notation as:

$$\tau = \mu[(\nabla \otimes U) + (\nabla \otimes U)^\top] - \frac{2}{3}\mu(\nabla \cdot U)\mathbb{I}$$

The unit dyadic, which has the same effect as the Kronecker delta is denoted by $\mathbb{I}$. Substituting the relation for stress tensor in governing equations, the well-known Navier-Stokes equations are obtained.

### 3.1.2 Reynolds Decomposition and Favre Averaging

In order to obtain the exact solution of pressure and the velocity of the flow field, the closed set of four instantaneous conservation equations obtained by applying the Navier-Stokes equation for mass and momentum in three coordinate directions, must be directly solved (DNS) without any form of modelling. However, due to the wide spectrum of length and time scales in turbulent flows, this approach needs extremely fine computational grids and ultra-fine time steps. Within the limits of current computing performance, it is extremely difficult to directly solve the above equations applied to a complex turbulent reacting flow in an engine. Hence, for practical engineering analyses, several alternative techniques such as LES and RANS are adapted.

It is possible to collapse the instantaneous property $\phi(x, y, z, t)$ into two components: a time averaged mean quantity $\bar{\phi}(x, y, z)$ and a superimposed fluctuating component $\phi'(x, y, z, t)$, defined by the following relations.

$$\phi(x, y, z, t) = \bar{\phi}(x, y, z) + \phi'(x, y, z, t)$$

$$\bar{\phi}(x, y, z) = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_t^{t+\Delta t} \phi(x, y, z, t) \, dt$$
The over bar (\( \overline{\cdot} \)) denotes a time averaged quantity and the prime (\( ' \)) denotes a turbulent fluctuating component. It is assumed that the time step \( \Delta t \) is greater than the characteristic time of turbulence, whilst smaller than the characteristic time of mean flow. The above procedure is usually called the Reynolds decomposition and the time averaged Navier-Stoke equations are referred as Reynolds Averaged Navier Stoke (RANS) equations. There are several immediate drawbacks of Reynolds averaging applied to variable density flows (Poinsot & Veynante 2005 and Kuo 2005). Among that, the main implication is associated with the resulting terms correlating density fluctuations, such as \( \overline{\partial (\rho'u')}/\partial x \) term in the continuity equation. This requires additional modelling and in fact, physically means a mass interchange across the mean streamline. This is somewhat contradictory with the usual concept of streamline and sometimes results in modelling errors. Therefore, an alternative approach called Favre averaging is adapted, where density weighted time averaging is considered. This procedure is primarily suited for variable density flows; specifically for reacting flows with heat transfer. Relations of the Favre averaging may be specified as:

\[
\phi(x, y, z, t) = \overline{\phi}(x, y, z) + \phi''(x, y, z, t)
\]

\[
\overline{\phi} = \frac{\rho \phi}{\rho} \text{ where } \overline{\rho \phi}(x, y, z) = \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_t^{t+\Delta t} \rho \phi(x, y, z, t) \, dt
\]

\[
\overline{\rho \phi''}(x, y, z, t) = 0
\]

The symbol tilde (~) denotes the Favre averaged quantities, while the double quotation (\( '' \)) represents the Favre fluctuating turbulent components. It should be noted that, Favre averaging leads to the relation \( \overline{\rho \phi''} = 0 \), but \( \overline{\phi''} \neq 0 \). All the instantaneous flow properties except density and the pressure (which are Reynolds averaged) are decomposed using above relations and substituted in the Navier-Stokes equations to obtain Favre averaged governing equations: the most useful form in practice.

Favre averaging has several distinct advantages. Unlike Reynolds averaging, it suppresses the density fluctuations leading to a significant simplification of the averaged equations (Cant & Mastorakos 2008). Furthermore, it reduces the number of turbulent correlations compared to the Reynolds averaging and for incompressible flows, both methods yield the same set of equations. In IC engines, where there is a significant variation in density, modelling should naturally have to be accomplished using the Favre averaging techniques. The code used in the present study solves the Favre averaged Navier-Stokes equations with necessary
modifications to suite for IC engine combustion. In the next few sections, the governing
equations solved in the present study are briefly discussed highlighting the important
assumptions and special terms where relevant.

3.1.3 Species Mass Conservation

The Favre averaged equation for the conservation of mass fraction $Y_m$ of species $m$ in reacting
flows may be expressed in the following form:

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{U}) = -\nabla \cdot (\bar{\rho} Y_m^u \bar{U}^u) - \nabla \cdot (\bar{\rho} Y_m V_m) + \bar{\omega}_{m,\text{source}}$$  \hspace{1cm} (3.19)

The first term in left hand side is the net mean rate of change of species mass and the second is
the rate of change of species mass within the control volume due to direct convective fluxes.
In order to close this equation, the three unknown terms on the right hand side should be
modelled. The first term $\nabla \cdot (\bar{\rho} Y_m^u \bar{U}^u)$ is due to the turbulent advection and the second term is
the mass exchange rate due to diffusion. When applied to IC engines, the source term may
comprise of two parts due to chemical reactions and fuel spray.

$$\bar{\omega}_{m,s} = \bar{\omega}_{m,\text{spray}} + \bar{\omega}_{m,\text{chem}}$$  \hspace{1cm} (3.20)

The spray term is non-zero only for the fuel species as spray droplets hardly contains other
species than the fuel. For premixed combustion, the spray term is always zero. Modelling the
chemical source term is the most important and most challenging task of combustion
simulation. Chapters 4 and 5 are mainly devoted to describe the techniques adopted in this
study to model the combustion source term.

The ability to diffuse or the diffusivity varies for each species. In fact, the diffusion is affected
not only by the concentration gradient (ordinary diffusion) but also by the thermal gradient
(thermal diffusion or Soret effect) and the pressure gradient (Pressure diffusion) (Turns 1996).
If unequal diffusivities are assumed for each species, it requires solving $N^2$ number of linear
equations for all the spatial points at each instant for an unsteady system having $N$ number of
species. Practically, this task is computationally exhaustive; hence, the usual engineering
approach is to assume the Fick’s law of diffusion with equal diffusivity for all species. This
law relates the tendency of species to move towards the low concentration regions with a
magnitude proportional to the concentration gradient. Moreover, it neglects the thermal and
pressure diffusion.
Under these assumptions, the laminar molecular diffusive flux in the $x$ direction can be expressed as:

\[
\rho \bar{Y}_m \bar{V}_{i,m} = -\rho \bar{D}_l \frac{\partial \bar{Y}_m}{\partial x} \approx -\bar{\rho} \bar{D}_l \frac{\partial \bar{Y}_m}{\partial x}
\] (3.21)

\[
\bar{D}_l = \frac{\mu}{\bar{\rho} S_{Cl}}
\] (3.22)

where, $V_{i,m}$ is the $x$ components of the diffusion velocity and $D_l$ is the coefficient of laminar diffusivity considered to be equal for all species. It may also be expressed as the ratio of the molecular dynamic viscosity $\mu$ and the mean density times laminar Schmidt number $S_{Cl}$. In order to calculate the molecular viscosity of the reacting gas mixture, the Sutherland (Sutherland 1893) formula given in Eq. (3.23) is used, based on the approximation that the resultant viscosity of the gas mixture is same as air viscosity at all engine operating conditions. This assumption is normally valid for engines as the total fuel mass is negligible compared to the trapped in-cylinder air mass.

\[
\mu = \frac{A_1 T^{3/2}}{T + A_2}
\] (3.23)

This experimental correlation provides the variation of molecular viscosity of air at elevated temperatures. $A_1$ and $A_2$ are constants having the values $1.457 \times 10^{-5}$ $gcm^{-1}s^{-1}K^{-0.5}$ and $110K$ respectively.

Note that, the molecular diffusion owing to fluctuating mass fraction and diffusivity have been neglected here, assuming the gradient in the mass density field is small. The collective expression for all the three components of the diffusion velocity in three dimensions is written using vector notations as:

\[
\nabla \cdot (\rho \bar{Y}_m \bar{V}_m) = -\nabla \cdot (\bar{\rho} \bar{D}_l \nabla \bar{Y}_m)
\] (3.24)

It is customary to use the classical gradient hypothesis to close the turbulent scalar fluxes, where the turbulent mass flux is assumed to be proportional to the mean concentration gradient. The flux and the gradient terms are related by the turbulent diffusivity $D_t$ defined by the Eq. (3.25) – (3.27).

\[
\bar{\rho} \bar{Y}_m' u'' = \bar{\rho} \bar{Y}_m'' u' = -\bar{\rho} \bar{D}_t \frac{\partial \bar{Y}_m''}{\partial x}
\] (3.25)
Chapter 3: Simulation of Turbulent Reacting Flows

\[ \overline{D_t} = \frac{\mu_t}{\bar{\rho} Sc_t} \] (3.26)

\[ \nabla. (\bar{\rho} Y''' U'') = -\nabla. (\overline{D_t \nabla Y_m}) \] (3.27)

Turbulent Schmidt number \( Sc_t \), is often taken to be constant. This is reasonable for shock wave free flows with moderate and low levels of heat transfer rates. The most common values at boundary layer for \( Sc_t \) are 0.89 or 0.9, while a value of 0.5 is more appropriate near the edge of the boundary layer (Wilcox 1998). Use of a varying Schmidt number would be able to represent more realistic local heat and mass transfer characteristics. Nevertheless, following the standard practice, a constant value equals to 0.9 is used in this study. The turbulent viscosity or the eddy viscosity \( \mu_t \) in Eq. (3.26) is the equivalent counterpart of the molecular viscosity for turbulence. This is somewhat an artificially defined parameter and a proper expression is given later in this chapter.

### 3.1.4 Global Mass Conservation

The global mass conservation or the continuity equation is obtained by summing up all the species conservation equations. The spray source term is zero for premixed combustion. Since the total mass of the system is conserved, all the chemical source terms in the right hand side cancel out with each other and the resultant relation would be:

\[ \frac{\partial \bar{\rho}}{\partial t} + \nabla. (\bar{\rho} \bar{U}) = 0 \] (3.28)

### 3.1.5 Momentum Conservation

The Favre averaged equation for the momentum transport in \( x \) direction is given by:

\[ \frac{\partial}{\partial t} (\bar{\rho} \bar{u}) + \nabla. (\bar{\rho} \bar{u} \bar{U}) + \nabla. (\bar{\rho} u'' U''') + \frac{\partial \bar{\rho}}{\partial x} \frac{\partial \bar{\tau}_{xx}}{\partial x} - \frac{\partial \bar{\tau}_{yy}}{\partial y} - \frac{\partial \bar{\tau}_{xz}}{\partial z} = \bar{\rho} g_x \] (3.29)

where, the vector \( U'' = u''i + v''j + w''k \). The specific body force vector \( g \) represents gravitational effects and often neglected in gaseous flow modelling. Expression given in the Eq. (3.12) may be Favre averaged to obtain a relation for viscous stresses. Usually, the viscous stress terms involving turbulent fluctuations are neglected based on the magnitude arguments. Thus, the resultant stress tensor remains in the same form as given by:

\[ \bar{\tau} = \mu \left[ \nabla \otimes \bar{U} + (\nabla \otimes \bar{U})^\dagger \right] - \frac{2}{3} \mu (\nabla \bar{U}) \] (3.30)
If the body forces are neglected, the closure of momentum equation only requires an expression for $\nabla \cdot (\rho \overline{u''u''})$ terms: often known as Reynolds stresses or turbulent stresses, as they dimensionally similar to the stresses. Estimation of the turbulent stress tensor is the central problem of turbulence modelling. Extensive research on this subject has resulted in several closure models known as turbulence closures. However, none of these models can be recognized as universal, as their performances are application dependent. A separate comprehensive discussion on the modelling of Reynolds stress terms is presented in Sec. 3.2.

### 3.1.6 Internal Energy Conservation

Favre averaged equation for the conservation of specific internal energy $\tilde{l}$, based on the first law of thermodynamics (exclusive of chemical energy), may be written in the form:

$$\frac{\partial}{\partial t} (\tilde{\rho} \tilde{l}) + \nabla \cdot (\tilde{\rho} \tilde{l} \tilde{U}) = -\nabla \cdot (\tilde{\rho} \tilde{l}''\tilde{U}'') - \tilde{p} \nabla \cdot \tilde{U} - (\tilde{p} \nabla \cdot \tilde{U}'') - \nabla \cdot \tilde{q} + (\nabla \otimes \tilde{U})^T : \tilde{\tau} + (\nabla \otimes \tilde{U}'') : \tilde{\sigma}'' + \dot{Q}_{LS}$$

(3.31)

The heat flux vector is composed of four main contributions: heat conduction, enthalpy diffusion, the Dufour effect and radiative heat flux. A heat flux is induced in the direction of species concentration due to the Dufour effect and may be assumed to be negligible in combustion processes compared to the other modes of heat transfer (Warnatz et al. 1996). Radiative heat transfer is also usually neglected in engine combustion simulations, although it can be significant in some combustion systems, as demonstrated by Malalasekera et al. (2002) and Henson & Malalasekera (2000). The adapted Favre averaged heat flux vector is given by:

$$\tilde{q} = -\mathcal{K} (\nabla \tilde{T}) - \tilde{p} (\tilde{D}_l + \tilde{D}_t) \sum_m h_m (\nabla \tilde{Y}_m)$$

(3.32)

where, $\mathcal{K}$ is the thermal conductivity of the reacting mixture defined by the relation:

$$\mathcal{K} = \frac{\mu C_p}{Pr_l}$$

(3.33)

$Pr_l$ is the laminar Prandtl number and $h_m$ is the specific enthalpy of the species $m$. The term $\mathcal{K} (\nabla \tilde{T})$, based on the Fourier’s law of conduction, corresponds to the heat flux by means of three dimensional conduction through the reacting medium. Heat flux caused by both laminar and turbulent diffusive mass transfer is taken care by the remaining term in Eq. (3.32). Note that, contributions from the fluctuating diffusivities and temperature gradients have been
neglected here. Moreover, the terms involving gradients in the fluctuating quantities of mass and enthalpy, arising due to Favre averaging are also neglected, assuming the magnitude is small compared to remaining terms. This assumption further leads to neglect the fluctuating viscous dissipation term \(( \nabla \otimes \mathbf{U''} ) : \mathbf{\sigma''} \) and the fluctuating pressure-velocity term \(( \overline{\rho \nabla \cdot \mathbf{U''}} ) \), where, \( \mathbf{\sigma''} \) is the fluctuating component of the viscous stress tensor. Chemical heat source term is modelled in combination with the mass source term of the species mass conservation in Eq. (3.19). The closure of the only remaining unknown correlation \(( \nabla \cdot \overline{\rho l'' \mathbf{U''}} ) \), is also normally based on the gradient flux approximation. Assuming the turbulent specific internal energy flux is proportional to the mean internal energy gradient:

\[
\nabla \cdot \left( \overline{\rho l'' \mathbf{U''}} \right) = -\nabla \cdot \left( \frac{\mu_t}{Pr_t} \nabla \overline{\mathbf{I}} \right) \tag{3.34}
\]

where, \( Pr_t \) is the turbulent Prandtl number.

### 3.1.7 State Relations

State relationships of thermodynamic variables in gas mixture are evaluated assuming ideal gas conditions. Following the Dolton’s law of partial pressure and universal gas law of ideal gases, the total pressure is calculated by summing up all the partial pressure contributions of each species as given below:

\[
\overline{p} = \overline{\rho R_u \overline{T}} \sum_{m} \left( \frac{\overline{Y_m}}{W_m} \right) \tag{3.35}
\]

\( R_u \) is the universal gas constant having the value 8.31447 \( (J mol^{-1} K^{-1}) \) and \( W_m \) \( (g mol^{-1}) \) is referred to the molecular weight of species \( m \).

Values for specific enthalpy of species \( m \) of reacting mixture at temperature \( \overline{T} \) are taken from JANAF tables of Stull & Phropert (1974). Specific enthalpies have been tabulated in JANAF tables at 100 \( K \) temperature intervals from absolute zero to 5000 \( K \) for each species. The values are linearly interpolated in order to obtain the specific enthalpy for an intermediate temperature within the range. It is expected that, the average temperature at any point inside the combusting mixture may always falls within the above limits. This is often valid for IC engine combusting flows, except during spark assisted ignition (see Chapter 4 for more details). The time span, in which the above extreme situations prevail, hardly exceeds few millisecond and alternative techniques with suitable simplifications are used to handle such excessively high temperatures.
Specific internal energy of species \( m \) is calculated using the following relation.

\[
I_m(\bar{T}) = h_m(\bar{T}) - \frac{R u \bar{T}}{W_m}
\]  (3.36)

Total internal energy of a species mixture is given by the summation of specific internal energies of all species:

\[
I(\bar{T}) = \sum_m \bar{y}_m I_m(\bar{T})
\]  (3.37)

Calculated specific internal energy values are then used to estimate the new temperature field \( \bar{T}(x, y, z) \) in the domain. Consequently, the values for constant volume specific heat capacity are obtained by the following relation.

\[
c_v(\bar{T}) = \frac{dI}{dT}
\]  (3.38)

Having calculated \( c_v \), the relation given by Eq. (3.39) is used to calculate the specific heat ratio \( \gamma \) and the constant pressure heat capacity \( c_p \).

\[
\gamma = \frac{c_p}{c_v} = 1 + \frac{\bar{p}}{\bar{\rho} c_v \bar{T}}
\]  (3.39)

### 3.2 Turbulence Model

The fundamental problem of turbulent modelling is finding a procedure to calculate Reynolds stresses. An exact transport equation of the following form for the Reynolds stress component \( \bar{\rho} u'' v'' \) may be derived (Jones & Whitelaw 1982):

\[
\frac{\partial}{\partial t}(\bar{u}'' \bar{v}'') + \bar{\rho} \bar{U} \cdot \nabla (\bar{u}'' \bar{v}'')
= -(\nabla \cdot \bar{\rho} u'' u'' \bar{U}'') - \bar{u}'' \frac{\partial \bar{\rho}}{\partial y} - \bar{v}'' \frac{\partial \bar{\rho}}{\partial x} + \left[ u'' \frac{\partial \bar{p}'}{\partial y} + v'' \frac{\partial \bar{p}'}{\partial x} \right]
- \bar{\rho} u'' (\bar{U} \cdot \nabla \bar{v}) - \bar{\rho} v'' (\bar{U} \cdot \nabla \bar{u}) - \bar{\rho} \varepsilon_{xy}
\]  (3.40)

Evaluation of these highly nonlinear terms requires various modelling assumptions. Several closure models are available with varying degree of complexity. Second moment closure models or generally known as Reynolds stress equation model (RSM) is the most complex and potentially the most general approach. Six different transport equations of the above form for each of the Reynolds stress component, together with an additional transport equation for
scalar dissipation have to be solved in this method. Consequently, the RSM model can grasp most of the turbulent characteristics compared to the other models, but the usage is limited due to considerable computational cost. A comprehensive review of second moment closure models may be found in Launder (1989).

The computational demand of RSM model can be reduced by approximating the Reynolds stresses by algebraic expressions. In practice, this procedure is called the Reynolds algebraic stress model (ASM). The usual practice is to iteratively solve the six linear equations for Reynolds stresses and two transport equations for turbulence kinetic energy $k$ and its rate of dissipation $\varepsilon$, which are two additional variables arise when modelling the Reynolds stresses. The alternative method proposed by Launder & Spalding (1974) uses the Boussinesq’s relation, which correlates the Reynolds stresses through a linear expression and solves two additional transport equations for $k$ and $\varepsilon$. In general, the standard $k - \varepsilon$ can perform consistently better than the ASM model in many applications (Versteeg & Malalasekera 2007). As a result, it is the most popular reactive flow modelling technique today. KIVA also employs the standard $k - \varepsilon$ model with modifications to account for volumetric expansions (Torres & Trujillo 2006). An optional RNG $k - \varepsilon$ model is also available, which can produce better results than standard $k - \varepsilon$ model in certain applications (Versteeg & Malalasekera 2007).

### 3.2.1 Selection of a Turbulence Model

Among the various other turbulence models, the standard $k - \varepsilon$ model was chosen for RANS based modelling of this study due to the following reasons.

- The $k - \varepsilon$ model has been used in numerous multidimensional studies in IC engine combustion and extensively validated against experimental data. Identified strengths and deficiencies have been well documented, so that a firm basis is available for further development.
- The existing $k - \varepsilon$ model in the present code can be modified with relatively less effort to accommodate the present requirements. Whereas, substantial modelling effort is essential to employ an advanced turbulence model. At the same time, it involves similar amount of work in validating the implementation.
- The additional modelling effort in using an alternative model does not guarantee the expected improvements in accuracy with respect to the operating/modelling conditions in the present test cases.
• Present developments in the combustion sub models are yet to be tested in RANS platform or to be investigated in the application of IC engine combustion. Therefore, the most appropriate method is to test them under a universally accepted standard turbulent implementation.

• Being a new code, $k - \varepsilon$ turbulence model of KIVA-4, has not yet been sufficiently validated with respect to its new unstructured mesh configuration. Hence, this study makes a basis for validating the performance of present $k - \varepsilon$ implementation in realistic engine configurations.

Therefore, in the following sections, the discussion has been limited to $k - \varepsilon$ turbulent model, which is the principal turbulence model used in this study.

### 3.2.2 Closure of the Reynolds Stresses

Reynolds stress closure of the standard $k - \varepsilon$ turbulence model requires adopting the Boussinesq relation with suitable generalisation for compressible flows. It assumes the same linear relationship between the stresses and strains as used in laminar viscous stress modelling, but uses a different proportionality constant $\mu_t$ called the eddy viscosity or turbulent viscosity. The Favre averaged Reynolds stress component due to the fluctuating velocity components $u''$ and $v''$ may be written as:

$$
-\rho u'' v'' = -\bar{\rho} u'' v'' = \mu_t \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right) - \frac{2}{3} \left[ \mu_t (\nabla \cdot \bar{U}) + \bar{\rho} k \right] \delta_{xy}
$$

(3.41)

The additional term in the right hand side is to recover the correct expression for turbulence kinetic energy $k$ defined as:

$$
k = \frac{1}{2} \left( u''^2 + v''^2 + w''^2 \right)
$$

(3.42)

In compact tensor notation, the mean Reynolds stress tensor $\bar{\tau}''$ is written in the form:

$$
\bar{\tau}'' = \mu_t \left[ (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^T \right] - \frac{2}{3} \left[ \mu_t (\nabla \cdot \bar{U}) + \bar{\rho} k \right] I
$$

(3.43)

Then the turbulent viscosity at each point in the flow field is defined by the relation:

$$
\mu_t = c_{\mu} \bar{\rho} \frac{k^2}{\varepsilon}
$$

(3.44)
where, $\varepsilon$ is the rate of dissipation of turbulence kinetic energy and $c_\mu$ is an empirical constant having the value 0.09. In the $k-\varepsilon$ turbulent model two separate transport equations are solved for turbulence kinetic energy and its rate of dissipation.

### 3.2.3 Transport of Turbulence Kinetic Energy

Derivation of an exact transport equation for turbulence kinetic energy involves a fair amount of algebra, but for brevity, a summarized procedure is presented here. Possible simplifying assumptions are also discussed where appropriate. It is possible to obtain an equation for the turbulence kinetic energy transport by considering the exact partial differential equation for Reynolds stresses. Summing up the resulting three equations for ($u''u''$), ($v''v''$) and ($w''w''$) together with some algebraic manipulations, the following model equation for $k$ is obtained.

\[
\frac{\partial}{\partial t} (\bar{\rho}k) + \nabla \cdot (\bar{\rho}k \bar{U}) = -\frac{1}{2} \nabla \cdot (\bar{\rho}k \bar{U}'') - U'' \cdot \nabla \bar{p} - \bar{\rho}u'' (U'' \cdot \nabla \bar{u}) - \bar{\rho}v'' (U'' \cdot \nabla \bar{v}) - \bar{\rho}w'' (U'' \cdot \nabla \bar{w}) - \bar{\rho} \varepsilon
\]

(3.45)

Expressions for the diffusion term, production term and the pressure work term are needed in order to close the above equation. Diffusion of fluctuating turbulence kinetic energy is commonly modelled using the gradient approximation.

\[
-\frac{1}{2} \nabla \cdot (\bar{\rho}k U'') = \nabla \left( \frac{\mu_{eff}}{S c_k} \nabla k \right)
\]

(3.46)

where, $S c_k$ is the equivalent Schmidt number for turbulence kinetic energy and $\mu_{eff}$ is the effective viscosity defined as the sum of the laminar and turbulent viscosities, which indeed provides the combined effect of laminar and turbulent transport.

The production terms of turbulence kinetic energy can be expanded in the following format:

\[
-\bar{\rho}u'' (U'' \cdot \nabla \bar{u}) = -\bar{\rho}u'' \left[ (u''i + v''j + w''k) \left( \frac{\partial \bar{u}}{\partial x} i + \frac{\partial \bar{u}}{\partial y} j + \frac{\partial \bar{u}}{\partial z} k \right) \right]
\]

(3.47)
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\[-\bar{\rho} u'' (\bar{U}'', \nabla \bar{u}) = -\left( \bar{\rho} \bar{u}'' u'' \right) \frac{\partial \bar{u}}{\partial x} - \left( \bar{\rho} \bar{u}'' v'' \right) \frac{\partial \bar{u}}{\partial y} - \left( \bar{\rho} \bar{u}'' w'' \right) \frac{\partial \bar{u}}{\partial z} \tag{3.48} \]

The other production terms are also rearranged in the same way. It is interesting to see that the terms within brackets in the right hand side of the Eq. (3.48) represent the Reynolds stresses. Those terms may be closed by substituting the relation given in Eq.(3.43). Finally, the pressure work term is also neglected upon magnitude arguments leading to the following simplified form.

\[ \frac{\partial}{\partial t}(\bar{\rho} k) + \nabla \cdot (\bar{\rho} k \bar{U}) = \nabla \cdot \left( \frac{\mu_{eff}}{Sc} \nabla k \right) + \tau : (\nabla \bar{U}) - \frac{2}{3} \bar{\rho} k \nabla \cdot \bar{U} - \bar{\rho} \varepsilon + \dot{W}^{spary} \tag{3.49} \]

The additional source term \( \dot{W}^{spary} \) is to represent the change in turbulence kinetic energy due to the injecting fuel spray. Since the present attention is limited to premixed combustion the source term \( \dot{W}^{spary} \) is set to zero.

### 3.2.4 Transport of Dissipation Rate of Turbulence Kinetic Energy

An exact transport equation for the rate of dissipation of turbulence kinetic energy: \( \varepsilon \), can be derived starting from the fundamental conservation equations, but it is exceedingly difficult to find a closure without rigorous assumptions. In the interest of brevity, only the final model equation is presented here. Alternatively, a model form for the \( \varepsilon \) equation may be devised from dimensional analysis, intuition and analogy, such that it is expected to contain similar terms to the \( k \) equation (Henson 1998). Therefore, the final form of the transport equation for the rate of dissipation of turbulence kinetic energy would be:

\[ \frac{\partial}{\partial t}(\bar{\rho} \varepsilon) + \nabla \cdot (\bar{\rho} \varepsilon \bar{U}) \]

\[ = \nabla \cdot \left( \frac{\mu_{eff}}{Sc} \nabla \varepsilon \right) + \frac{\varepsilon}{k} \left[ c_{\varepsilon_1} \tau : (\nabla \bar{U}) - c_{\varepsilon_2} \bar{\rho} \varepsilon + c_s \dot{W}^{spary} \right] \tag{3.50} \]

\[ - \left( \frac{2}{3} c_{\varepsilon_1} - c_{\varepsilon_2} \right) \bar{\rho} \varepsilon \nabla \cdot \bar{U} \]

where, \( Sc \) is the equivalent Schmidt number for \( \varepsilon \) and \( c_{\varepsilon_1}, c_{\varepsilon_2} \) and \( c_s \) are additional model constants to be found through experimental comparison. Extensive studies carried out using the above model equations for thin shear layer and recirculating flows in various applications have suggested the values given in Table 3.1 for the above model constants (Amsden et al. 1989).
Despite of the pronounced popularity, there are some well-known deficiencies of the standard $k - \varepsilon$ model, which may hinder the reliability of predictions.

- Closure of the $k - \varepsilon$ model implicitly assumes homogeneous isotropic turbulence at high Reynolds numbers (Poinsot & Veynante 2005). Hence, the present formulation is inadequate to describe complex non-linear stress strain interactions driven by largely anisotropic turbulent flows.
- Poor predictions have been recorded in cases, where extra strains involve such as curved boundary layers and swirling flows (Versteeg & Malalasekera 2007).
- As a result of wall shear stresses, a steep gradient in the velocity field is induced making the on-wall velocity nearly zero. Thus, in general, the local Reynolds numbers are minimal near solid boundaries. Standard $k - \varepsilon$ model originally derived for high Reynolds number flows performs poor in such circumstances.
- Due to the near-wall steep gradient of flow properties, a massively fine spatial grid resolution is required if the flow field is to be adequately resolved through a turbulence model. This procedure is highly impractical for an engine like application as it unduly increases the total cell count beyond the capable limits of current computing. Thus, as a compromise, algebraic wall models should be used.

Besides, development of turbulent models is out of the focus of the present study. Therefore, based on the high Reynolds number assumption, the conventional $k - \varepsilon$ model combined with simplified wall layer models is employed in this work.

### 3.2.5 Further Refinements in Model Equations

Favre averaged equations are updated using the modifications suggested in the previous sections to suite premixed SI engine combustion simulations and rewritten here for completeness with some rearrangements.

#### Species Mass Conservation

\[
\frac{\partial}{\partial t}(\bar{\rho}\bar{Y}_m) + \nabla.(\bar{\rho}\bar{Y}_m \bar{U}) - \nabla.(\bar{\rho} \frac{\mu_t}{Sc_t} \nabla \bar{Y}_m) - \nabla.(\bar{\rho} \frac{\mu}{Sc_l} \nabla \bar{Y}_m) = \bar{\omega}_{m,chem} \tag{3.51}
\]

Often, the laminar diffusive fluxes: $\bar{\rho}D_l \nabla \bar{Y}_m$, are small in magnitude compared to the turbulent fluxes: $\bar{\rho}D_t \nabla \bar{Y}_m$, at sufficiently high Reynolds numbers. Hence, the molecular diffusive terms are usually neglected or roughly approximated. It is possible to retain the effects of molecular diffusion by using the effective viscosity concept used earlier in Eq.
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(3.46). The laminar and the turbulent diffusive fluxes are combined together via an effective turbulent viscosity defined by the relation:

\[
\nabla \left( \bar{\rho} \frac{\mu_t}{Sc_t} \nabla \bar{Y}_m \right) + \nabla \left( \bar{\rho} \frac{\mu}{Sc_t} \nabla \bar{Y}_m \right) = \nabla \left( \bar{\rho} \frac{\mu_{eff}}{Sc} \nabla \bar{Y}_m \right)
\]

(3.52)

Laminar and turbulent Schmidt numbers may have different values and vary depending on the application, but for the simplicity, a single value equal to 0.9 is assumed. Therefore, the final form of the species mass conservation is given by:

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{u}) - \nabla \cdot (\bar{\rho} \frac{\mu_{eff}}{Sc} \nabla \bar{Y}_m) = \bar{\omega}_{m,chem}
\]

(3.53)

**Momentum Conservation**

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{u}) + \nabla \cdot (\bar{\rho} \bar{u} \bar{U}) - \nabla \cdot \bar{\tau} = \frac{\partial \bar{p}}{\partial x} - \frac{\partial P_{xx}}{\partial x} - \frac{\partial P_{yx}}{\partial y} - \frac{\partial P_{zx}}{\partial z} = \bar{\rho} \bar{g}_x
\]

(3.54)

\[
\bar{\tau} = \mu \left( (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^\top \right) - \frac{2}{3} \mu (\nabla \cdot \bar{U}) \mathbb{I}
\]

(3.55)

\[
\bar{\tau}'' = \mu_t \left( (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^\top \right) - \frac{2}{3} \left[ \mu_t (\nabla \cdot \bar{U}) + \bar{\rho} \bar{k} \right] \mathbb{I}
\]

(3.56)

It is evident from the Eq. (3.55) and Eq. (3.56) that both turbulent and viscous stress tensors have the similar format, except the turbulence kinetic energy term in Eq. (3.56). If the effect of that particular term is considered explicitly, an effective stress tensor may be defined:

\[
\bar{\tau}_{eff} = \mu_{eff} \left( (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^\top \right) - \frac{2}{3} \left( \nabla \cdot \bar{U} \right) \mathbb{I}
\]

(3.57)

Thus, the combined momentum equation in three dimension is given as:

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{U}) + \nabla \cdot (\bar{\rho} \bar{U} \bar{U}) = -\nabla \bar{p} - \nabla \left( \frac{2}{3} \bar{\rho} \bar{k} \right) + \nabla \cdot \bar{\tau}_{eff} + \bar{\rho} \bar{g}
\]

(3.58)

where, \( \circ \) denotes the tensor dot product.

**Specific Internal Energy**

\[
\frac{\partial}{\partial t} (\bar{\rho} \tilde{I}) + \nabla \cdot (\bar{\rho} \tilde{I} \bar{U}) = -\left( \nabla \cdot (\bar{\rho} \tilde{I}'''' \bar{U}'''') \right) - \bar{p} \nabla \cdot \bar{U} - \nabla \cdot \bar{q} + \left( \nabla \otimes \bar{U} \right)^\top \cdot \bar{\tau} + \bar{Q}_{ls}
\]

(3.59)
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\[-(\nabla, \bar{\rho} U'' U'') = \nabla \left( \frac{\mu_t}{P_{rt}} \nabla \bar{I} \right) = \nabla \left( \frac{\mu_t c_p}{P_{rt}} \nabla \bar{T} \right) \tag{3.60}\]

\[\bar{q} = -\mathcal{K} (\nabla \bar{T}) - \left( \frac{\mu_{eff}}{Sc} \right) \sum_{m} \bar{h}_m \left( \nabla \bar{Y}_m \right) \tag{3.61}\]

The gradient flux approximation assumes that, the internal energy flux arising from turbulent convection is proportional to the internal energy gradient. However, for ideal gases, the specific energy gradient may be equal to the temperature gradient in the reactive mixture as shown in Eq. (3.60). As ideal gas conditions have already been assumed in the present study, the same approximation is employed. Further, the Eq. (3.60) and (3.61) can be combined by defining the effective conductivity, such that:

\[\mathcal{K}_{eff} = \mathcal{K} + \frac{\mu_t c_p}{P_{rt}} = \frac{\mu_{eff} c_p}{P_{rt}} \tag{3.62}\]

\[\bar{q}_{eff} = -\mathcal{K}_{eff} (\nabla \bar{T}) - \left( \frac{\mu_{eff}}{Sc} \right) \sum_{m} \bar{h}_m \left( \nabla \bar{Y}_m \right) \tag{3.63}\]

Accordingly, suitable approximations have now been stated for all the unknown turbulence correlations. However, further analysis of the transport equations for specific internal energy and turbulence kinetic energy in their present form exposes that, both contain source contributions from the viscous stresses. In physical point of view, this indicates a production of internal energy in both equations. To be consistent with the concept of turbulence kinetic energy dissipation, the viscous stress source term is substituted by \(\bar{\rho} \varepsilon\) assuming, turbulence kinetic energy is produced by viscous stresses and later dissipated into internal energy. Thus the final simplified form of the internal energy equation is:

\[\frac{\partial}{\partial t} (\bar{\rho} I) + \nabla \cdot \bar{\rho} \bar{U} \bar{U} = -\bar{p} \nabla \bar{U} - \nabla \cdot \bar{q}_{eff} + \bar{\rho} \varepsilon + \dot{\bar{Q}}_{l,chem} \tag{3.64}\]

3.2.6 The Working Set of Equations

Favre averaging with suitable approximations and rearrangements yields a largely simplified version of turbulent Navier-Stokes equations. Symbolically, they are identical to the laminar form, but can be distinguished by the magnitudes of transport coefficients, which are much large for turbulent flows compared to laminar counterparts. For the completeness, all the equations in their final form are presented here with the values of constants used in the present study. Note that, only the source terms relevant to premixed SI engine combustion are presented here.
Species Mass Conservation
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{U}) - \nabla \cdot \left( \bar{\rho} \frac{\mu_{eff}}{S_c} \nabla \bar{Y}_m \right) = \bar{\omega}_{m,chem}
\] (3.65)

Global Mass Conservation
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{u}) = 0
\] (3.66)

Momentum Conservation
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{U}) + \nabla \cdot (\bar{\rho} \bar{U} \bar{U}) + \nabla \bar{p} + \nabla \left( \frac{2}{3} \bar{\rho} \bar{k} \right) - \nabla \cdot \bar{\tau}_{eff} = 0
\] (3.67)

Specific Internal Energy Conservation
\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{T}) + \nabla \cdot (\bar{p} \bar{U} \bar{U}) + \nabla \bar{q}_{eff} - \bar{\rho} \bar{\varepsilon} = \dot{\bar{Q}}_{l,chem}
\] (3.68)

\( k - \varepsilon \) Model Equations
\[
\frac{\partial}{\partial t} (\bar{\rho} k) + \nabla \cdot (\bar{\rho} k \bar{U}) = \nabla \cdot \left( \frac{\mu_{eff}}{S_{c_k}} \nabla k \right) + \tau_{eff} : (\nabla \bar{U}) - \frac{2}{3} \bar{\rho} k \nabla \cdot \bar{U} - \bar{\rho} \bar{\varepsilon}
\] (3.69)
\[
\frac{\partial}{\partial t} (\bar{\rho} \varepsilon) + \nabla \cdot (\bar{\rho} \varepsilon \bar{U}) = \nabla \cdot \left( \frac{\mu_{eff}}{S_{c_\varepsilon}} \nabla \varepsilon \right) + \frac{\varepsilon}{k} \left[ c_{e_1} \tau_{eff} : (\nabla \bar{U}) - c_{e_2} \bar{\rho} \varepsilon \right] - \frac{2}{3} \left( c_{e_1} - c_{e_3} \right) \bar{\rho} \varepsilon \nabla \cdot \bar{U}
\] (3.70)

where, the effective stress tensor and the effective heat flux vector:
\[
\bar{\tau}_{eff} = \mu_{eff} \left[ (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^T - \frac{2}{3} (\nabla \cdot \bar{U}) I \right]
\] (3.71)
\[
\bar{q}_{eff} = -k_{eff} (\nabla \bar{T}) - \left( \frac{\mu_{eff}}{S_{c_t}} \right) \sum_m \bar{r}_m (\nabla \bar{Y}_m)
\] (3.72)

with effective transport coefficients defined by:
\[
\mu_{eff} = A_1 \bar{T}^{3/2} \frac{k^2}{\bar{T} + A_2} + c_{\mu} \bar{\rho} \frac{k^2}{\varepsilon}
\] (3.73)
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\[ \mathcal{K}_{eff} = \frac{\mu_{eff} c_p}{Pr_t} \]  \hspace{1cm} (3.74)

Table 3.1: Model constants of the standard \( k - \varepsilon \) turbulence model

<table>
<thead>
<tr>
<th>( c_\mu )</th>
<th>( c_{\varepsilon 1} )</th>
<th>( c_{\varepsilon 2} )</th>
<th>( c_{\varepsilon 3} )</th>
<th>( Sc_k )</th>
<th>( Sc_\varepsilon )</th>
<th>( Sc_\tau )</th>
<th>( Pr_t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.44</td>
<td>1.92</td>
<td>-1.0</td>
<td>1.0</td>
<td>1.3</td>
<td>0.9</td>
<td>0.9</td>
</tr>
</tbody>
</table>

### 3.3 Boundary Conditions

The flow inside an engine is entirely wall bounded, except at port openings, where mass exchange processes with the surrounding take place. The walls may be stationary, such as cylinder walls and head or may be moving in the case of valve faces or piston face. In such boundaries, special conditions have to be imposed into the governing equations to correctly compute the flow field. These conditions may either be based on physical considerations or due to numerical reasons. In this section, the measures taken to incorporate these boundary effects into the governing equations are described.

#### 3.3.1 Modelling Near Wall Turbulence

Presence of the wall friction creates a boundary layer on a solid surface, making a characteristic steep gradient in flow properties. Resolving the boundary layer gradient for adequate details with a complete set of transport equation is unaffordable due to enormous spatial discretisation requirement. Thus, for the economy and convenience, wall functions: one dimensional analytical solutions of largely simplified governing equations, are solved to approximate the boundary layer behaviour. However, the validity of the wall functions in practice is highly questionable. Usually, they are derived based on the flow characteristics over a flat plate, assuming quasi steady flow at high Reynolds number with no chemical reactions in the gas or wall surface. In particular, the flow inside engine combustion chamber is highly irregular and, may have several moving stagnation points (Henson 1998). Mostly, a larger area of the chamber walls are also curved and cornered. Hence, the in-cylinder boundary layer flow is essentially expected to differ from the flat plate behaviour. Nevertheless, these simplified relations are still used due to the lack of a better alternative approach (Heywood 1988). Procedures described by Amsden \textit{et al.} (1989) and Amsden (1997) are used in the present study in boundary layer mass and heat transfer calculations.
3.3.2 Boundary Layer Velocity Field

Velocity boundary conditions on grid walls are introduced in two forms: the value of flow velocity is modified according to the wall velocity and the stress tensor is updated with the explicitly calculated wall stresses. Note that, Favre and time averaged notations (tilde and over-bar) have been omitted hereafter for notational convenience. Unless otherwise stated, all state variables denote corresponding mean flow properties. The wall normal flow velocity is set to be equal to the wall velocity given by:

\[
U \cdot \mathbf{n} = U_w \cdot \mathbf{n}
\]  

(3.75)

where, \( \mathbf{n} \) is the unit wall normal vector. Consequently, the flow velocity normal to a stationary wall becomes zero, whereas it is equal to the wall velocity at moving walls. The effect of wall boundaries on other two velocity components, which are tangential to the wall, is included via wall shear stresses. The local wall Reynolds number \( \zeta \), defined at a distance \( y \) from the wall is given by:

\[
\zeta = \frac{\rho \nu y}{\mu_l}
\]  

(3.76)

\[
\nu = U - U_w
\]  

(3.77)

The velocity \( \nu \) is the relative flow field velocity with respect to the wall, where the wall velocity is moving at velocity of \( U_w \).

However, the law of the wall is applied only for the first cell layer adjacent to the wall. Hence, the \( y \) value corresponds to the distance measured from the wall to the opposite face of the wall cell. The flow velocity and the shear speed \( u^* \) are correlated as follows.

\[
\frac{|\nu|}{u^*} = \begin{cases}
\frac{1}{\kappa} \ln \left( c_{lw} \zeta^{7/8} \right) + B, & \zeta > \zeta_c \\
\zeta^{1/2}, & \zeta \leq \zeta_c
\end{cases}
\]  

(3.78)

Constants \( B = 5.5, c_{lw} = 0.15, \kappa = 0.4327 \) and are given the standard values. The critical wall Reynolds number is taken to be \( \zeta_c = 114 \) and it separates the viscous sublayer and the logarithmic layer of the boundary region. It is implicitly assumed that \( y \) is small enough to be in one of the prescribed regions. Accordingly, tangential components of the wall stresses are computed from the expression below.

\[
\tau_w - (\tau_w \cdot \mathbf{n}) \mathbf{n} = \rho (u^*)^2 \frac{\nu}{|\nu|}
\]  

(3.79)
3.3.3 Temperature Boundary Conditions

Imposing boundary conditions for the enthalpy equation requires calculation of wall heat flux at the boundary layer. The following relations were used to estimate heat loss at solid walls $Q_{wall}$, following Launder & Spalding (1974).

$$ Q_{wall} = \frac{\mu_{air}c_pF}{Pr_l y} (T - T_w) \quad (3.80) $$

where, $T_w$ is the constant wall temperature and $Pr_l$ is the laminar Prandtl number. The function $F$ is given by:

$$ F = \begin{cases} \frac{\zeta' Pr_l/Pr_t}{1/k \ln(\zeta')} + B + 11.05\left(Pr_l/Pr_t - 1\right), & \zeta' < \zeta_c' \\ 1.0, & \zeta' \geq \zeta_c' \end{cases} \quad (3.81) $$

$$ \zeta' = \frac{\rho c_p 1/4 k^{1/2} y}{\mu_{air}} \quad (3.82) $$

The characteristic temperature Reynolds number $\zeta'$ at a wall cell is defined in terms of the turbulence kinetic energy at a distance $y$ from the wall. The critical value for the temperature Reynolds number $\zeta_c'$ is found to be 11.05. Typically, a value of 0.74 is assigned for laminar Prandtl number in engine applications (Amsden et al. 1989).

Certain amount of energy is dissipated as heat at wall boundary attributable to the wall friction. This loss is added to the internal energy equation as a sink term given by the following equation.

$$ f_{wall} = \tau_w \cdot v \quad (3.83) $$

$f_{wall}$ is the heating rate per unit area of wall.

3.3.4 $k - \epsilon$ Boundary Conditions

In calculating turbulent flow near walls, boundary conditions are required to solve $k - \epsilon$ equations. Generally, these conditions depend upon the wall Reynolds number but, the following simplified conditions are used assuming local equilibrium of production and dissipation of turbulence kinetic energy.
Diffusive kinetic energy fluxes are set to zero in the wall normal direction at wall cell, based on physical reasoning.

\[ \nabla k \cdot \mathbf{n} = 0 \]  \hspace{1cm} (3.84)

The dissipation of the turbulence kinetic energy at wall is explicitly computed from the following algebraic relation (Amsden et al. 1989).

\[ \varepsilon = \frac{c_{\mu}^{3/4} \kappa^{3/2}}{\kappa \gamma} \]  \hspace{1cm} (3.85)

### 3.3.5 Open Boundaries

Simulation of an open system requires specifying flow properties at the interface to the atmosphere. Two types of boundary conditions: pressure in/outflow and velocity in/outflow, could be used for this purpose. The choice of a suitable open boundary condition is problem dependent. For example, pressure boundaries may be used in engine intake flow calculations, whereas, a velocity inlet boundary may be used at the inlet of a steady flow problem.

#### Intake and Exhaust Ports

Conditions at the intake and exhaust port openings must be prescribed in engine applications. The best method is to simulate the entire breathing systems including pipes, manifolds and plenums up to the opening to the atmosphere. However, this requires massively parallel computer codes running in high-performance computing clusters. (see Granet et al. (2012) for example). A low cost alternative is to simulate only the port sections by imposing a prescribed pressure value: \( p_{amb} \), at the opening. \( p_{amb} \) may either be a mean cycle averaged value or a crank resolved time varying profile. A measured port pressure signal or the pressure obtained through one dimensional system analysis can also be used for this purpose. Alternatively, it can be assumed that the port is connected to a large plenum at constant pressure. In each of these cases \( p_{amb} \) may have to be adjusted in order to obtain the desired mass flow rate.

#### Inflow and Outflow Boundaries

In non-engine applications, such as channel flow problems, a prescribed inflow velocity may be used as the inflow condition. Note that, the inflow velocity is assumed to be normal to the boundary plane. Outlet can be defined as a pressure boundary, where \( p_{amb} \) acts at a distance \( x \) outside the boundary. In this case, the pressure of the boundary cells is calculated by linear interpolation (Amsden et al. 1989):
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\[ p = \frac{x \cdot p_{amb} + y \cdot p_0}{x + y} \]  

(3.86)

where, \( p_0 \) is the pressure of the computational cell at the start of the current iteration, of which the cell centre is located \( y \) distance away from the boundary. Setting \( x = 0 \) leads the pressure of the boundary cell layer to become \( p_{amb} \). However, it is not recommended as it perfectly reflects acoustic waves in subsonic flow calculations, such that unrealistically large pressure fluctuation may be induced in upstream flow. A large reduction of acoustic wave reflection can be achieved by setting \( x \) equals to the characteristic size of the computational mesh. For example, \( x \) may be taken as the length of the channel in a channel flow problem. In addition, for all situations, it is required to specify the turbulent length scale and turbulence kinetic energy at the boundary, so that \( k - \varepsilon \) equations are properly defined.

3.4 Numerical Scheme

The finite volume approximations of the governing equation were solved using the Arbitrary Lagrangian and Eularian (ALE) method (Hirt et al. 1974). This is a largely conservative scheme with sufficient flexibility to deal with moving and deforming meshes. Flow variables were resolved the in a staggered grid formulation. All the variables, except velocity, are located in cell centres, whilst the velocity is on cell nodes. Governing equations discretized in integral form, are solved in there different stages: A, B and C. The first two phases are computed using Lagrangian methods, assuming that the computational cell faces are moving with the fluid flow. Particularly in phase A, the influence of fuel spray and chemical reactions, which appear in the form of source terms in governing equations are explicitly computed. Then in stage B, the diffusion terms are computed using a semi implicit method. Stage C: the rezoning phase, solves advection terms using an Eularian method. Historical development of the numerical scheme of KIVA code and related references can be found in Amsden et al. (1989), Amsden (1993, 1997) and Torres & Trujillo (2006). A brief description of the present numerical scheme is provided here to facilitate upcoming discussions.

3.4.1 Integral Form of Governing Equations

Recast below in their integral form are the governing equations detailed in section 3.2. Solution procedure is based on the discretized version of these equations. Note that, these equations have been rearranged into non-conservative form (Anderson 2009), where advection terms are embedded in to the substantial derivative. In addition, several volume integrals of the gradient terms have been converted in to surface integrals using the Gauss Divergence theorem.
Species Mass

$$\frac{D}{Dt} \int_V \rho Y_m \, dV = \int_S \left( \rho \frac{\mu_{\text{eff}}}{Sc} \nabla Y_m \right) \, dA + \int_V \dot{w}_{m,\text{chem}} \, dV$$  \hspace{1cm} (3.87)

Global Mass

$$\frac{D}{Dt} \int_V \rho \, dV = 0$$  \hspace{1cm} (3.88)

Momentum

$$\frac{D}{Dt} \int_V \rho U \, dV = -\int_S \left( p + \frac{2}{3} \rho k \right) \, dA + \int_S \tau_{\text{eff}} \cdot \mathbf{A} \, dA$$  \hspace{1cm} (3.89)

Specific Internal Energy

$$\frac{D}{Dt} \int_V \rho l \, dV = -\int_V p \nabla \cdot \mathbf{U} \, dV - \int_S q_{\text{eff}} \, dA + \int_V \rho \varepsilon \, dV + \int_V \dot{Q}_{l,\text{chem}} \, dV$$  \hspace{1cm} (3.90)

$k - \varepsilon$ Model Equations

$$\frac{D}{Dt} \int_V \rho k \, dV = \int_S \left( \frac{\mu_{\text{eff}}}{Sc} \nabla k \right) \, dA + \int_V \left[ \tau_{\text{eff}} \cdot (\nabla \cdot \mathbf{U}) \right] \, dV - \int_V \left( \frac{2}{3} \rho k \nabla \cdot \mathbf{U} \right) \, dV$$  \hspace{1cm} (3.91)

$$\frac{D}{Dt} \int_V \rho \varepsilon \, dV = \int_S \left( \frac{\mu_{\text{eff}}}{Sc} \nabla \varepsilon \right) \, dA + \int_V \frac{\varepsilon}{k} \left[ c_{\varepsilon_1} \tau_{\text{eff}} \cdot (\nabla \cdot \mathbf{U}) - c_{\varepsilon_2} \rho \varepsilon \right] \, dV$$  \hspace{1cm} (3.92)

$\mathbf{A}$ denotes the surface area vector and $S$ is the closed surface area, on which the integral is performed. In practice, for a hexahedral computational element $S$ is the area bounded by the six cell faces. $\mathbf{A}$ is defined for a given cell face as:

$$\mathbf{A} = A_x i + A_y j + A_z k$$  \hspace{1cm} (3.93)

where, $A_x$, $A_y$ and $A_z$ are the projected areas of the cell surface in $yz$, $xz$ and $xy$ planes respectively.
3.4.2 Lagrangian Phase Discretization

The Lagrangian phase comprises of two stages: stage A and B. Transport equations arranged in non-conservative form are discretized and solved in this stage. The discretization process presumes that the thermodynamic properties are uniformly distributed within the cell. As already noted, the Lagrangian description considers that the cell faces are moving with the flow velocity, such that no advection occurs. Hence, the advection terms automatically become zero for this stage. The temporal discretization scheme is first order accurate and the spatial discretisation scheme is second order accurate. A brief overview of the discretized equations is provided in this section. A comprehensive discussion can be found in Torres & Trujillo (2006).

Species Mass

The stage A species equations are discretized as given in Eq. (3.94) using the control volume approach. In the present staggered grid formulation, scalar variables are located in cell centres. Hence, the volume enclosed by the computational cell is taken as the control volume for scalars. The super scripts n and A denote the conditions at the beginning and at the end of the stage A respectively. The duration of the current global time step is symbolized by $\Delta t$ and $M$ is the mass of the control volume.

\[
\frac{Y_m^A - Y_m^n}{\Delta t} = \bar{\omega}_{m,\text{chem}}
\]  

(3.94)

Values of all the source terms are explicitly computed in stage A and equations are updated before moving to stage B. The discretized species equation for stage B can be given by:

\[
M^B \frac{Y_m^B - Y_m^A}{\Delta t} = \sum_f \left( \frac{\mu_{eff}}{Sc} \right)^n \nabla[\phi_D Y_m^B + (1 - \phi_D)Y_m^A] \cdot A_f^n
\]  

(3.95)

Conditions at the end of the stage B are designated by superscript $B$. The summation $f$ in the right hand side is over all the faces of the computational cell. The variable implicitness parameter $\phi_D$ has been introduced in order to control the degree of implicitness of the solution. A fully explicit solution may be obtained by setting it to zero, while the solution will be fully implicit if it is set to 1.0. The explicit solution is less accurate for a given number of iterations, but less time consuming and might become unstable. Implicit solution is unconditionally stable and higher in accuracy, but computationally demanding as an iterative solution procedure is required. However, a semi implicit solution can be obtained by setting $\phi_D$ to an intermediate value, so that a sufficient accuracy and stability with a reasonable
computational time is obtained. The estimation of $\phi_D$ is based on the diffusion Courant number $C_D$ given by:

$$C_D = \frac{\mu_{eff}}{\rho} \frac{\Delta t}{\Delta x^2}$$  \hspace{1cm} (3.96)

The derivation of an expression for $\phi_D$ needs a lengthy discussion; hence, omitted from this report. Relevant procedures can be found in Amsden et al. (1989).

**Specific internal Energy**

Specific internal energy equation is also discretized in a similar format. The same variable implicitness parameter is used for both temperature and mass diffusion. In general, the only source term is due to chemical reactions. However, wall heat dissipation terms have also to be considered for near wall cells.

$$\frac{(MI)^A - (MI)^n}{\Delta t} = \dot{Q}_{chem} V^n$$  \hspace{1cm} (3.97)

$$M^B \frac{I^B - I^A}{\Delta t} = M^B \varepsilon^A - \left( \frac{p^B + p^n}{2} \cdot \frac{V^B - V^n}{\Delta t} \right)$$

$$+ \sum_f \kappa_{eff} \nabla [\phi_D T^B + (1 - \phi_D) T^A] \cdot A^n_f$$  \hspace{1cm} (3.98)

$$- \sum_m \left[ \sum_f \left( \frac{\mu_{eff}}{Sc} \right) h_m \nabla [\phi_D Y^B_m + (1 - \phi_D) Y^A_m] \cdot A^n_f \right]$$

**Momentum**

The distribution of the velocity field is computed by solving the momentum equation. In the present staggered grid formulation, velocity is placed on cell vertices. Hence, the employed control volume is formed out of several cell portions, which share the particular vertex. In an unstructured grid, the number of cell portions differs upon the number of attached cells to that vertex. For instance, there are 8 cell portions in a vertex control volume in a structured hexahedron grid. Each cell contributes with a one eighth of its volume to form the momentum control volume. In addition, these eight portions make 24 momentum cell face segments. Therefore, the integration surface of the momentum equation should be on all the face segments.
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\[ \frac{M_B^v U^B - M_B^v U^n}{\Delta t} = - \sum_c \sum_{\beta_c} \left\{ \left[ \phi_p p^p + (1 - \phi_p) p^n \right] + \frac{2}{3} \rho_A^A k^A \right\} A_{\beta_c}^n \]

\[ + \sum_c \sum_{\beta_c} \left[ \phi_D \tau_{eff}^B + (1 - \phi_D) \tau_{eff}^A \right] o A_{\beta_c}^n \]  

(3.99)

Note that, the density here corresponds to the averaged density over all the connected cell portions. Summation \( \beta_c \) is over all the face segments of the given cell \( c \). The variable implicitness parameter for pressure is given by \( \phi_p \). It performs a similar role as \( \phi_D \), but determined as a function of sound speed courant number \( C_s = \frac{C \Delta t}{\Delta x} \). The isentropic speed of sound is denoted by \( C \). Solution of the momentum equation is coupled with a separate pressure solver. Therefore, during the iteration process the pressure \( p^P \) is updated appropriately. In the absence of fuel spray, conditions of the momentum equation do not change during the phase A. For non-premixed combustion with fuel spray, momentum change due to droplet motion has to be separately accounted for as a phase A source term.

**k – \( \varepsilon \) Equations**

\[ \frac{M_B^B k^B - M_A^A k^A}{\Delta t} = - \frac{2}{3} \rho_B^B \left[ \frac{V^B - V^n}{\Delta t} \right] \left[ (1 - V) k^n + U k^B \right] \]

\[ + V^n \left\{ \phi_D \tau_{eff} : (\nabla U) \right\}^B + (1 - \phi_D) \left\{ \tau_{eff} : (\nabla U) \right\}^A \]  

(3.100)

\[ + \sum_f \mu_{eff} \nabla \left[ \phi_D k^B + (1 - \phi_D) k^A \right] \cdot A_f^n - M_B^B \frac{\varepsilon^n}{k^n} k^B \]

The factor \( U \) is taken to be 1, when \( V^B > V^n \), otherwise zero. Similarly, the turbulent dissipation rate equation can be discretized as follows.
\[
\frac{M^B \varepsilon^B - M^A \varepsilon^A}{\Delta t} = -\left(\frac{2}{3}c_{\varepsilon_1} - c_{\varepsilon_3}\right) \rho^B \frac{V^B - V^n}{\Delta t} [(1 - \gamma)\varepsilon^n + \varepsilon \varepsilon^B] \\
+ c_{\varepsilon_1} \varepsilon^n V^n \left\{ \phi_B [\tau_{eff} : (\nabla, U)]^B + (1 - \phi_B) [\tau_{eff} : (\nabla, U)]^A \right\} \\
+ \sum_f \frac{\mu_{eff}}{S_{\varepsilon}} \nabla \left[ \phi_B \varepsilon^B + (1 - \phi_B) \varepsilon^A \right] \cdot \mathbf{A}_f^B - c_{\varepsilon_2} M^B \frac{\varepsilon^n}{k n} \varepsilon^B
\]

Source terms arising from spray become zero for premixed combustion. Hence, phase A calculations are omitted. If fuel injection is present, change in turbulence kinetic energy and the dissipation rate should be considered with appropriate source terms.

During the Lagrangian phase, the cell faces are assumed to move with fluid, so that \( V^B \) is different from its initial volume \( V^n \) at the start of the time step. \( V^B \) can be computed from the ideal gas relations given by:

\[
V^B = \frac{M^B}{p^B} RT^B
\]

or according to Lagrangian approximation, assuming the final volume: \( V^{LAG} \), is equal to the initial volume plus the displacement of cell faces.

\[
V^{LAG} = V^n + \Delta t \sum_f (U \cdot \mathbf{A}_f)^B
\]

Hence, \( p^B \) can be estimated by equating the two volumes \( V^{LAG} \) and \( V^B \). However, the estimated pressure values affects the internal energy equation so as the temperature \( T^B \). Therefore, the pressure estimation has to be iteratively accomplished until a sufficient tolerance is reached.

### 3.5 Solution Algorithm

The coupled set of equations: Eq. (3.94) – (3.99), for mass, energy, pressure and the velocity fields are then iteratively solved using the conjugate residual method (O’Rourke & Amsden 1986) following semi-implicit pressure linked equations (SIMPLE) algorithm (Patankar & Spalding 1972). Once a predefined level of convergence is achieved the \( k - \varepsilon \) equations: Eq.(1.100) and (1.101), are solved. At the end of the convergence of \( k - \varepsilon \) iterations, transition to the phase C occurs.
In stage C, the cell faces displaced from their original location during the Lagrangian phase, are rezoned back to a predefined computational mesh at the next global time step. In a stationary domain problem, the mesh is moved back to the original mesh configuration and in engines the new mesh points may be defined by the piston and valve motion. In this phase, the advection scalar and momentum fluxes are interchanged between cells. The quasi second order upwind (QSOU) scheme was employed in the present study for both scalar and momentum fluxing. Partial donor cell (PDC) fluxing scheme, which needs a lesser computing cost is also available as an option. However, the PDC scheme is not used as it was found to be less accurate compared to the QSOU scheme (Amsden et al. 1989). In addition, the phase C iterations were performed in number of sub cycled time steps much smaller than the global time step. The Courant stability criterion \( u\Delta t_{sub}/\Delta x < 1 \) was used in determining the sub cycle time step \( \Delta t_{sub} \). After \( \Delta t/\Delta t_{sub} \) number of sub cycles the iteration marches to the next time step.

### 3.6 Summary

- Discussion in this chapter has mainly focused to introduce RANS governing equations for combusting flows and their adaptation to suite premixed SI engine combustion modelling.
- In the current modelling work, transport equations for species mass, momentum and specific internal energy are solved together with ideal gas assumptions.
- The \( k – \varepsilon \) turbulence model customized for engine modelling is chosen to close the turbulent stress tensor, due to its proven success in engine related problems.
- Governing transport equations discretised in their integral form, are solved following an ALE approach, where solution process is carried out in three phases: A, B and C.
- Phase A and B are considered to be Lagrangin, where cell faces are assumed to move with the flow.
- In phase A, all source terms are explicitly computed and in phase B diffusion terms are computed.
- Advection terms are evaluated in the phase C, which is considered to be Eularian. The mesh is rezoned from their Lagrangian position to the new location in number of sub cycle iterations. QSOU scheme was used for both scalar and momentum flux calculations.
- Equations are iteratively solved by using a conjugate residual method and pressure velocity coupling is made with the SIMPLE algorithm.
Combustion process in SI engines is extremely complex, so that hardly a single mathematical model can grasp all the associated phenomena. The typical approach is to use a combination of several sub models, where each model is tailored to simulate a distinct aspect. Combustion process in a spark ignition engine may be divided into two main stages: the developing stage and the fully developed stage. Spark breakdown, arc discharge, glow discharge, incipient flame kernel formation and its early stage propagation under the rising influence of turbulence are considered as the developing stage. When the size of the flame kernel is sufficiently large enough to be wrinkled by the larger turbulent eddies, the flame is said to be fully developed. Combustion in these two phases shows fundamental differences, so that the each phase needs to be dealt with a separate sub model. The discussion in this chapter has been limited for the simulation of the first phase: the developing stage. The considerations and modelling strategies of the second stage: the fully developed stage, are explained in the next chapter.

The basis for the present formulation of spark ignition and flame kernel growth sub model and its progress towards the implementation in KIVA-4 code is presented in this chapter. The section 4.1 is devoted to discuss the physical aspects of ignition phenomenon and section 4.2 provides an introduction to its modelling process. Described in section 4.3 - 4.7 is the present implementation of the ignition sub model, which has been considerably modified from its original formulation to make it more appropriate for engine combustion. A brief summary of this chapter is also provided in section 4.8.
4.1 Spark Ignition and Flame Kernel Formation

The combustion process in an SI engine is initiated by depositing heat into a flammable mixture, typically in the form of an electrical arc discharge in sub-microsecond time scale. A conventional automotive ignition system may induce a potential difference of 10,000-30,000 V across spark electrodes at breakdown (Basshuysen 2009 & Rajgupt 2005). The energy release rate during breakdown is very high, such that an ionized plasma kernel is formed at a temperature as high as 60,000 K (Maly 1994). The features of the nascent flame kernel are observed to be primarily dependent on the supplied breakdown energy. However, in general, its size does not differ much from the order of 0.5-1.0 mm in automotive applications (Heywood 1994).

The spark evolution process may be split into three phases. Initial breakdown and the subsequent arc discharge are the first two phases, that last no longer than few microseconds. These two phases are more efficient in transferring heat into the surrounding gas mixture. The third phase: glow discharge, exists about 2-3 ms and corresponds to the visible illumination. Overall energy transfer efficiency of present-day ignition systems is very low; utmost 30%, due to significant heat losses to the spark plug (electrodes). However, most of the times, the very high level of temperature in the plasma kernel is capable of effectively initializing oxidising reactions, leading to a self-sustained flame. This process results in a rapid release of chemical energy stored in the combustible mixture, establishing an active flame kernel expanding in the outward direction. Plasma support tends to fade away over the time (~300 μs). Thus, the flame kernel rapidly cools down from its high temperature to a much lower adiabatic level. Chemical reactions at breakdown and arc discharge phases are of highly complex in nature and resolving involves high temperature plasma physics. General combustion chemistry is only applicable when the kernel temperature is sufficiently low, i.e. when there is no significant plasma formation (Maly 1994).

Under general circumstances, the initial flame kernel is often observed to be spherical (Xu et al. 1994) and initial flame propagation exhibits a laminar like behaviour. In the presence of strong non-homogeneity in the fuel mixture, emerging multiple localized flame kernels may also be witnessed along the spark channel (Dahms et al. 2009). The incipient flame kernel is always susceptible to external influences due to its small size (Loye & Bracco 1987). Sometimes it may result in an extinguishment, if the heat loss to the electrodes is too high or the turbulence intensity in the vicinity is too severe to survive. The flame kernel can also be convected away from the electrodes by the local bulk flow. In such conditions, particularly in
engines, the flame kernel is significantly wrinkled and deformed into arbitrary shapes (Herweg & Ziegler 1990). Couple of other interesting observations can also be made in engine environments, which demonstrate the effects of surrounding solid boundaries, i.e. the flame holder effects. Even in cases, where the flame is rapidly convected away from the spark centre, the flame kernel often seems to remain attached to the spark electrodes. On the other hand, the presence of a curved boundary in the vicinity, makes the flame kernel to follow the boundary profile forming a horn of plenty or cornucopia (Herweg & Maly 1992).

Indisputably, the consequences of turbulence are significant from the very beginning of the spark discharge, but flame wrinkling and stretching become evident and dominant only after the flame dimension is larger than the integral length scale of turbulence. After this stage, the gradual transition from the developing stage to the fully developed stage occurs. In general, the size of the flame kernel at transition is about 5 mm in radius and it may take 5 to 10 crank degrees to reach this state at 1500 to 3000 rpm (Heywood 1994). Physical nature of a fully developed turbulent flame is significantly different from its kernel stage and is separately discussed in the next chapter.

4.2 Modelling the Early Stage of Flame Development

Accurate modelling of spark discharge and the flame kernel development is crucial in order to predict the actual flame propagation on a more physical basis. In general, more than 95% of fuel is consumed during the fully developed phase of combustion and only a less than 5% is reacted during the early flame development. However, the burned gas condition at transition has a major impact on the prediction of the main combustion model. Essentially, the ignition and flame kernel models provide the initial conditions for the main combustion model, which eventually predicts the flame propagation and species reaction rates during the bulk of the combustion duration. Heywood (1994) and Fan & Reitz (2000a) have clearly demonstrated the necessity of an appropriate ignition sub model to achieve sufficiently accurate simulation results.

Modelling the complete ignition process is always a tedious task due to the complexity of physics involved. It needs to account for spark channel breakdown, radical formation and recombination, surface chemistry, mixture inhomogeneity, heat dissipation and turbulent-chemistry interactions. Hence, usually in engineering applications, a vastly simplified approach is taken, which replicates only the major outcomes of the actual ignition process. The flame kernel size at its initial stage is very small; typically less than 1 mm comparable to the electrode gap. Consequently, extremely fine mesh resolutions are needed in order to
accurately resolve the flame surface with a complete set of balance equations. This approach dramatically increases the computational load, which is still a significant encumber to be handled by the present day computers. On the other hand, ignition and early flame propagation is just nearly a few hundredths of a full cycle engine simulation time; hence, the use of such a technique is impractical. As an alternative solution, simplified sub-grid scale models are preferred.

Numerous types of ignition models with varying degree of complexity, considering various aspects of ignition process have been proposed. By way of being the simplest method, many studies including Amsden et al. (1989) and Henson (1998), simulated the ignition by depositing internal energy into a selected number of computational cells, which approximately represent the spark kernel volume, until the maximum cell temperature reaches a cut-off limit (1600 K). The reaction rate was evaluated by an Arrhenius type model. A similar alternative is to burn the fuel up to a decided level in a selected number of cells to match with the initial kernel volume (Gubba et al. 2008). Neither, the spark breakdown nor complex physics in the early flame propagation is normally considered in this approach; the species reaction rate is predicted using the main combustion model itself.

Relatively simple, yet convincing approach is to neglect the early breakdown and arc discharge stages and simulate only the kernel development stage. In fact, this has been the current standard practise in SI engine modelling and found to produce reasonable results. Often, flamelet models are used for this purpose, where the flame front is assumed to be a thin surface. The main challenge in this type of modelling is to estimate the total flame area within a computational cell, so that the mass burn rate can be taken as proportional to the flame area times the flame propagation speed. Pischinger & Heywood (1990) solved a balance equation for the mean flame kernel area and it was scattered among individual cells using an error function type distribution. Andreassi et al. (2003) proposed to solve for the flame radius growth assuming a spherical expansion. Subsequently, the geometrically intersected surface area with a computational cell was calculated, to approximate the local flame area. In the method suggested by Falfari & Bianchi (2007), the flame surface is represented by a spherical triangulated surface. The surface traverses the outward direction at the flame propagation speed and local flame area within a computational cell is computed by calculating the number of triangles enclosed by the cell. However, the use of this approach needs to maintain a connectivity data base for the triangulated surfaces. Also, the error in local flame area estimation rapidly increases with the flame radius, as the triangle sizes increase with time. Fan & Reitz (2000b) proposed to represent the flame surface by a set of spherically distributed
Lagrangian particles, which move at the flame propagation speed. Local flame area was computed using the ratio of the total area of the sphere and the number of particles within a cell.

None of the above models considered the bulk flow convection effects and, the effect of turbulence was incorporated by using a flame wrinkling factor. The Arc and Kernel Tracking (AKTIM) model suggested by Duclos & Colin (2001) follows a similar concept but, provisions for accounting convection effects has been made. In addition, several simplified sub models have also been suggested to introduce the electrical characteristics of the ignition system. The AKTIM is shown to be a decent model for spark ignition modelling, but it requires a considerable amount of measured data from the ignition system as input parameters. However, these data is often unavailable, even in the present case, and difficult to measure in practice. Consequently, an alternative formulation based on the Discrete Particle Ignition Kernel (DPIK) model (Fan & Reitz 2000a) is proposed here.

### 4.3 A Realistic Approach for the DPIK Model

The procedure adopted here follows the concepts of DPIK model proposed by Fan & Reitz (2000a, 2000b) and further developed by Tan & Reitz (2003). This model has been successfully implemented and validated by Stiesch et al. (2001), Tan et al. (2003), Teraji et al. (2005) and Liu et al. (2006) in SI engine applications. The DPIK model assumes a spherical flame kernel, whose flame front represented by a set of Lagrangian marker particles. These particles expand outward at a velocity equal to the summation of mean turbulent flame velocity and the plasma expansion velocity.

Several immediate deficiencies exist in the DPIK model (hereafter, called the standard version). It merely predicts only the displacement speed of the flame front. The effects of turbulence are incorporated only in the form of turbulent velocity. Convection of the kernel and wrinkling of the flame front due to bulk flow motion are not explicitly considered. As already highlighted, these effects are predominant, if the spark location is positioned close to the cylinder wall, where greater convection effects are possible due to high swirl velocity. On the other hand, the presence of a solid boundary in the neighbourhood induces flame holder effects. Herweg & Maly (1992) have demonstrated its significance in engine flame wrinkling via both experimental imaging and numerical simulations. In a computational model, these phenomena can be simulated only by suitably accounting for the bulk flow effects. Moreover, the standard DPIK model has completely omitted the modelling of both the breakdown and arc discharge phases and the characteristics of the electrical circuit. Heat losses to the
electrodes have also been shrunk into a single efficiency coefficient. However, incorporation of all these effects in great detail requires significant modelling work. As a first step, present work considers only the first two issues: the flame wrinkling and convection due to local bulk flow motion. Measures required in addressing other concerns are also appropriately discussed providing relevant references. Development of the present flame kernel model is now described from section 4.3.1 onwards.

### 4.3.1 Onset of the Flame Kernel

Following the conventional approach, the breakdown and arc discharge phases and the associated plasma chemistry were neglected in the present formulation. The ignition is initiated by depositing a fully burned spherical gas volume having a diameter equal to the inter electrode gap. It has been often observed that, the initial kernel dimension is close to the inter-electrode gap. Therefore, the overall error introduced by this assumption is expected to be a minimal. Sher *et al* (1992) suggested a method to estimate the onset kernel radius in terms of breakdown energy and the thermodynamic properties of the surrounding gas mixture. A similar method has also been proposed by Duclos & Colin (2001) based on experimental results of Verhoeven (1995). However, these relations need certain input parameters from the ignition system, such as the breakdown voltage and current through the secondary circuit. A detailed model to calculate the energy discharge in spark ignition has been proposed by Yasar (2001), considering the electromagnetic behaviour of the ignition system. Such parameters are unavailable for the present ignition system and therefore, the above simplified method was adopted. Nevertheless, the above references should provide guidance for such a comprehensive implementation in the future.

### 4.3.2 Mean Flame Kernel Surface Area

DPIK model considers the flame front to be very thin, so that it separates the burn and unburned gas regions. For the simplicity, it further postulates that, the flame kernel is spherical. This assumption is no longer used in this study and instead, the flame kernel is taken to be of any arbitrary closed volume, continuously deformed by the bulk flow motion. Moreover, the flame kernel is assumed to be a simple thermodynamic system, whose boundary is represented by a set of Lagrangian marker particles as shown in Figure 4.1. It should be noted that, this approach does not resolve the flame structure or the arc discharge process. It starts the calculations after the initial spark breakdown phase, ideally after few microseconds. Further, it assumes that, there is no heat transfer taking place across the flame.
front surface, while the conditions inside the system are uniform with fully burned gases in equilibrium.

![Diagram of ignition flame kernel represented by a set of Lagrangian marker particles](image)

Figure 4.1: Ignition flame kernel represented by a set of Lagrangian marker particles

The burned gas temperature within the kernel is also assumed to be at adiabatic flame temperature, though in reality, this is only a rudimentary approximation. Figure 4.2 shows a schematic view of the equivalent thermodynamic system of the spark kernel.

![Diagram of simplified thermodynamic system of the flame kernel](image)

Figure 4.2: Simplified thermodynamic system of the flame kernel. Flame front is taken to be the boundary of the system

Rate of change of flame kernel mass $m_k$, which is essentially the unburned gas consumption rate, is given by:

$$\dot{m}_k = \frac{dm_k}{dt} = \rho_u A S_{eff}$$  \hspace{1cm} (4.1)
where, \( A \) is the total flame area and \( \rho_u \) is the unburned gas density. The effective flame propagation speed \( S_{eff} \) is the resultant flame traverse speed and is equal to the summation of laminar flame speed \( S_l \) and the plasma expansion speed \( S_{plasma} \). However, the estimation of the actual flame area is a difficult task at this stage, as it should account for both the effects of turbulent and bulk flow wrinkling. As the size of the kernel is smaller than both the larger turbulent eddies and computational cell dimension, the flame area cannot be computed with a sufficient accuracy using conventional methods. Consequently, \( A \) is replaced by \( A_k \): the mean flame surface area. To be consistent with flame speed definitions, the laminar flame speed is now replaced with the turbulent flame speed \( S_t \). Accordingly, the mass burn rate and the effective flame speed are recast as:

\[
\dot{m}_k = \rho_u A_k S_{eff} \quad (4.2)
\]
\[
S_{eff} = S_t + S_{plasma} \quad (4.3)
\]

In this chapter, subscript \( k \) represents the flame kernel and should not be confused with the subscript \( k \) used to represent the \( z \) direction in Cartesian space or the turbulent kinetic energy in Chapter 3.

In the original version of the DPIK model, the mean flame area and the mean kernel volume are respectively taken to be the surface area and the volume of the sphere formed by the marker particles. However, in the present formulation, these relations are not valid, as the flame kernel is no longer assumed to be spherical. Therefore, the kernel volume was considered to be equal to the total burned gas volume \( V_k \) and, is estimated by evaluating the following integral over the entire domain \( \Omega \):

\[
V_k = \int_{\Omega} \bar{\epsilon} dV \quad (4.4)
\]

\( \bar{\epsilon} \) is the mean progress variable and is a function of the mass averaged progress variable \( \bar{\epsilon} \) and the burned and unburned gas densities. Exact expressions for the mean and mass averaged progress variables are given in section 4.3.3, followed by a comprehensive discussion.

Similarly, two other expressions are required to estimate the flame kernel surface area and the radius. As kernel particles are now free to move with flow, the shape of the flame kernel is not definite and hence, no radius can be defined as in the case of a sphere. Consequently, at this point, an equivalent radius \( r_k \) is defined, such that the burned gas volume is equal to the volume of the sphere whose radius is \( r_k \).
\[ r_k = \left( \frac{3V_k}{4\pi} \right)^{1/3} \tag{4.5} \]

Mean kernel surface area is then related to \( r_k \) as:

\[ A_k = 4\pi r_k^2 \tag{4.6} \]

Bradly et al. (2003) have verified via experimental flame kernel imaging that, this approach is capable of calculating mean flame area with a reasonable degree of accuracy, even with moderate levels of turbulence.

### 4.3.3 Progress of the Reaction

It is possible to define the degree of reaction taken place in premixed combustion, at a given location, in terms of the mean progress variable \( \bar{c} \). Progress variable has the value 0 in fresh gas side and reaches to 1 at fully burned region or may be the other way around depending on the definition. Several different formulae have been proposed for the definition of progress variable. Reduced temperature, reduced fuel mass fraction and reduced product mass fractions are among frequently used definitions. For the present study, the definition based on the fuel mass fraction is considered.

\[ \bar{c} = \frac{\bar{Y}_{f,u} - \bar{Y}_f}{\bar{Y}_{f,u} - \bar{Y}_{f,b}} \tag{4.7} \]

\( Y_{f,u} \) and \( Y_{f,b} \) are the fuel mass fraction in fresh and fully burned gases respectively, whereas \( Y_f \) is the currently available fuel mass fraction at the point considered. Subscripts \( u \) and \( b \) denotes conditions at unburned and burned gas conditions respectively. Note that, the mean progress variable here is calculated using mean mass fractions. To relate Favre averaged quantities to mean quantities, a separate relation has to be obtained. After Bray & Moss (1977), the following relationship is widely used in the literature for this purpose.

\[ \bar{c} = \frac{(1 + \tau)\bar{c}}{1 + \tau\bar{c}} \tag{4.8} \]

\[ \tau = \frac{\bar{\rho}_u}{\bar{\rho}_b} - 1 = \frac{\bar{T}_b}{\bar{T}_u} - 1 \tag{4.9} \]

\( \tau \) is the heat release factor defined in terms of the ratio between fresh and burned gas densities \( \rho_u \) and \( \rho_b \) respectively. If the pressure is assumed to be equal in both burned and unburned gas regions, it may be recast in terms of fresh and burned gas temperatures \( T_u \) and \( T_b \) as well.
4.3.4 Volumetric Expansion Rate of the Flame Kernel

Eq. (4.10) given below, has been obtained by applying the time varying ideal gas equations to the flame kernel. It is possible to derive Eq. (4.11) by taking the time derivative of the definition of the mass density, in relation to the flame kernel: \( m_k = \rho_k V_k \), and combining with Eq. (4.1) - (4.3).

\[
\frac{1}{\rho_k} \frac{d\rho_k}{dt} = \frac{1}{p} \frac{dp}{dt} - \frac{1}{T_k} \frac{dT_k}{dt}
\]  

\[
\frac{dV_k}{dt} = \frac{\rho_u}{\rho_k} A_k \left( S_t + S_{plasma} \right) + V_k \left( \frac{1}{T_k} \frac{dT_k}{dt} - \frac{1}{p} \frac{dp}{dt} \right)
\]

\p is the pressure inside the kernel, assumed to be equal to the average pressure within the combustion chamber and \( T_k \) is the kernel temperature. The burned gas density inside the kernel is denoted by \( \rho_k \).

It is reasonable to assume that, the relative pressure increase due to combustion during the ignition period is negligible (Fan & Reitz 2000a). This is justified due to the fact that, the breakdown phase characterized by high temperatures lasts only a few nanoseconds and the flame kernel development phase is limited to a few crank degrees. As it was already mentioned, the temperature inside the kernel is assumed to be constant, in the order of adiabatic temperature. These assumptions further simplify Eq. (4.11) and the resultant equation for the flame kernel expansion rate is given below.

\[
\frac{dV_k}{dt} = \frac{\rho_u}{\rho_k} A_k \left( S_t + S_{plasma} \right)
\]  

Substitution for the flame kernel area and volume leads to the following relation in terms of the mean flame kernel radius.

\[
\frac{dr_k}{dt} = \frac{\rho_u}{\rho_k} \left( S_t + S_{plasma} \right)
\]

There is no an immediate use of this equation in the present model. These relations are used in the next section to evaluate the plasma expansion speed.

4.3.5 Approximation for the Plasma Velocity

Plasma velocity can be estimated by the control volume analysis of the flame kernel. During the ignition, energy balance for the volume surrounded by the flame kernel surface gives:
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\[ Q_k + (h_u + \frac{1}{2} v^2) \dot{m}_k = \frac{dE_k}{dt} + p_k \left( \frac{dV_k}{dt} \right) \]  \hspace{1cm} (4.14)

where, \( \dot{Q}_k \) is the net energy transfer rate into the flame kernel by external means. \( E_k \) is the total internal energy content of the kernel. \( h_u \) and \( v \) respectively stand for the enthalpy and velocity of the unburned gas at the flame surface boundary and account for the energy carried into the flame kernel by mass entrainment. The last terms means the work done by the expansion process of the flame surface.

Net rate of heat transfer into the ignition kernel \( \dot{Q}_k \) is the summation of spark energy discharge rate \( \dot{Q}_{\text{spark}} \), heat release rate by the burning fuel \( \dot{Q}_{\text{chem}} \) and the rate of heat loss to the spark electrodes \( \dot{Q}_{\text{electrodes}} \).

\[ \dot{Q}_k = \dot{Q}_{\text{spark}} + \dot{Q}_{\text{chem}} - \dot{Q}_{\text{electrodes}} \]  \hspace{1cm} (4.15)

Compared to the enthalpy of unburned gases, the order of magnitude of the kinetic energy content in entrained gases is negligible. Thus, the term \( v^2 \) can be eliminated from Eq. (4.14) and recast as:

\[ \dot{Q}_{\text{spark}} + \dot{Q}_{\text{chem}} - \dot{Q}_{\text{electrodes}} = \left( \frac{dE_k}{dt} \right) - h_u \dot{m}_k + p_k \left( \frac{dV_k}{dt} \right) \]  \hspace{1cm} (4.16)

Since the total internal energy of the kernel \( E_k \) is the product of specific internal energy \( U_k \) and the kernel mass \( m_k \), \( dE_k/dt \) term in Eq. (4.16) can be expressed as:

\[ \frac{dE_k}{dt} = m_k \frac{dU_k}{dt} + U_k \dot{m}_k \]  \hspace{1cm} (4.17)

The expansion work term in Eq. (4.16) can be rearranged using Eq. (4.13) to obtain the expansion rate of mean flame kernel radius as:

\[ p_k \frac{dV_k}{dt} = 4\pi r_k^2 p_k \frac{dr_k}{dt} = p_k 4\pi r_k^2 \frac{\rho_u}{\rho_k} (S_t + S_{\text{plasma}}) \]  \hspace{1cm} (4.18)

Once Eq. (4.15) - (4.18) are combined, the resultant would be:

\[ \dot{Q}_{\text{spark}} + \dot{Q}_{\text{chem}} - \dot{Q}_{\text{electrodes}} \]

\[ = m_k \frac{dU_k}{dt} + U_k \dot{m}_k - h_u \dot{m}_k + p_k 4\pi r_k^2 \frac{\rho_u}{\rho_k} (S_t + S_{\text{plasma}}) \]  \hspace{1cm} (4.19)

This equation provides an expression to calculate the plasma velocity in terms of other parameters. Calculation of the mass transfer rate into the kernel is quite a complex task;
hence, it is replaced with an alternative expression in the next few steps, to obtain a straightforward description.

If no spark energy is supplied into the flame kernel and no heat is lost into the electrodes, Eq. (4.19) becomes:

\[
\dot{Q}_{\text{chem}} = m_k \frac{dU_k}{dt} + U_{ad} \dot{m}_{\text{chem}} - h_u \dot{m}_{\text{chem}} + p_k 4\pi r_k^2 \frac{\rho_u}{\rho_k} S_t
\]  

(4.20)

As there is no heat loss taken place across the flame front, the internal thermodynamic properties within the kernel reach adiabatic conditions. Hence, the specific internal energy is replaced with the corresponding adiabatic value \( U_{ad} \). In these particular conditions, the mass transfer rate into the kernel is only due to the flame surface propagation and, is assumed to be equal to the turbulent burning rate \( \dot{m}_{\text{chem}} \):

\[
\dot{m}_{\text{chem}} = 4\pi r_k^2 \rho_k S_t
\]  

(4.21)

Combining Eq. (4.19) - (4.21) the following relation is obtained,

\[
\dot{Q}_{\text{spark}} - \dot{Q}_{\text{electrodes}} = U_k \dot{m}_k - U_{ad} \dot{m}_{\text{chem}} + h_u (\dot{m}_{\text{chem}} - \dot{m}_k) + 4\pi r_k^2 \frac{\rho_u}{\rho_k} S_{\text{plasma}}
\]  

(4.22)

Previously, at the beginning of the derivation, it was assumed that the temperature within the flame kernel is uniform and adiabatic and this leads to \( U_k = U_{ad} \). Further, the difference in mass burn rates in two cases \( \dot{m}_k - \dot{m}_{\text{chem}} \) is caused due the increased flame speed imposed by plasma. Hence, it is concluded that,

\[
\dot{m}_k - \dot{m}_{\text{chem}} = \rho_u 4\pi r_k^2 S_{\text{plasma}}
\]  

(4.23)

Finally, Eq. (4.22) is rearranged to calculate the plasma velocity (Fan & Reitz 2000a):

\[
S_{\text{plasma}} = \frac{\dot{Q}_{\text{spark}} - \dot{Q}_{\text{electrodes}}}{4\pi r_k^2 \left[ \rho_u (U_k - h_u) + p_k \frac{\rho_u}{\rho_k} \right]}
\]  

(4.24)

where, \( \dot{Q}_{\text{spark}} - \dot{Q}_{\text{electrodes}} \) represents the net energy transfer rate into the flame kernel, which is the summation of spark discharged energy deposition rate and the heat loss rate to the electrodes. The best way of estimating the rate of spark energy deposition is by comprehensive modelling of the ignition circuit following Duclos & Colin (2001) or Yasar (2001). This may require accurate estimation of spark plug surface area exposed to the
combustion chamber, convective coefficient between spark plug surface and in-cylinder gas mixture and the characteristics of the secondary ignition circuit. Alternatively, it is possible to estimate the overall energy transfer rate by introducing an efficiency factor for the whole energy transfer process given by:

\[
\dot{Q}_{\text{spark}} - \dot{Q}_{\text{electrodes}} = \dot{Q}_{\text{ign}} \eta_{\text{ign}}
\]

where, \(\dot{Q}_{\text{ign}}\) is the total energy discharge rate during the ignition process and \(\eta_{\text{ign}}\) is the efficiency of energy transfer rate to the flame kernel. For the present study, the latter method is implemented. \(\eta_{\text{ign}}\) was assumed to be 30% as suggested by Heywood (1994) and Dahms (2009). \(\dot{Q}_{\text{ign}}\) was calculated assuming an energy discharge of 60 mJ within a period of one crank degrees in engine applications, which corresponds to a typical transistor controlled ignition (TCI) system, as measured by Herweg & Maly (1992).

### 4.3.6 Species Consumption Rate During the Ignition Period

Source term \(\dot{\omega}_{\text{chem,m}}\) in the species mass conservation equation for species \(m\) in a given computational cell during the ignition period was modelled as:

\[
\dot{\omega}_{m,\text{chem}} = C_{\text{IGN}} \rho_u Y_m A_k (S_t + S_{\text{plasma}}) \Sigma_{\text{cell}}
\]

where, \(C_{\text{IGN}}\) is a model constant typically with a large value like 10, as in Tan et al. (2003) and Fan and Reitz (2000b) and also in the present study, to ensure complete combustion within the flame kernel. \(Y_m\) is the mass fraction of species \(m\) in unburned gas and \(\Sigma_{\text{cell}}\) is the flame surface density: available flame surface area per unit volume, within the computational cell.

As mentioned earlier, the flame surface is represented by a set of Lagrangian marker particles that move outward from the electrode at the flame kernel expansion rate. Since these particles are uniformly distributed over the entire flame surface, the fraction of the flame surface enclosed by a given cell at a given instance can be approximated by counting the number of marker particles within that cell, at that particular moment. If the total flame surface is represented by \(N_{\text{total}}\) number of particles, the flame surface density of a cell with volume \(V_{\text{cell}}\) is given by:

\[
\Sigma_{\text{cell}} = \frac{N_{\text{cells}} A_k}{N_{\text{total}} V_{\text{cell}}}
\]
where, \( N_{\text{cells}} \) is the number of particles contained within the cell at the considered instance. Note that, \( N_{\text{cells}} \) is a dynamic time varying parameter, so that it has to be estimated at every time step for each cell. For this reason, the following algorithm was developed to be used in the present study.

### 4.3.7 Tracking the Particle Motion

Assuming the flame surface is convected away by the bulk flow at a speed equal to the mean local flow velocity (Duclos & Colin 2001), each particle was assigned the averaged flow velocity \( S_{\text{flow}} \) interpolated on to the particle location. Thus, \( S_{\text{eff},p} \), the effective local propagation velocity vector of a given particle is modelled as:

\[
\vec{S}_{\text{eff},p} = \vec{S}_t + \vec{S}_{\text{plasma}} + \vec{S}_{\text{flow},p}
\]  (4.28)

\( S_{\text{flow},p} \) is the interpolated flow velocity vector on the marker particle.

\[
S_{\text{flow},p}(u, v, w) = \sum_{i=1}^{32} \left[ \frac{S_i(u, v, w)}{d_i^\varphi} \right] \div \sum_{i=1}^{32} \left( \frac{1}{d_i^\varphi} \right) \]  (4.29)

\( S_{\text{flow},p}(u, v, w) \) was estimated using the inverse distance interpolation technique, considering a maximum of 32 neighbouring cell vertices. It was assumed that the tendency of turbulent and plasma velocity of a given particle is always to propagate towards the originally assigned direction; i.e., in the absence of bulk flow effects, flame kernel remains spherical. \( S_i(u, v, w) \) is the velocity vector at \( i^{\text{th}} \) vertex and \( d_i \) is the distance to vertex \( i \) from the particle location. The weighting power of the inverse distance \( \varphi \) was taken as 2.0 as suggested by Sadarjoen et al. (1994). This procedure results in a floating flame kernel with an irregularly wrinkled flame surface.
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Figure 4.3: A Lagrangian ignition kernel particle inside a typical hexahedron computational cell

In order to find the number of particles in a given cell, the following algorithms were developed. For brevity, only the main logic sequences are presented here. Figure 4.3 shows an arbitrary particle \( P \) within a hexahedral computational cell. If the point \( P \) is within the cell, coordinates of the particle \( (x_p, y_p, z_p) \) should satisfy the following criteria.

Let,

\[
\begin{align*}
  x_{\text{max}} &= \max(x_1, x_2, x_3 \ldots \ldots x_8) \\
  x_{\text{min}} &= \min(x_1, x_2, x_3 \ldots \ldots x_8) \\
  y_{\text{max}} &= \max(y_1, y_2, y_3 \ldots \ldots y_8) \\
  y_{\text{min}} &= \min(y_1, y_2, y_3 \ldots \ldots y_8) \\
  z_{\text{max}} &= \max(z_1, z_2, z_3 \ldots \ldots z_8) \\
  z_{\text{min}} &= \min(z_1, z_2, z_3 \ldots \ldots z_8)
\end{align*}
\]

Then,

\[
x_{\text{min}} < x_p < x_{\text{max}} \quad \text{AND} \quad y_{\text{min}} < y_p < y_{\text{max}} \quad \text{AND} \quad z_{\text{min}} < z_p < z_{\text{max}} \quad (4.30)
\]

where, \( (x_i, y_i, z_i) \) is the spatial coordinates of \( i^{th} \) cell vertex. It is worth mentioning that, some of the particles lying outside a computational cell can also satisfy these conditions, as illustrated in the Figure 4.4. However, this logic can still be used as an initial filter to select a cluster of probable particles. It was found that this initial filtration results in a considerable reduction in computational time taken for particle search. Subsequently, the selected set of particles is checked for the following exact condition, which is satisfied only by the particles residing inside the computational cell.
As depicted in the Figure 4.3, if the point \( P \) is located in the same side as \( G \) with respect to face \( ABCD \), then the angle \( \theta \) is always acute \((0 < \theta < \pi/2)\); where vertex \( G \) is selected, such that path \( A \rightarrow B \rightarrow C \rightarrow D \) is anticlockwise as seen from \( G \). The angle \( \theta \) is measured between the vector \( \overrightarrow{AP} \) and \( \eta \): the unit normal vector to the face \( ABCD \). This further infers that, \( \cos \theta \) lies within zero and one. This condition is satisfied by all the 6 cell faces if and only if the particle is located inside the cell volume. The mathematical formulation of these logical conditions can be described as follows.

Unit normal vector to the face \( ABCD \): \( \eta \) is obtained by evaluating the vector product of \( \overrightarrow{AB} \) and \( \overrightarrow{BC} \).

\[
\eta = \frac{\overrightarrow{AB} \times \overrightarrow{BC}}{|\overrightarrow{AB} \times \overrightarrow{BC}|}
\]

\( \overrightarrow{AB} \times \overrightarrow{BC} = \begin{bmatrix} i & j & k \\ (x_b - x_a) & (y_b - y_a) & (z_b - z_a) \\ (x_c - x_b) & (y_c - y_b) & (z_c - z_b) \end{bmatrix} = ai + bj + ck
\]

Position vector \( \overrightarrow{AP} \) may be written as:

\[
\overrightarrow{AP} = (x_p - x_i)i + (y_p - y_i)j + (z_p - z_i)k
\]
\begin{align*}
|\overrightarrow{AP}| &= \sqrt{(x_p - x_1)^2 + (y_p - y_1)^2 + (z_p - z_1)^2} 
\end{align*}

(4.34)

The value of \( \cos \theta \) may be estimated from the scalar product of \( \overrightarrow{AP} \) and \( \eta \).

\begin{align*}
\overrightarrow{AP} \cdot \eta &= |\overrightarrow{AP}| \cos \theta = a(x_p - x_1) + b(y_p - y_1) + c(z_p - z_1) \\
\cos \theta &= \frac{a(x_p - x_1) + b(y_p - y_1) + c(z_p - z_1)}{|\overrightarrow{AP}|} 
\end{align*}

(4.35)\hspace{1cm}(4.36)

If the particle \( P \) is inside the cell, then for each \( \cos \theta_i \) for all six cell faces:

\begin{align*}
0 < \cos \theta_i < 1 \quad ; \quad i = 1,2,3,4,5,6
\end{align*}

(4.37)

Accordingly, all the particles which meet this constraint are considered to recline within the particular cell. Alternatively, it is also possible to verify whether a particle is inside a cell by evaluating the volume of six pyramidal volumes formed by joining the particle location and the six cell faces as described in Amsden et al. (1989) for spray droplet tracing. However, this method was not used in this study, as subroutines developed for mesh conversion in Chapter 3 can be easily adapted to implement the proposed vector based method. Both methods require similar number of computing operations; hence no significant difference in computational demand.

The larger the number of particles used to represent the flame surface, the higher will be both the accuracy of the computed local flame surface density and the computational cost. Therefore, a compromise is required. For the present study, 4000 marker particles were used. Starting locations and the outward direction of motion of the particles were randomly initialized on a surface of a sphere according to Eq. (4.38) and (4.39). Initial sphere radius \( r_0 \), which is the nascent kernel radius, is taken as 0.5 mm, due to Heywood (1994).

\begin{align*}
P(x_{pi}, y_{pi}, z_{pi}) &= (r_0 \cos \alpha_i \sin \beta_i, r_0 \sin \beta_i \sin \alpha_i, r_0 \cos \beta_i) \\
0 < \alpha_i < 2\pi \text{ and } 0 < \beta_i < \pi
\end{align*}

(4.38)\hspace{1cm}(4.39)

\( \alpha_i \) and \( \beta_i \) are the randomly assigned direction angles of \( i^{th} \) particle during the initialisation. \( r_0 \) is measured with respect to the centre of the spark volume, which is located at the spark position.

Particle tracking and interpolation algorithms usually involve large repetitive loops that will be in the order of the product of marker particle count and the number of mesh cells.
Therefore, it consumes considerable amount of computational time if implemented serially. To overcome this problem, all the tracking and interpolating logics were coded using the OPEN-MP parallel programming techniques and as a result, a huge reduction of the computational time was achieved.

4.4 Turbulent Flame Speed

Prediction of the chemical source term in ignition model using Eq. (4.26) requires the estimation of turbulent flame propagation speed $S_t$, for which several closure models are found in the literature; including Gülder (1990), Herweg & Maly (1992), Liu et al. (1993), Zimont et al. (1998) and Peters (1999). However, relatively a large number of successful applications have been reported on the model proposed by Herweg & Maly (1992) in SI engine applications. Besides, this has been specifically developed for turbulent flame speed predictions in the course of early flame kernel growth in SI engines. Therefore, in this study, the model proposed by Herweg & Maly (1992) is adapted.

In general, the turbulent flame speed is related to the laminar flame speed by the following relation.

$$\frac{S_t}{S_l} = \frac{A_f}{A_t} = \Xi$$

(4.40)

$A_f$ is the actual flame area and $A_t$ is the mean projected flame area in the propagation direction. The flame wrinkling factor $\Xi$ is defined as the ratio between $A_f$ and $A_t$. Hence, the calculation of the turbulent flame speed requires expressions for the laminar flame speed and the flame wrinkling factor.

4.4.1 Stretch and Curvature Effects on Flame Kernel Propagation

Up to this point, the term laminar burning velocity was used without any specific definition. However, the laminar velocity used in all the previous cases corresponds to the strained laminar burning velocity at mean strain. To be precise, this implies a flame propagation speed, which changes with the applied strain level (or stretch) on the flame surface. Flame stretch rate may be defined as the rate of change of flame surface area per unit flame surface. In practice, it is virtually impossible to observe a perfectly unstrained (zero stretch) flame front, but ideally, a one-dimensional planar flat flame and a stationary spherical flame front are two examples for unstrained flames. Stresses applied on the flame front are twofold. Naturally, the flame front tends to propagate spherically; hence, a curved flame front with a gradually increasing surface area is formed. This results a self-induced stress on the spherical flame
front. The other is the aerodynamic stresses, which lead to flame wrinkling. Stresses usually reduce the flame propagation speed and excessive stresses could lead to extinction. Sometimes, it has been noted that, laminar flame speed becomes higher before the extinction (Stahl & Warnatz 1989).

Relationship between the strained laminar burring velocity $S_l$ and the unstrained laminar burning velocity $S^0_l$ can be defined as:

$$S_l = I_0 S^0_l \quad (4.41)$$

where, $I_0$ is the stretch factor, which depends on the local turbulence level and the flame geometry. Modelling of $I_0$ requires the knowledge of certain quantities such as Karlovitz number and Damköhler number, which relate the degree of interaction of turbulence on combustion. Discussion on these aspects has been left for the next chapter. Therefore, only the expression for $I_0$ is given in this section.

As an alternative formulation, it is now possible to describe the turbulent flame speed as a summation of stained laminar flame speed and $f(u', L_i, ...)$: a function to account for the effect of turbulence and other related parameters.

$$S_l = I_0 S^0_l + f(u', L_i, ...) \quad (4.42)$$

Subjected to the same set of assumptions made during the derivation of ignition model, it has been proved by Herweg & Maly (1992) that, the function $f(u', L_i)$ can be expressed as follows during the flame kernel formation period.

$$f(u', L_i, ...) = \sqrt{I_0 \left(\frac{u'}{u' + S^0_l}\right) \left[1 - \exp\left(-\frac{r_k}{L_i}\right)\right] \left[1 - \exp\left(-\frac{\Delta t}{T_{0G}}\right)\right] \left(\frac{u'}{S^0_l}\right)^{5/6} S^0_l \quad (4.43)$$

Accordingly, the flame wrinkling factor $\Xi$ during the early development stage may be given by the following equation.

$$\Xi = I_0 + I_0^{1/2} \left(\frac{u'}{u' + S^0_l}\right)^{1/2} \left[1 - \exp\left(-\frac{r_k}{L_i}\right)\right]^{1/2} \left[1 - \exp\left(-\frac{\Delta t}{T_{0G}}\right)\right]^{1/2} \left(\frac{u'}{S^0_l}\right)^{5/6} \quad (4.44)$$

where, $u'$ is the turbulent intensity for isotropic turbulence, $\Delta t$ is the time elapsed after the spark discharge, $L_i$ is the integral length scale of turbulence and $T_{0G}$ is the characteristic time given by the relation:
The stretch factor $I_0$ is estimated as (Herweg & Maly 1992):

$$I_0 = 1 - \left( \frac{\delta_l}{15L_i} \right)^{3/2} \left( \frac{u'}{S_i^0} \right)^{3/2} - 2 \frac{\delta_l \rho_u}{r_k \rho_b}$$

(4.46)

$\delta_l$ represents the laminar flame thickness and taken to be equal to the ratio between the laminar kinematic viscosity $\nu$ and the unstrained laminar flame speed.

$$\delta_l = \frac{\nu}{S_i^0}$$

(4.47)

The speciality of this turbulent speed relation is that, it accounts for the effects of strain, turbulent intensity and characteristic time and length scales during the flame kernel growth, whereas many other models consider only one or few of these aspects, or simply neglect the strain effects on flame propagation. Figure 4.5 shows the effect of turbulence, combustion and geometric parameters of the flame kernel in determining the magnitude of the stretch factor.

It can be seen that, $I_0$ has a minimum value at the onset of ignition and gradually increases towards a saturated value with the increasing flame radius. This saturation limit is inversely proportional to the turbulent intensity. Higher turbulent levels could result in a much lower $I_0$.
value, which makes the strained laminar flame speed substantially different from its unstrained value.

### 4.5 Unstrained Laminar Flame Speed

Unstrained laminar flame speed is a function of fuel mixture composition, temperature and pressure. There are some theoretical relations for calculating the laminar flame speed (Williams 1985 & Mitani 1980), however it is often found that empirical correlations produce much better results, when applied to a range of operating conditions in real world applications. In experiments, the flame traverse speed is measured for different curvature stretch rates in the absence of aerodynamic stretche (turbulence), usually for spherically expanding flames in combustion bombs. Subsequently, the measured speed $S_t$ and the unstrained laminar speed is correlated using the Markstine length scale $L_{Ma}$, as given below in Eq. (4.48) assuming a linear relationship (Kuo 2005). However, this linear relationship is valid only for small values of curvature strains as suggested by the asymptotic analysis of Bush & Fendell (1970) and Williams (1985).

$$S_t = S_t^0 - L_{Ma} K_C$$

(4.48)

The curvature stretch rate $K_C$ for spherical flames can be computed by simple flame analysis as:

$$K_C = \frac{1}{A} \frac{dA}{dt} = \frac{2}{r} \frac{dr}{dt}$$

(4.49)

where, $A$ is the flame area and $r$ is the radius of the spherical flame. The intercept of the graph between the curvature stretch and the measured flame speed gives the flame speed at zero stretch and the gradient is the Markstine length. It should be noted that, the Markstine length varies with flow and fuel properties. Several expressions are found in the literature to evaluate $L_{Ma}$, but their applicability is highly restricted. For example, the relation proposed by Calvin & Joulin (1983) is valid only under the conditions of constant viscosity with single-step chemistry in lean mixtures.

In the literature, there is no sufficient data set or a suitable empirical correlation for unstretched burning velocity of different fuel types, which can be applicable for a range of operating conditions. Some work has been carried out to find a proper empirical correlation by Bradley et al. (2003), but its validity has been tested only for a very limited range of conditions. Consequently, all present-day simulation studies have used some form of well-established laminar flame correlations such as, Metgalchi & Keck (1982) and Gülder (1984).
Unfortunately, these correlations have been derived to predict the measured flame speeds in the absence of turbulence; hence, no correction has been made for curvature strain. However, for fully developed flames, the effect of curvature stresses is negligible compared to the turbulent stresses. Therefore, these correlations more or less predict the unstrained laminar velocity in such situations. In fact, DNS confirm that (Haworth & Poinsot 1992), the ratio between strained unstrained and flame speeds remains close to the unity. Thus, some models simply neglect this aspect.

Geometric stresses are much larger in the early stage of flame propagation, where the flame radius is significantly small. In these situations, use of such uncorrected correlations may produce a substantial influence on the predictions. However, these correlations are still universally used in flame kernel modelling due to lack of a proper relation (see Herweg & Maly (1992), Fan & Reitz (2000a) and Heywood (1994) for examples). The correlation proposed by Gülder (1984) is used in this study to approximate the unstrained laminar burning velocity. As already noted, this correlation has also not been compensated for curvature effects, however shown to be the best fit for extensive set of experimental measured flame speeds. It has also been found to predict much better at high unburned gas temperatures, compared to the widely used Metgalchi & Keck (1982) correlation, which often over predicts in such conditions (see Gülder 1984). This correlation has been validated for a range of fuel-air equivalence ratios from 0.7 to 1.4 at a pressure of 1.0-100 atm and a temperature range of 298-900 K. Typically, homogeneous charge SI engines operate almost near stoichiometric conditions. On the other hand, the in-cylinder mean pressure and unburned gas temperature in SI engines fall within these validated limits. Therefore, Gülder’s expression can effectively be used to compute the unstrained laminar burning in engines. The laminar flame speed estimated using this empirical correlation is denoted by $S_l$.

The Gülder (1984) correlation for the laminar burning velocity is often stated in the following form:

$$S_l = S_0 \left( \frac{T}{T_0} \right)^\alpha \left( \frac{P}{P_0} \right)^\beta (1 - \omega R_f)$$

$$S_0 = z.w. \phi^n \exp[-\xi(1 - 1.075)^2]$$

where, $S_0$ is a reference laminar velocity measured at reference pressure $P_0$ and reference temperature $T_0$. The local fuel-air equivalence ratio is denoted by $\phi$ and $R_f$: the residual gas
mass fraction, has been incorporated to account for the effects of inert diluents. All other parameters are fuel specific model constants and given in the Table 4.1.

Table 4.1 Model coefficients of the laminar burning velocity correlation

| Model constants | \( z \) | \( w \) (\( cms^{-1} \)) | \( \eta \) | \( \xi \) | \( \alpha \) | \( \beta \) | \( \sigma \) | \( P_0 \) (bar) | \( T_0 \) (K) |
|-----------------|-----|-----------------|-----|-----|-----|-----|-----|-----|-----|-----|
| Isooctane       | 1   | 46.58           | -0.326 | 4.48 | 1.56 | -0.22 | 2.10 | 1.0 | 300 |
| Propane         | 1   | 44.60           | 0.120  | 4.95 | 1.77 | -0.20 | 2.10 | 1.0 | 300 |

Predicted laminar burning velocity by this correlation for different unburned gas conditions are shown in the Figure 4.6 and Figure 4.7. Effect of the fuel type and the diluent content is also illustrated. It is interesting to note that, maximum flame speed is achieved for slightly rich mixtures, as a consequence of dissociation reactions at elevated temperatures. These reactions cause CO\(_2\) to split into CO and O increasing the oxygen content and thereby accelerating chemical reactions.

![Figure 4.6: Predicted laminar flame speed for iso-octane at different unburned gas (a) temperatures and (b) pressures values](image)

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Figure 4.7: (a) Effect of residual gas on the laminar flame speed
(b) Comparison of predicted laminar flame speed for propane and iso-octane

4.6 Calculation of Burned and Unburned Gas Properties

Pressure inside the engine cylinder is often considered to be uniform for low Mach number flows. Hence, both the burned and the unburned gas pressures have the same values. Consequently, both these pressures were taken as the local cell pressure value. $T_u$: the unburned gas temperature is estimated based on adiabatic compression with a polytropic index $\gamma$ according to Eq. (4.52). Reference conditions $T_1$ and $p_1$ are respectively taken to be the unburned gas temperature and pressure computed in the previous iteration.

$$T_u = T_1 \left( \frac{p_1}{p_u} \right)^{1-1/\gamma}$$

(4.52)

The local specific heat capacity value changes with the combustion product composition within a computational cell. Hence, the local $\gamma$ value cannot be used to determine the local unburned gas temperature after combustion has started in the corresponding cell. Hence, a mass averaged $\gamma$ value computed within the unburned region, where $\tilde{c} = 0$, is used to overcome this difficulty. The unburned gas density is computed by the ideal gas relation with an averaged molecular weight $W_m$ for the gas mixture. $W_m$ is computed just before the combustion starts.

$$\rho_u = \frac{m_u}{v_u} = \frac{p_u W_m}{R_u T_u}$$

(4.53)
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$m_u$ and $v_u$ correspond to the mass of unburned gases and their volume within a computational cell and they may be estimated by combining with the following relations.

$$m_u = \bar{\rho}v_c(1 - \bar{\varepsilon}) \tag{4.54}$$

$v_c$ is the local cell volume and $\bar{\rho}$ is the mean density within the cell. Consequently, the local burned gas density can be estimated from:

$$\rho_b = \frac{\bar{\rho}v_c\bar{\varepsilon}}{v_c - v_u} \tag{4.55}$$

In a similar way, the internal energy of the burned gas kernel could be determined by:

$$U_k = \frac{U - (1 - \bar{\varepsilon})U_u}{\bar{\varepsilon}} \tag{4.56}$$

where, $U$ is the mean internal energy of the cell and $U_u$ is the internal energy of remaining unburned gases within the cell.

### 4.7 Transition of the Flame Kernel to a Fully Developed Flame

When the flame radius is large enough to be influenced by the surrounding turbulence, it is considered to be a fully developed flame. Some of the assumptions made in the flame kernel modelling no longer hold for the developed stage. Hence, a separate sub model to handle the fully developed flame propagation should be activated. Several transition criteria from flame kernel to the fully developed combustion state may be found in the literature. Some such conditions are the time elapsed after the spark, flame kernel radius reaching a predetermined value, temperature of the computational cells in ignition region exceeding a user defined threshold or a reaching the burned fuel mass to a specific amount of the total fuel mass (Palipana 2000). In the present study, the transition is considered to take place when the flame radius is greater than the mean integral scale of turbulence: a well-established criterion following Duclos & Colin (2001), Tan & Reitz (2003) and Teraji et al. (2005). Certainly, this is in good agreement with the experimental observations: which says that, turbulent flame wrinkling is dominant when the flame radius is in the order of the turbulent integral scale.

Integral scale, which represent the mean size of larger turbulent eddies, is a universally applied parameter in combustion modelling. Though, the exact relation between the length scale used in a CFD simulation and the actual integral length scale of a flow field is still an unsolved problem. Hence, several relations can be found in the literature for these purposes. Consequences of these expressions in combustion modelling are much noticeable in
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modelling the fully developed phase. Hence, a detailed discussion on this aspect is made in the next chapter.

4.8 Summary

- A model form for simulating the spark ignition and the early stage of flame propagation was developed based on the desecrate particle ignition kernel model.
- Negligence of the bulk flow convection effects and the assumption of a perfectly spherical flame front were identified as major draw backs of the standard DPIK model.
- As a solution, a methodology was developed to account for the bulk flow convection and wrinkling effects and the non-spherical nature of the flame front.
- The flame front was modelled using a set of Lagrangian particles which follows the path of the flame propagation.
- Particles travel at the resultant velocity of turbulent flame speed, plasma expansion speed and the local bulk flow velocity.
- The flame area is estimated to be the equivalent surface area of the burned gas volume.
- Particle motion was tracked by vector based parallelized computer algorithms and the local flame surface density and the reaction rate were estimated proportional to the number of marker particles within a computational cell.
- Transition to the main combustion model occurs when the flame kernel radius is large enough to be wrinkled by the larger eddies of turbulent.
Combustion in homogeneous charge spark ignition engines is essentially an ideal practical example for turbulent premixed combustion. Effects of combustion are mainly incorporated into the governing equations via source terms in species and enthalpy equations. In practise, computing these source terms are the most challenging task in combustion modelling. Chemical reactions, flame-turbulent interactions and flame-wall interactions are some of the key parameters to be accounted for in such a modelling exercise.

This chapter explains the present approach to estimate the reaction rate term. Section 5.1 provides the theoretical aspects and categorisation of flames considering the physical nature. Use of flame surface density modelling for reaction rate term calculation is discussed in section 5.2. The approach of the Bray-Moss-Libby (BML) (Bray et al. 1984) model for flame surface density calculation and its issues related to engine combustion modelling are highlighted is presented in section 5.3. Suggested solutions for those problems during the present work and their implementation are described in detail, starting from section 5.4. Development of a new model for evaluating the flame wrinkling scale is discussed in section 5.5 and 5.6. Development of a new correlation to estimate the flame quenching rate near cold boundaries is presented in section 5.7. Explained in section 5.8 are the chemical reaction mechanisms used in this study for the modelling of fuel oxidisation and other associated reactions. A concluding summary is presented in section 5.9.
5.1 Regimes of Premixed Turbulent Combustion

Effect of turbulence on combustion may be viewed as an interaction between flame fronts and turbulent eddies of various sizes. Eddies in a turbulent flow field may vary in size from Kolmogorov scale: the smallest, to the integral scale: the largest. The representative time scale of an eddy of size $r$ is defined by:

$$\tau_t(r) = \frac{l(r)}{u'(r)}$$  \hspace{1cm} (5.1)

where, $l(r)$ and $u'(r)$: the characteristic length and velocity scales of the eddy respectively, are functions of its size $r$ (Poinsot & Veynante 2005).

How fast the chemical reactions are, compared to the turbulent mixing in a premixed reactive flow field, can be identified by comparing the chemical and the integral turbulent time scales. Characteristic flame time or the chemical time scale can be defined using flame properties as:

$$\tau_c = \frac{\delta_l}{S_l^0}$$  \hspace{1cm} (5.2)

where, $\delta_l$ is the laminar flame thickness and $S_l^0$ is the unstrained laminar burning velocity. As a comparison measure, the ratio between the two time scales: the Damköhler number $Da$, is defined as:

$$Da(r) = \frac{\tau_t(r)}{\tau_c}$$  \hspace{1cm} (5.3)

The magnitude of the Damköhler number scatters from integral scale to the Kolmogorov scale. It is not yet clear that, what the most influential scale of turbulence is, in controlling the flame structure. However, it is possible to define two values for $Da(r)$ at extreme length scale limits; namely, at the Kolmogorov scale $\eta$ and the integral scale $L_i$.

$$Da = Da(L_i) = \frac{\tau_t(L_i)}{\tau_c}$$  \hspace{1cm} (5.4)

$$Ka = \frac{1}{Da(\eta)} = \frac{\tau_c}{\tau_t(\eta)}$$  \hspace{1cm} (5.5)

Damköhler number at integral scale is simply denoted by $Da$. The Karlovitz number $Ka$ corresponds to the reciprocal of Damköhler number at Kolmogorov scale. The characteristic
Kolmogorov time $t_\eta$, velocity $u_\eta$ and length scale $\eta$ are defined in terms of kinematic viscosity $\nu$ and dissipation rate of turbulent kinetic energy $\varepsilon$ as:

$$t_\eta = \left(\frac{\nu}{\varepsilon}\right)^{1/2} \quad u_\eta = (\nu \varepsilon)^{1/4} \quad \eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$$  \hspace{1cm} (5.6)

Schmidt number $Sc$ defines the ratio between the rates of viscous and molecular diffusion. Conventionally, for scaling purposes, a unit Schmidt number is assumed for premixed flames, together with the laminar flame thickness defined by the ratio between the molecular diffusivity $D$ and the kinematic viscosity. In practise, the value of Schmidt number is application dependent, but in the order of unity.

$$Sc = \frac{\nu}{D} = 1$$  \hspace{1cm} (5.7)

$$\delta_t = \frac{D}{S_0^0} = \frac{\nu}{S_0^0}$$  \hspace{1cm} (5.8)

Eq. (5.4) and (5.5) can be recast using Eq. (5.6) and (5.7) to obtain the following expressions, in conjunction with the definition of $\varepsilon \propto k^{15}/L_i$; where, $k$ is the turbulent kinetic energy.

$$Da = \frac{L_i/u'}{\delta_t/S_0^0}$$  \hspace{1cm} (5.9)

$$Ka = \frac{(u'/S_0^0)^{3/2}}{(L_i/\delta_t)^{1/2}}$$  \hspace{1cm} (5.10)

Further, the Damköhler number and the Karlovitz number can be related to the integral scale turbulent Reynolds number $Re_t$ using the following relation.

$$Re_t = \frac{u'L_i}{\nu} = \left(\frac{u' \delta_t}{S_0^0}\right) \left(\frac{L_i}{\delta_t}\right)$$  \hspace{1cm} (5.11)

$$Re_t = Da^2 Ka^2$$  \hspace{1cm} (5.12)

Based on the relative intensity of turbulent-chemistry interaction, several families of flames are identified and often interpreted in the form of combustion regime diagrams. According to Poinset & Veynante (2005), several combustion regime diagrams have been proposed by various researchers including Barrera (1974), Bray (1980), Borghi (1984), Williams (1985) and Poinset et al. (1991) and Peters (1999). Figure 5.1 depicts an adapted version of the
combustion diagram suggested by Peters (1999). It is worth noting that, the criteria and regime limits used to distinguish different zones are solely based on the order of magnitude estimations and not on precise derivations. Further, a homogeneous isotropic turbulence field unaffected by the heat release due to chemical reactions is implicitly assumed, despite its unphysical nature.

Figure 5.1: Regimes of the premixed combustion. The operating range of the piston engines is highlighted by the dashed rectangular region. Adapted from Peters (1999)

Lines given by $Ka = 100$ and $Re_t = 1$ provide the boundaries for each region. Unit Damköhler number line and the operating range of a typical piston driven IC engines are also shown for clarity. When the turbulent Reynolds number is less than the unity, the effect of turbulence is insignificant on combustion thus a laminar combustion process is observed.

Large Damköhler numbers ($Da > 1$) imply that the time scale of chemical reactions are extremely small compared to the integral time scale of turbulence. Hence, the turbulence cannot influence the inner reacting structure of the flame front, but it distorts the flame surface by wrinkling. Consequently, the flame front may propagate in laminar burning
velocity and reaction rate is directly proportional to the product of laminar burning velocity and the overall flame surface area. Moreover, chemical reactions in this region may be modelled employing the classical infinitely fast chemistry assumptions. It should also be noted that, majority of the operating range of a typical piston operated IC engine lies within this region. Remarkably, not only piston engines but also most of the practical combustion devices such as gas turbines and industrial furnaces operate in the same region. Thus, for this regime, numerous models have been proposed for combustion simulations.

In the region where chemical time scale is much larger than the turbulent time scale, the Damköhler number becomes much smaller than the unity \((Da \ll 1)\). Therefore, the reactants and products are rapidly mixed with each other by turbulence eddies; hence, called the \textit{perfectly stirred reactor}. Usually, in modelling, instantaneous mixing is assumed for this region. The overall reaction rate is, then controlled by chemistry and can be easily modelled using a simplified Arrhenius type expression with a good accuracy (Poinsot & Veynante 2005).

Based on the Karlovitz number, above regions may be further classified into sub regions with characteristic properties. Only the conclusions of the regime analysis are given here. A detailed description of magnitude arguments used in classification can be found in Peters (2000).

- \(Ka < 1\) : implies the following properties of the flame front.
  - Chemical time scale is shorter than the any of the turbulent time scales.
  - Flame thickness is smaller than the smallest turbulent scale, the Kolmogorov scale.
  - Flame front is very thin with laminar like inner reacting structure.
  - It can be wrinkled by turbulence motion.
  - Based on the velocity ratio \(u'/S^0\), this regime is further divided in to two regions.
    - \(u' < S^0\): speed of the turbulent velocity fluctuations are not severe enough to wrinkle the flame until the flame surface crosses itself. A continuous, but wrinkled surface may be observed in the absence of flame quenching, hence the name \textit{wrinkled-flamelets} is given.
    - \(u' > S^0\): turbulent motion is strong enough to wrinkle the flame front until it crosses itself forming fresh and burned gas pockets. Flames in this region are called the \textit{corrugated flamelets}.
- Peters (1999) derived an expression for the smallest scale of the turbulent eddy that can locally interact by wrinkling the flame front in flamelet region. This scale is termed as the Gibson scale $L_G$ and expressed by the following relation.

$$L_G = \frac{S_l^{0.3}}{\varepsilon}$$  \hspace{1cm} (5.13)

Using the relation $\propto u'/L_i$, $L_G$ can be recast as:

$$L_G = C_G L_i \left(\frac{S_l^{0.3}}{u'}\right)^3$$  \hspace{1cm} (5.14)

where, $C_G$ is a proportionality constant.

- $Ka > 1$ and $Da > 1$ : means that the turbulent time scale is larger than the chemical time scale. On the other hand, the flame brush thickness is also larger than the smallest scale of turbulence: the Kolmogorov scale. Hence, Kolmogorov eddies can enter in to the pre heat zone and widen the flame thickness, However, the inner reaction zone thickness is still smaller than the Kolmogorov scale and, remains unaffected. Therefore, this regime is called the *thin reaction zone* or *thicken wrinkled flame* regime.

- $Da < 1$ : infers that the chemical time scale is larger than the turbulent time scale and flame properties are chemistry dependent. No further discussion is made here on this as the focus of the present research is only on the operating range of the piston engines.

As explained above, turbulent flame interaction shows different characteristics based on how strong the turbulence is. Developing a unified modelling approach to accurately predict the flame behaviour in all the regions is an extremely difficult task. Therefore, individual regions are catered separately with customized approaches, mostly on application basis.

### 5.2 Estimation of the Unburned Gas Consumption Rate

From the discussion in section 5.1, it is clear that the flamelet combustion can be assumed for a vast majority of operating conditions of premixed SI engine. Indeed, this has become the most common approach (Poinsot & Veynante 2005). Several studies including Abu-Orf & Cant (2000) and Zhao *et al.* (1994a) have followed this concept and obtained promising results. In this study too, a flamelet approach is used to model the premixed combustion in SI engines.
It should be noted here that, Favre average symbol ‘tilde’ (~), has been omitted in this chapter for the simplicity. Therefore, all the turbulent quantities shown here are Favre averaged values unless otherwise explicitly stated.

In the flamelet regime, assuming a thin flame front, with infinitely fast chemistry, the instantaneous unburned mass consumption rate per unit volume \( \bar{\omega} \), in the absences of flame quenching due to strain can be written by:

\[
\bar{\omega} = I_0 \rho_u \delta t \frac{\delta A}{\delta V}
\]  

(5.15)

where, \( \delta A \) is the total flame surface area within the infinitesimal volume \( \delta V \) and \( \rho_u \) is the unburned gas density. Factor \( I_0 \) accounts for the turbulent and curvature strain effect on the flame propagation speed. If \( \Sigma \) represents the available mean flame surface area per unit volume (i.e. \( \delta A/\delta V \)), the above equation can be rearranged to obtain the following equation.

\[
\bar{\omega} = I_0 \rho_u S_1^0 \Sigma
\]  

(5.16)

Here, \( \Sigma \) is called the flame surface density (FSD). Closure of the Eq. (5.16) requires modelling of the unstrained laminar flame speed, stretch factor \( I_0 \) and flame surface density. In this study, the experimental correlation proposed by Gülder (1984) is used for modelling the unstrained laminar burning velocity. A detailed description of the model equations has been presented in Chapter 4 of this thesis. Thus, the discussion here is limited to the modelling of flame surface density and \( I_0 \).

It is possible to solve a complete balance equation following Trouve & Poinsot (1994) or Cant et al. (1990) for FSD, incorporating detailed models for flame-turbulent interaction. This is one of the most accurate methods as evident from the results of Choi & Huh (1998) and Teraji et al. (2009), but associates a significant computational overhead. FSD balance equations often involve several case dependent model constants, which need to be fine-tuned to match the operating conditions on case by case basis. On the other hand, simple algebraic models that describe the main features of flame surface density have become handy for its less computational cost and lesser number of tuning constants. In fact, these simple models have found to outperform more complex formulations, such as solving a balance equation for \( \Sigma \), in some engine related applications (Zhao et al. 1994a). Consequently, the present study develops an algebraic model form to compute the flame surface density and the mean species consumption rate.
More precisely, the work presented here, aims to formulate a new combustion model based on
the well-known Bray-Moss-Libby (BML) model (Bray et al. 1984). Theoretical and
experimental based modifications have been suggested, such that the BML model can be
applied to wall-bounded combustion modelling eliminating the wall flame acceleration
problem, which is an inherent issue in the standard BML model. Estimation of integral length
scale of turbulence has been made dynamic, so that allowance for spatial inhomogeneity of
turbulence is made. A new dynamic formulation has also been proposed based on the
Kolmogorov-Petrovski-Piskunov analysis and fractal geometry to evaluate the mean flame
wrinkling scale. In addition, a novel empirical correlation to quantify the quenching rates
within the influenced zone of the quenching region near solid boundaries has been derived
based on experimentally estimated flame image data. Starting from the next section, a
comprehensive discussion is made on the development of the present formulation.

5.3 The Bray Moss Libby (BML) Model

Bray et al. (1984) identified that the mean reaction rate at a point in a reacting flow field is
mostly dependent on the number of flamelet crossings per unit time (i.e. the crossing
frequency of the flame front) than the local mean temperature or the species mass fraction. In
other words, they experimentally observed that, the highest reaction rate occurs at point B in
the Figure 5.2 (b), rather than at the points A or C.

Figure 5.2: Measured temperature signal vs. time (a) at points A, B and C in (b). $T_1$ is the
minimum, $T_2$ is the maximum and $\bar{T}$ is the time averaged measured temperatures
Figure 5.2(b) shows three spatial points: A, B and C, where point A is located in the unburned gas region, B within flame brush and C in the burned gas region. Plotted in Figure 5.2(a) are the time evolutions of measured temperature signals at corresponding points. Interestingly, these temperature profiles were of the square wave form as shown. $\bar{T}$ denotes the measured time mean temperature at the corresponding location. It is easily understood that, the point B corresponds to the most number of flamelet crossings per unit time, whereas points A and C have a minimum number of such crossings, even though the point C is entirely within the high temperature burned gas region. This observation lead to the conclusion that, the mean reaction rate can be modelled as the product of flamelet crossing frequency $f_x$ and the reaction rate per unit flamelet crossing $\dot{\omega}_x$, as given below.

$$\bar{\omega} \propto \dot{\omega}_x f_x \quad (5.17)$$

### 5.3.1 Spatial Flamelet Crossing Frequency

Having identified the relationship between temporal flamelet crossing frequency and the mean reaction rate, the association between the spatial flamelet crossing frequency and the mean reaction rate is now established. Instantaneous flame surface crossing an iso-progress variable surface on a given two dimensional plane is shown in Figure 5.3.

![Instantaneous flame front crossing a mean iso-progress variable surface.](image)

**Figure 5.3:** Instantaneous flame surface crossing a mean iso-progress variable surface. $L_y$ is the integral scale of flame wrinkling.

Along the iso $\bar{c}$ curve, the distribution of the instantaneous progress variable $c$ is again found to be of the square wave form (Cant & Bray 1988). Therefore, as the reaction rate at a spatial location is proportional to the number of flamelet crossings, it is argued that the reaction rate...
per unit length of the mean progress variable curve is also proportional to number of flame front crossings.

Consequently, the overall reaction rate may be specified in terms of spatial crossing frequency \( n_y \) as:

\[
\overline{\dot{\omega}} \propto \dot{\omega}_x n_y
\]  

(5.18)

where, \( n_y \) is the number of flamelet crossings per unit length (spatial frequency of flamelet crossings). If \( L_y \) is the integral scale of flame wrinkling or the wavelength of the square wave function (see Figure 5.3), \( n_y \) can be written as (Bray et al. 1989):

\[
n_y = \frac{g\bar{\varepsilon}(1 - \bar{\varepsilon})}{L_y}
\]  

(5.19)

If the mean spatial distribution of flamelet crossing points on the iso-\( \bar{\varepsilon} \) surface is exponential, \( g \) is taken to be 2.0 or if a symmetric beta probability distribution is assumed, a value of 1.0 may be taken. In practise, this distribution is found to vary in-between symmetric and exponential range.

Aluri et al. (2005) have used \( g = 1.0 \) for Bunsen flame simulations; but, at the expense of tuning some of the other modal constants to match with experimental results. Having arrived at a different set of values ranging from 1.7 to 2.2 Chang et al. (2001) and Shy et al. (1996) suggested further investigation to identify a suitable value for \( g \). Abu-Orf & Cant (2000) and Watkins et al. (1996) have used a value of 1.5 while, Ranasinghe & Cant (2000) have used 1.0; all with reasonable success in SI engine applications. However, studies of Chew et al. (1990) and Patel & Ibrahim (2002) show that, scatter of crossing lengths are more biased towards an exponential distribution with an average \( g \) value of around 1.7-2.0. Further, they suggested that it would be better approximated for varying degree of reactions by \( g = 1 + 2\bar{\varepsilon} \). Accordingly, this expression is adopted for the present study.

5.3.2 Flame Wrinkling Length Scale

Integral scale or the characteristic scale of flame wrinkling \( L_y \), is modelled using the empirical relation given in Eq. (5.20), which is originally suggested by Bray (1990), merely based on the simulation results of Chatè (1987) and Chatè & Cant (1988). Remarkably, this expression has been able to produced good qualitative results with standard model constants and, quite good quantitative agreements when they are fine-tuned. The expression relies on the argument that the flame wrinkling length scale is a direct function of both integral scale of
turbulence and laminar flame speeds as shown by Figure 5.4. This may be justified, as the higher laminar flame speeds tends to smooth out the turbulent fluctuations, thereby increasing the wrinkling scale.

\[
L_y = C_b L_i \left( \frac{S'_t}{u'} \right)^n
\]  

(5.20)

Originally, Bray (1990) proposed a value of 1.0 for \( n \), though different fine-tuned values are found in the literature: for example, Aluri et al. (2005) suggested a value of 1.2. \( C_b \) is an adjustable model constant in the order of unity. Generally the integral scale is modelled as:

\[
L_i = C_L u^3 / \varepsilon
\]  

(5.21)

where, \( C_L \) is a model constant.

Figure 5.4: Wrinkling of flame front due to the interaction between the flame front and flow eddies

The above relation for \( L_y \): initially proposed for stagnation flames, seems to over predict the reaction rate (extremely high values) near solid boundaries, when applied to engine like wall bounded systems. Physically, this is totally unrealistic, as flames tend to extinguish at walls due to thermal quenching. Therefore, alternative expressions have been proposed by Watkins et al. (1996), Bailly et al. (1996) and Abu-Orf & Cant (2000). The deficiencies of the expressions in Eq. (5.20) and (5.21) have been one of the major concerns addressed in the present study. Hence, an improved formalism is derived for \( L_y \) in this work, as described in a latter section.
5.3.3 Flame Surface Density

Closure of the reaction rate model still requires modelling $\dot{\omega}_x$: the mean reaction rate for a unit flamelet crossing. Finding an expression for $\dot{\omega}_x$ is a difficult task. Thus, Bray et al. (1989) correlated the spatial flamelet crossing frequency to the mean flame surface density as:

$$ \Sigma = \frac{n_y}{|\sigma_y|} $$

(5.22)

where, $\sigma_y$ is the mean cosine angle between the tangent vector to the flame front and the mean iso $\tilde{c}$ surface at the location of flamelet crossing, i.e. $\sigma_y = \cos \alpha$ with reference to the Figure 5.3. In the past, $\sigma_y$ was considered to be a universal constant having a value of 0.5. Chang et al. (2001) and Shy et al. (1996) experimentally found its value to be 0.65. However, a value of 0.7 has been used by Lahjaily et al. (1998) as revealed by DNS studies. In this work also, a value of 0.7 was found to produce better results. The final model equation for the flame surface density as suggested by the standard BML model is of the following form:

$$ \Sigma = \frac{g}{|\sigma_y|} \frac{1 + \tau}{(1 + \tau \tilde{c})^2} \tilde{c}(1 - \tilde{c}) $$

(5.23)

5.3.4 Estimation of the Stretch Factor

As previously briefed in Chapter 4, the strain effects on flame propagation are twofold: geometric strain effects and turbulent strain effects. Generally, the effect of strain on the laminar flame speed is taken to be negative, i.e. strain hinders the unstrained laminar speed. Note that, there are some exceptions, where this assumption contradicts (Stahl & Warnatz 1989). Haworth & Poinson (1992) showed from DNS result that, $I_0$ remain close to unity in all levels of turbulence, thus some modelling studies simply neglect the $I_0$ by setting it to be unity. An accurate method to obtain values for $I_0$ is to use laminar flamelet libraries, but this needs to maintain a database of turbulent and flame properties for a range of conditions in the reacting flow. To avoid this difficulty, Bray (1990) proposed a relationship for $I_0$ by curve fitting the experimental data of Abdel-Gayed et al. (1989), assuming the only influencing factor on strain is the Karlovitz number. However, this relation is applicable only for very high turbulence levels and not suitable for engine combustion. In addition, several other expressions for $I_0$ have been reported in Chung & Law (1988), Wu et al. (1993) and Law et al. (1986). All these models are found to produce reasonable results in most of the engineering combustion problems.
According to Law et al. (1986), $I_0$ can be expressed as:

$$I_0 = 1 - \left[ \frac{\delta_t}{S_l^0 Le} + \left( \frac{1}{Le} - 1 \right) \left( \frac{\delta_t T_a}{S_l^0 Le 2T_{ad}} \right) \right] K_E$$  \hspace{1cm} (5.24)

where, $K_E$ is the effective strain rate and $T_a$ is the activation temperature of the combustion reaction. $T_{ad}$ is the adiabatic temperature of the flame. The Lewis number $Le$ interprets the relative intensity of molecular and heat diffusion. Most of the technically interested flames have a Lewis number close to unity. Thus, unity Lewis number is a common assumption in engineering combustion modelling. Accordingly, the above relation is reduced to Eq. (5.25).

$$I_0 = 1 - \left( \frac{\delta_t}{S_l^0} \right) K_E$$  \hspace{1cm} (5.25)

The effective strain rate could be split into two parts for explicit representation of geometric (curvature) strain rate $K_C$ and the turbulent strain rate $K_T$.

$$K_E = K_C + K_T$$  \hspace{1cm} (5.26)

$K_C$ is defined as the rate of increase of the flame surface area per unit flame surface area:

$$K_C = \frac{1}{A} \frac{dA}{dt}$$  \hspace{1cm} (5.27)

For spherically propagating flames with a radius $r$, $K_C$ is reduced to:

$$K_C = \frac{2}{r} \frac{dr}{dt}$$  \hspace{1cm} (5.28)

Compared to the order of magnitude of turbulent strain, geometric strain rate is negligible for fully developed flames, but could be higher or in a similar order during the flame kernel development. Thus, $K_C$ is often neglected in fully developed phase and explicitly modelled in the early stage of flame propagation.

Turbulent strain rate $K_T$ is often called Karlovitz stretch factor and, can be computed from the expression below (Matthews & Chin 1991).

$$K_T = \frac{u'}{L_\lambda}$$  \hspace{1cm} (5.29)

The Taylor micro scale $L_\lambda$ is related to the integral scale $L_i$ by:
where, $A$ is a model constant estimated to be 40.4 by Abdel-Gayed & Bradley (1985), correlating experimental data. It should be noted that, the expression used for $I_0$ in Chapter 4 during the flame kernel formation has been derived by accounting for both geometric and turbulent strain effects.

### 5.3.5 Application of the BML Model to Wall Bounded Systems

The BML model and its variants have been successfully used in premixed combustion modelling studies for many years. Application of the original BML model for the simulation of open-stagnation flames has shown to be capable of producing comparably good results. However, its applications in wall bound combustion problems are rare. This is due to the ‘near wall flame acceleration problem’, or in simple terms, predicting excessively higher unphysical reaction rates near solid boundaries. In reality, this is unacceptable, as flames tend to extinguish at walls due to thermal quenching.

BML model assumes isotropic homogeneous turbulence. Thus, its application in the core region of the flame (where sufficiently homogeneous turbulent can be expected) provides satisfactory results. Conversely, near solid boundaries, the homogeneous assumption is no longer valid, owing to the presence of a sharp gradient of turbulent properties. Furthermore, the turbulent intensity $u'$ rapidly decreases towards zero, which eventually leads to very small values of the integral scale given by $L_i \sim u'^{3/2}/\varepsilon$. Consequently, the flame wrinkling scale $L_y$ also becomes very small making flame surface density infinite; so as the reaction rate.

A number of alternative forms of the BML model have been suggested in the literature to overcome this problem, but most of them are based on ad-hoc assumptions. For example, in the work of Watkins et al. (1996) and Abu-Orf & Cant (2000) the flame wrinkling is assumed to be an empirical function of laminar flame thickness and the turbulent intensity. Necessary damping of the reaction rate near walls is artificially embedded via an exponential correlation. The fundamental disadvantage of these substitutions is that they neglect the well-known direct dependency of the integral scale of turbulence on the flame wrinkling. Thus, improvements are suggested in this study as described later.
5.3.6 Some Concerns about the BML Model Parameters

Expression for the flame surface density and the mean wrinkling scale of the BML model have already been stated in the previous sections. Those expressions are repeated here in Eq. (5.31) and (5.32).

\[
\Sigma = \frac{g}{|\sigma_y|} \frac{1 + \tau}{(1 + \tau \bar{c})^2} \frac{\bar{c} (1 - \bar{c})}{L_y}
\]

(5.31)

\[
L_y = C_b L_i \left( \frac{S_t}{u'} \right)^n
\]

(5.32)

Model constants reported in the literature are summarised in Table 5.1. Some of the points mentioned below have already been discussed, but presented here for comparison purposes and to capture a global picture of the situation.

Careful observation of the values in Table 5.1 indicates that \( g \) is much closer to 2.0, showing an exponential distribution of flamelet crossing frequency. In addition, the mean cosine angle between the flame front and the normal to the iso-\( \bar{c} \) surface of the flame \( \sigma_y \), is biased more towards 0.7 showing a distinct deviation from original value of 0.5. These trends have further been verified by the DNS results and experiments of Chew et al. (1990) and Deschamps et al. (1996). On the other hand, the scatter of model parameters \( C_b \) and \( n \) is high and no any reasonable mean value can be seen. This has become a major implication on standard BML model and all the above authors strongly suggest an alternative description for the flame wrinkling scale. In fact, Abu-Orf & Cant (2000), Ranasinghe & Cant (2000) and Watkins et al. (1996) have already used correlation based empirical equations, in order to calculate the wrinkling scale with the allowance for flame quenching at walls.

### Table 5.1 BML model constants found in the literature

<table>
<thead>
<tr>
<th>Author</th>
<th>Application</th>
<th>( g )</th>
<th>( \sigma_y )</th>
<th>( C_b )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bray (1990) ( ^{\text{xy}} )</td>
<td>Bunsen flames</td>
<td>1 or 2</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Aluri et al. (2005) ( ^{\dagger} )</td>
<td>Bunsen flames</td>
<td>1</td>
<td>0.5</td>
<td>1</td>
<td>1.2</td>
</tr>
<tr>
<td>Chang et al. (2001) ( ^{\dagger} )</td>
<td>Cruciform burner</td>
<td>1.79-1.83</td>
<td>0.65</td>
<td>0.23</td>
<td>0.36</td>
</tr>
<tr>
<td>Shy et al. (1996) ( ^{\dagger} )</td>
<td>Surface stabilized flames</td>
<td>2</td>
<td>0.65</td>
<td>12.3</td>
<td>0.41</td>
</tr>
<tr>
<td>Ghenai et al. (1996) ( ^{\dagger} )</td>
<td>Open conical flames</td>
<td>1.5</td>
<td>0.7</td>
<td>0.85-0.3( \bar{c} )</td>
<td>0.45+0.2( \bar{c} )</td>
</tr>
<tr>
<td>Abu-Orf &amp; Cant (2000) ( ^{\dagger} )</td>
<td>SI engine combustion</td>
<td>0.5</td>
<td>0.5</td>
<td>( AE^* )</td>
<td>( AE^* )</td>
</tr>
<tr>
<td>Ranasinghe &amp; Cant (2000) ( ^{\dagger} )</td>
<td>SI engine combustion</td>
<td>0.5</td>
<td>0.5</td>
<td>( AE^* )</td>
<td>( AE^* )</td>
</tr>
<tr>
<td>Watkins et al. (1996) ( ^{\dagger} )</td>
<td>SI engine combustion</td>
<td>1.5</td>
<td>0.5</td>
<td>( AE^* )</td>
<td>( AE^* )</td>
</tr>
<tr>
<td>Patel (2001) ( ^{\dagger} )</td>
<td>Stagnation flames</td>
<td>1+ 2( \bar{c} )</td>
<td>0.5</td>
<td>1.0</td>
<td>6D-13</td>
</tr>
</tbody>
</table>
Therefore, having identified the problematic nature of the current expression for flame wrinkling scale in the BML model, a new formulation is proposed here in this study. This approach is based on the fundamental theories of fractal modelling of combustion. It allows integrating dynamic variations of local wrinkling scale caused by the inhomogeneity of turbulence. Consequently, a brief note on the fractal modelling of turbulent combustion is presented below in the next section to support the understanding of present modelling approach.

5.4 Fractal Flame Model (FFM) for Turbulent Combustion

Most shapes found in nature exhibit self-similar characteristics; so do turbulent flame fronts. Fractal geometry provides an accurate statistical description of the geometric properties of highly contoured and roughened curves and surfaces with self-similarity features (Gouldin 1987). Thus, fractal explanations of turbulent combustion are materialized. Even in SI engines, where turbulence rigorously interacts with the flame front, the universal fractal behaviour has been observed (Mantzaras et al. 1989 & Hall et al. 1992). In the flamelet region with thin flame fronts, where low and moderate turbulence levels are present, Gouldin (1987) showed that under homogeneous isotropic turbulence, the actual mean flame front area \( A_f \) can be estimated from:

\[
A_f = A_i = A_o \left( \frac{\epsilon_o}{\epsilon_i} \right)^{D-2}
\]

(5.33)

where,

- \( \epsilon_i \) — Inner cut off length scale
- \( \epsilon_o \) — Outer cut off length scale
- \( A_i \) — Measured flame surface area using the inner cut off length scale
- \( A_o \) — Measured flame surface area using the outer cut off length scale
- \( D \) — Fractal dimension of the flame surface

\( \epsilon_i \) and \( \epsilon_o \) denote the smallest and the largest possible flame wrinkling scales. The fractal dimension \( D \) is a quantitative measure of how wrinkly the surface is. Thus, the value of \( D \) is equally influenced by the relative intensity of all sizes of wrinkling scales.
Various length scales of turbulence contribute in different proportions for wrinkling the flame front. As a first guess, the smallest scale of turbulence; the Kolmogorov length scale, may be assumed to be the inner cut off length scale of flame wrinkling. Even though, it is still unclear what the minimum length scale of flame wrinkling in engine like conditions, a length scale slightly larger than the Kolmogorov scale is found to be the inner cut off limit for grid stabilized and V-shaped flames by Gouldin (1987) and Murayama & Takeno (1989). Further, they suggested it to be in the order of 1.3 times of Kolmogorov scale or occasionally as much as 5.8 times for lean mixtures. Peters (1999) argued that, within the flamelet region, the Gibson scale should be considered as the inner cut off scale. Despite this, both the Kolmogorov and Gibson scales are equally employed in modelling though. A number of other expressions have also been suggested for $\varepsilon_i$ by several authors including Poinot et al. (1991) and Roberts et al. (1993). A comparison of these models can be found in G"uder & Smallwood (1995). Further, the outer cut off scale is recognized to be larger than the integral scale, sometimes as twice in IC engines (Mantzaras 1989). Nonetheless, during the early stage of flame kernel development, the maximum flame wrinkling scale cannot be larger than the flame dimension, due to the fact that the scales larger than the flame size cannot wrinkle the flame. However, following Peters (1999), the Gibson scale and the integral scale of turbulence are considered to be respectively the minimum and maximum scales of flame wrinkling during the fully developed combustion period in the present study as given in Eq. (5.34).

$$\frac{\varepsilon_o}{\varepsilon_i} = \frac{L_i}{L_G}$$

(5.34)

### 5.4.1 Fractal Dimension

Identifying the correct value for the fractal dimension $D$ in an application is the fundamental difficulty in fractal modelling. However, it is bound by the lower limit of 2.0: for perfectly smooth surfaces, and the upper limit of 3.0: for highly roughened surfaces. Figure 5.5 shows the measured fractal dimension by North & Santavicca (1990) in an SI engine. It indicates that, the fractal dimension scatters from 2.1 to 2.35 for the range considered.
Figure 5.5: Measured and curve fitted fractal dimension in an SI engine. Adapted from Zhao et al. (1994a)

Flame curvature is affected not only by the turbulence length scales, but also by the relative turbulence intensity to the laminar flame speed. Therefore, both of these effects must be considered when arriving at an expression for the fractal dimension. A direct prominent dependence of flame curvature on the integral length scales and a substantial dependence on the square root of $u'/S_l$ has been clearly observed by Lee et al. (1992). This provides a justification for the following heuristic relation suggested by North & Santavicca (1990):

$$D = D_t \frac{S_l^0}{u' + S_l^0} + D_t \frac{u'}{u' + S_l^0}$$

(5.35)

where, $D_t$ is the fractal dimension for a smooth surface and $D_t$ is the maximum possible fractal dimension for the flamelet under consideration. Based on the experimental results, a value of 2.0 for $D_t$ and a 2.35 for $D_t$ are suggested, though values as high as 2.41 have also been proposed for $D_t$ by Francke et al. (1990). Value of 2.0 for $D_t$ seems logically correct as it is defined on a smooth surface, but in practice a value of 2.05 is found to produce better overall results (Santavicca 1989).

However, over the years, several modifications have been proposed to Eq. (5.35) and Zhao et al. (1994a) suggested the following relations after curve fitting the data in Figure 5.5.
At a glance, it seems that the above expression neglects the effect of laminar flame speed yet, it is implicitly accounted for by the turbulent Reynolds number. Under the unit Schmidt number assumption, $Re_t$ can be written as:

$$Re_t = \frac{u'\bar{l}_i}{v} = \left(\frac{u'}{S_i^0}\right)\left(\frac{\bar{l}_i}{\delta_i}\right)$$

Due to the considerable success after Zhao et al. (1994a) and Palipana (2000) in SI engine combustion modelling, the above relation for the fractal dimension is used in the present study.

### 5.4.2 Turbulent Flame Speed of the Fractal Model

By definition, the ratio between the turbulent flame speed and the laminar burning velocity is equal to the ratio of total flame surface area $A_f$ to the mean flame surface area $A_t$ projected towards the propagation direction, as given in Eq. (5.38). Following fractal theories of combustion (Matthews et al. 1991), the inner and outer cut off flame areas may be related to the flame speeds according to Eq. (5.39). The parameter $C_t$ is dependent on the nature of the turbulence of the flow field, but often assumed to be an adjustable constant.

$$\frac{S_t}{S_i} = \frac{A_f}{A_t} = C_t \frac{A_f}{A_0}$$  \hspace{1cm} (5.38)

$$\frac{S_t}{S_i} = C_t \left(\frac{\varepsilon_0}{\varepsilon_i}\right)^{D-2}$$  \hspace{1cm} (5.39)

Combining the two equations, a resultant expression for the turbulent velocity of the FFM model can be obtained as follows. $I_0$ has been introduced to make allowances for strain effects on the laminar flame speed.

$$S_{t,FFM} = C_t I_0 S_i^0 \left(\frac{\varepsilon_0}{\varepsilon_i}\right)^{D-2}$$  \hspace{1cm} (5.40)

This turbulent flame speed relation is used in the following section in obtaining a fractal based expression for the mean flame wrinkling scale.
5.5 A Novel Fractal Based Description for the BML Model

The mean flame wrinkling scale or the integral scale of flame wrinkling; introduced in the BML model, is often seen to be affected by the whole spectrum of turbulence. Mean integral scale of flame wrinkling is typically much larger than the integral scale of turbulence (Kuo 2005), but sometimes, it can be even smaller than the turbulent integral scale (Shy et al. 2000). Thus to make the modelling results more accurate, effect of all the possible scales on flame wrinkling should be introduced (Poinsot & Veynante 2005). The fractal dimension is a quantitative index of the degree of flame wrinkling induced by the entire turbulence spectrum. Thus, a fractal based description of $L_y$ should implicitly account for such influences.

5.5.1 Kolmogorov – Pertovsky – Piskunow (KPP) Analysis

KPP analysis provides a theoretical tool to compare different combustion models via the turbulent burning velocity. Detailed descriptions of this analysis are found in Hackberge and Gosman (1984), Fichot et al. (1993), Duclos et al. (1993) and Poinsot & Veynante (2005). Assuming a frozen turbulence field, unaffected by the combustion heat release, a balance equation for the statically one dimensional, steadily propagating turbulent flame can be written using the mean reaction progress variable (Poinsot & Veynante 2005).

$$\rho_u S_t \frac{\partial \tilde{c}}{\partial x} = \bar{\rho} \frac{\nu_{eff}}{Sc_{eff}} \frac{\partial^2 \tilde{c}}{\partial x^2} + \tilde{\omega} \tag{5.41}$$

$\rho_u$ is the fresh gas density and $\bar{\rho}$ is the mean gas density. KPP analysis aims to find an exponential solution for the above equation at the leading flame edge, where $\tilde{c}$ goes to zero. Under these conditions, it is possible to assume that all the other variables except derivatives are constants. Then, if $\tilde{\omega} = \rho_u \omega_0 \tilde{c}$, where $\omega_0$ is a constant, there exists an exponential solution for the above equation if the discriminant $\Delta$ is greater than or equals to zero:

$$\Delta = S_t^2 - 4 \frac{\nu_{eff}}{Sc_{eff}} \omega_0 \geq 0 \tag{5.42}$$

It should be noted that, $\bar{\rho}$ is assumed equal to $\rho_u$ at the very edge of the flame front. The KPP theorem shows that, the actual solution of the Eq. (5.41) corresponds to the lowest turbulent speed given by:

$$S_t = \sqrt{\frac{4 \nu_{eff}}{Sc_{eff}} \omega_0} \tag{5.43}$$
5.5.2 KPP Turbulent Speed of the BML Model and FFM Model

Reaction rate expression of the BML model can be expressed in the form:

\[ \bar{\omega} = \rho_u l_0 S_i^0 \Sigma = \frac{\rho_u l_0 S_i^0}{\sigma_y} g \frac{1 + \tau}{(1 + \tau \bar{c})^2} \frac{\bar{c}(1 - \bar{c})}{C_b L_i \left( \frac{S_i^0}{u'} \right)^{\pi}} \]  \hspace{1cm} (5.44)

When \( \bar{c} \) goes to zero, neglecting higher order terms of \( \bar{c} \), the reaction term can be rearranged to obtain the following.

\[ \bar{\omega} = \rho_u \omega_0 \bar{c} = \frac{\rho_u l_0 S_i^0}{\sigma_y} g \frac{1 + \tau}{C_b L_i \left( \frac{S_i^0}{u'} \right)^{\pi}} \bar{c} \]  \hspace{1cm} (5.45)

Therefore, according to the KPP theorem turbulent speed of the BML model would be:

\[ S_{t,BML} = \sqrt{\frac{4 \nu_{eff} l_0 S_i^0}{Sc_{eff}} \frac{g}{\sigma_y} \frac{1 + \tau}{C_b L_i \left( \frac{S_i^0}{u'} \right)^{\pi}}} \]  \hspace{1cm} (5.46)

It is possible to interpret \( \nu_{eff}/Sc_{eff} \) as a function of integral scale and the root mean square turbulent velocity fluctuation (Bray 1990).

\[ C_{eff} u'L_i = \frac{\nu_{eff}}{Sc_{eff}} \]  \hspace{1cm} (5.47)

where, \( C_{eff} \) is a constant. The final expression of the BML turbulent flame speed is:

\[ S_{t,BML} = \sqrt{\frac{4 C_{eff} u'L_i S_i^0}{\sigma_y} \frac{g}{g} \frac{1 + \tau}{C_b \left( \frac{S_i^0}{u'} \right)^{\pi}}} \]  \hspace{1cm} (5.48)

An expression for the turbulent velocity predicted by the fractal model was already derived in the previous section. Thus, equating the turbulent velocities of both models given by Eq. (5.48) and Eq. (5.40) yields:

\[ C_t l_0 S_i^0 \left( \frac{\varepsilon_0}{\varepsilon_i} \right)^{D-2} = \sqrt{\frac{4 C_{eff} u'L_i S_i^0}{\sigma_y} \frac{g}{g} \frac{1 + \tau}{C_b \left( \frac{S_i^0}{u'} \right)^{\pi}}} \]  \hspace{1cm} (5.49)
In the early stage of fractal modelling, the parameter $C_t$ was considered to be a constant (Gouldin 1987). However, later it was recognized that this would result in modelling deficiencies as shown by Gülder & Smallwood (2000) and Zhao et al. (1994a). Therefore, $C_t$ can be more accurately interpreted by assuming proportional to $(\frac{u'}{S_l})^{1/2}$, following Zhao et al. (1994a).

$$C_t = C_t' \left( \frac{u'}{S_l^0} \right)^{1/2} \quad (5.50)$$

If the minimum and maximum scales of flame wrinkling is represented using the Gibson scale and the integral scale respectively, the wrinkling ratio becomes,

$$\left( \frac{\varepsilon_0}{\varepsilon_i} \right)^{D-2} = C_G^{D-2} \left( \frac{u'}{S_l^0} \right)^{3(D-2)} \quad (5.51)$$

Substituting Eq. (5.50) and (5.51) in Eq. (5.49), the following final form is obtained.

$$C'_t I_0 C_G^{D-2} \left( \frac{u'}{S_l^0} \right)^{1/2} \frac{u'}{S_l^0}^{3(D-2)} = \frac{4C_{eff} I_0 g}{\sigma_y} \frac{1 + \tau}{C_b} \left( \frac{u'^{n+1}}{S_l^0} \right) \quad (5.52)$$

As the both sides of the equation are equal to each other, both sides must also be dimensionally the same. Consequently, by comparing the dimension, it is understood that:

$$n = 6D - 12 \quad (5.53)$$

In Bray’s (1990) original model, $C_t$ was assumed to be a constant. The inner and outer flame wrinkling scales were assumed to be integral and Gibson scales respectively. This resulted in $n = 6D - 13$. Further, the fractal dimension was assumed to be a constant with a value $D = 7/3$ and this yields $n = 1$. The fractal dimension is a variable in SI engine applications. Complex nature of in-cylinder combustion dynamics generates spatially and temporally varying flow properties. Thus, the use of a dynamic fractal dimension that can adjust itself according to in-cylinder conditions is essential. The relation suggested by Zhao et al. (1994a), for the fractal dimension given by Eq. (5.36) has such dynamic properties and used in the present modified BML model (known as Fractal-BML model (FBML) hereafter). Accordingly, this formulation limits the maximum possible $D$ value close to 2.35 and hence, the maximum attainable $n$ value would be about 2.1.
5.6 Integral Scale of Turbulence

Experimental observations suggest that, the integral scale in engines is proportional to the gap between the piston crown and the cylinder head during the compression, whereas in intake, it is proportional to the maximum valve lift. This will possibly provide a rough quantitative judgment on the mean value of $L_i$, but not on its spatial distribution. Traditionally in CFD, based on the dimensional arguments, the integral scale is assumed to be equal to the dissipation length scale of the turbulent model $L_\varepsilon$. Consequently, the integral scale can be expressed by:

\[ L_i = L_\varepsilon = C_L \frac{k^{1.5}}{\varepsilon} \]  \hspace{1cm} (5.54)

where, $C_L$ is a proportionality constant and its exact value is still not a well-defined quantity. Often, the value of $C_L$ is found to be code specific. Wilcox (1998) suggested $C_L$ to be taken as the $k-\varepsilon$ model constant $c_\mu = 0.09$, while Ikekami et al. (1987) used 0.16 assuming $C_L = c_\mu^{0.75}$. In contrast, the KIVA uses $C_L = c_\mu^{0.75}/\kappa = 0.4$ in estimating $L_\varepsilon$ (Amsden et al. 1989). The Von Karman constant $\kappa$ is taken as 0.4. It is questionable, how accurate the current turbulent length scale formula, if it is used to represent the integral scale in engine like applications where, rapid distortion of turbulence is dominant. However, in practise, the agreement between the $k-\varepsilon$ computed length scale and the actual integral scale is found to be very poor (Han & Reitz 1996).

Having identified this deficiency, Han & Reitz (1996) investigated the relationship of length scales predicted by the $k-\varepsilon$ model with the measured in-cylinder integral scales. In their work, the length scales measured using the LDV technique in a motored engine with a piston bowl was compared against the modelling results produced by $k-\varepsilon$ and RNG $k-\varepsilon$ models. It was evident that, neither model can satisfactorily predict the magnitude of the integral length scale nor its variation during the engine cycle. Adjustments of the proportionality constant $C_L$ were needed, based on engine speed and the initial conditions, to match with the experimentally measured values. Therefore, those results question the validity of the hypothesis that, integral scale is directly proportional to the turbulence length scale.

5.6.1 Modelling Integral Scale in Inhomogeneous Turbulence

The main contribution for the near wall singularity of the BML model is its use of classical definition of the integral scale to calculate the mean flame wrinkling scale given by Eq. (5.54). Initially, based on the dimensional arguments, the above expression has been derived
for homogeneous turbulence. In contrast, for practical applications, corrections must be made to account inhomogeneity (Lumbly 1992). In this regard, Sreenivasan’s (1984) work is brought to attention here.

Several experimental data sets of grid generated turbulence length scales were compared in his study and a functional dependence between the Taylor Reynolds number $\text{Re}_\lambda$ and the turbulent integral scale constant $C_L$ was found. For very large value of $\text{Re}_\lambda$; typically $\text{Re}_\lambda \geq 50$, $C_L$ asymptotically approaches to a value close to unity as shown by Figure 5.6. On the other hand, for small Reynolds numbers $C_L$ may be approximately expressed by the relation $(\pi/2)^{0.5}(15/\text{Re}_\lambda)$. Saffman (1968) has also shown a power law dependence between constant $C_i$ and $\text{Re}_\lambda$, which further verifies the dependency of $C_L$ on the local turbulence. This argument is further supported by DNS studies of Wu et al. (1985) and experimental results of Dinsdale et al. (1988) and Han & Reitz (1996), which confirmed that integral scale and Taylor macro scale $L_\lambda$ remain proportional to each other in rapidly compressed flows like engines.

Based on the observations of Sreenivasan (1984), Lindsted and Vos (1998) obtained the following curve-fit correlation, which is valid for the entire range of $\text{Re}_\lambda$.

Figure 5.6: Variation of measured values of the integral scale model constant $C_L$ with the Taylor Reynolds number $\text{Re}_\lambda$ for grid-generated turbulence. Adapted from Lindsted and Vos (1998)
where, $a$ and $b$ are constants having the values 5.715 and 72.051 respectively. $Re_\lambda$ may be estimated from:

$$Re_\lambda = \frac{u' L_\lambda}{\nu}$$

and the Taylor length scale $L_\lambda$ can be expressed as (Tennekes & Lumely 1972):

$$\varepsilon = 15 \nu u'^2 / L_\lambda^2$$

In an engine like environment, the scatter of $Re_\lambda$ is so wide varying its local values from near zero to very large numbers. Therefore, considering the universal applicability, the curve fit expression has been used in the present study for modelling the integral scale of turbulence. One of the main advantages of this expression is that it eliminates the singularity of the BML model at near zero turbulent intensity. Lindsted and Vos (1998) version of the BML model has already been benefited from these findings and has obtained comparable results in stagnation flame modelling at low Reynolds numbers.

### 5.7 A Novel Wall Flame Quenching Correlation

Flame wall interaction has been a fundamental problem of combustion studies for a long time. A flame front is quenched when approaches a cold wall due to excessive heat loss. In engine applications, it is believed that the unburned hydrocarbon formation is largely associated with wall quenching, which results in partial burning of fuels (Heywood 1988). The quenching phenomenon is expected to be a chemically driven problem. Rate of quenching is determined by the relative intensity of heat release from combustion and the rate of absorption of heat by the cold boundary. One of the important findings on flame wall quenching is the identification of the existence of two distinct quenching regions as illustrated in Figure 5.7. Closest to the wall, a total quenching region exists and in which, no reaction is ever taken place. Poinset et al. (1993), through DNS data, estimated the thickness of this region to be in correspondence to a Quenching Peclet number of 3.5, where the Peclet number is defined as the ratio between the flame power and the wall heat flux. A simplified expression for the local Peclet number may be obtained as:
where, $y$ is the distance from the wall and $\delta_l$ is the unstrained laminar flame thickness estimated based on dimensional arguments.

In the region located above the total quenching region, which is identified as the *influenced zone*, flame front senses the presence of the wall and subjected to partial quenching. Estimated Peclet number corresponding to the distance for the outer boundary of the influenced zone is in the order of 10.0 (Poinsit *et al.* 1993). Gruber *et al.* (2010) have published more supporting evidence for the existence of the two layers of quenching. Their DNS result indicates a total quenching zone thickness in the order of 3 flame thicknesses, while the influenced zone is found to be approximately 10 flame thicknesses. Poinsot *et al.* (1993) implemented his findings in the transport equation of equilibrium FIST model to modify the source term near solid boundaries. Their formulation is in the form of law of the wall model and the flame surface density of the first cell (which was assumed to be large enough, so that the quenching zone is totally inside the cell) was appropriately modified via a simplified relation. Applied in engine combustion, it was found to show a significant rate of reduction of flame surface density near solid boundaries.

Experimental investigations of Foucher *et al.* (2002) and Foucher & Russel (2005) provide a new insight into the understanding of flame wall interaction. Laser tomographic images taken...
during head-on wall quenching in an optical engine revealed the influenced zone thickness could be as high as in the order of 40 times the quenching zone thickness, which is quite large compared to DNS findings. Foucher & Rousselle (2005) extended their work in order to quantify their findings in Foucher et al. (2002). Using a fractal based method, they were able to evaluate active flame surface area in the influenced zone. The quenching rate parameter \( I_{QR} \) has been defined as the ratio between the length of the active flame and the total flame length. Referring to Figure 5.7 (b), this may be expressed as:

\[
I_{QR} = \frac{L_f}{L_f + L_q}
\]

(5.59)

where, \( L_f \) and \( L_q \) are respectively the active length and the quenched length of the flame front for a given length of a flamelet segment. Note that, \( I_{QR} \) is equal to zero within total quenching region and \( 0 < I_{QR} < 1 \) in the partial quenching zone. Both the total and partial flame quenching result in significantly reduced burning rates and incomplete burning of fuels. This suggests the necessity of introducing the wall-flame quenching effects in to the burning rate integral in modelling studies.

Foucher et al. (2002) experimentally verified that, the burning rate in the vicinity of a solid wall can be expressed in terms of the quenching rate as:

\[
\overline{\omega}_{chem,w} = \rho_0 I_0 S_i^0 A_f \times I_{QR}
\]

(5.60)

where, \( \overline{\omega}_{chem,w} \) is the near wall unburned gas consumption rate. Experimentally evaluated quenching rates by Foucher & Rousselle (2005) in head on flame quenching near the piston surface have been plotted in Figure 5.8.
The exhibited trend in variation of quenching rate with the distance from the wall for different air fuel ratios of methane-air mixtures was found to be reasonably linear near the wall and then, exponentially decay towards unity at the outer boundary of the influenced zone. Conditions of the flame, corresponding to the three cases examined by Foucher & Rousselle (2005) are shown in Table 5.2. Note that, some of these parameters were experimentally measured and the others have been estimated via a simple thermodynamic analysis (see Foucher & Rousselle (2005) for more details).

Table 5.2: Flame conditions (Foucher & Rousselle 2005)

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$P$ (bar)</th>
<th>$T$ (K)</th>
<th>$\delta_t$ ($\mu$m)</th>
<th>$Re_t$</th>
<th>$Da$</th>
<th>$Ka$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>10.4</td>
<td>600</td>
<td>27</td>
<td>527</td>
<td>16</td>
<td>1.42</td>
</tr>
<tr>
<td>0.9</td>
<td>9.8</td>
<td>633</td>
<td>18</td>
<td>454</td>
<td>29</td>
<td>0.71</td>
</tr>
<tr>
<td>1</td>
<td>9</td>
<td>600</td>
<td>16.4</td>
<td>455</td>
<td>35</td>
<td>0.60</td>
</tr>
</tbody>
</table>
Foucher & Rousselle’s (2005) estimation of $I_{QR}$ was completely based on experimental observations and no mathematical formulation was presented. In order to implement their findings in a computer code, a numerical formulation is needed. It was found in this study that, these results can be correlated quite well with a set of expressions given in Eq. (5.65) - (5.67). Following section provide a brief note on the development of these correlations.

Let, the non-dimensional normalized distance $D_Q$ be taken as:

$$D_Q = \frac{d - d_{cr}}{d_{max} - d_{cr}}$$  \hspace{1cm} (5.61)

$$0 \leq D_Q \leq 1$$  \hspace{1cm} (5.62)

where, $d$ is the distance measured from the solid wall, $d_{cr}$ is the thickness of the total quenching zone and $d_{max}$ is the distance to the outer boundary of the influenced zone. For physical and conceptual reasons following limitations are imposed.

$$D_Q = 0 \text{ when } d < d_{cr}$$  \hspace{1cm} (5.63)

$$D_Q = 1 \text{ when } d > d_{max}$$  \hspace{1cm} (5.64)

Figure 5.9 shows the graph between experimentally calculated quenching rate and the reduced distance $D_Q$. Note that, measured values of $d_{cr}$ and $d_{max}$ required in calculating $D_Q$ have been estimated from Figure 5.8. Surprisingly, it is clear from this figure that, the relation between $I_{QR}$ vs. $D_Q$ also shows the exact trend seen previously with $I_{QR}$ vs. $d$.

It can be noticed form Figure 5.9 that, $I_{QR}$ decays exponentially with the normalized distance and, is bound by the limits of zero and unity. To fit with these constraints the following relation is proposed.

$$I_{QR} = 1.0 - \frac{2.0}{1 + \exp(D_Q)^\alpha}$$  \hspace{1cm} (5.65)
It was further found that, the rate of decay of $I_{QR}$ increases as a function of the distance from the solid wall. Consequently, the exponent $\alpha$ was incorporated as in Eq. (5.66). The normalized distance $D_Q$ in the denominator ensures that $\alpha$ is appropriately scaled.

$$\alpha = \frac{\beta}{(1.0 - 0.6D_Q)} \quad (5.66)$$

Parameter $\beta$ accounts for the effects of fuel-air equivalence ratio $\phi$, in flame quenching and all the other numerical values were obtained by calibrating the model to the experimental data of Foucher et al. (2002).

$$\beta = 3.7 - 2|\phi - 1.0| \quad (5.67)$$

Here, $\beta$ is the only parameter that varies with the operating conditions. Expression for $\beta$ is arrived based on the assumption, that the minimum rate of quenching occurs at unity equivalence ratio. This assumption is valid as the variation of quenching Peclet number of many fuel types is symmetric about the unity equivalence ratio or has only a small offset (Lavoie 1978). For much accurate calculations, a fuel specific determination of $\beta$ is needed.
However, due to the unavailability of experimental data, Eq. (5.67) is assumed for all types of fuels used in the present study.

Figure 5.10 to Figure 5.12 show the comparison of curve fitted plots using the expression suggested in Eq. (5.65) - (5.67), for the considered experimental cases. It can be seen that the agreement is remarkably good for the entire quenching zone thickness.

![Graph](image-url)

**Figure 5.10:** Variation of parameter $\beta$ in Eq. (5.32) for varying equivalence ratios of the air fuel mixture: Case 1: $\phi = 1.0$ and $\beta = 3.7$
Figure 5.11: Variation of parameter $\beta$ in Eq. (5.32) for varying equivalence ratios of the air fuel mixture: Case 2: $\phi = 0.9$ and $\beta = 3.5$

Figure 5.12: Variation of parameter $\beta$ in Eq. (5.32) for varying equivalence ratios of the air fuel mixture: Case 3: $\phi = 0.8$ and $\beta = 3.3$
The usual practice in wall quenching studies is to represent the parameters in terms of the Peclet number. The region of interest; the quenching zone, is so small such that the variation of temperature, pressure and the other fluid properties can be negligible. This has been the basis of almost all the wall-quenching studies (Karrer 2010). Under those assumptions the unstrained laminar burning velocity and the kinematic viscosity of the fluid can also be considered as constants. Consequently, the unstrained laminar flame thickness $\delta_l$ can also be assumed as a constant in this region.

$$\delta_l = \frac{v}{S_l^0}$$  \hspace{1cm} (5.68)

Normalizing of the wall distance $d$ with respect to $\delta_l$ leads

$$D_Q = \frac{d - d_{cr}}{d_{max}} = \left(\frac{d}{\delta_l} - \frac{d_{cr}}{\delta_l}\right)$$  \hspace{1cm} (5.69)

Using Eq. (5.68), $D_Q$ is obtained in terms of the Peclet number.

$$D_Q = \frac{Pe - Pe_{cr}}{Pe_{max} - Pe_{cr}}$$  \hspace{1cm} (5.70)

The critical Peclet number $Pe_{cr}$, is usually termed the quenching Peclet number in the literature and represented here by $Pe_Q$. Once a suitable relation for $Pe_Q$ and $Pe_{max}$ is given, Eq. (5.70) can effectively be used in modelling studies to account for the reduction in burning rate near solid walls.

### 5.7.1 Quenching Peclet Number

Even though there have been many studies, a comprehensive mathematical formulation to evaluate the Peclet number at quenching conditions is yet to be found. Reviewing quenching distance measurements for various fuel types at different equivalence ratios, Lavoie (1978) proposed the following expression for head-on quenching distance.

$$Pe_Q = \frac{1.9}{\phi} \left(\frac{P}{3}\right)^{0.26 \min(1, \frac{1}{\phi^2})}$$  \hspace{1cm} (5.71)

It should be noted here that, this expression does not account for the effect of temperature variations in the quenching distances, which should essentially be embedded. For
stoichiometric propane air mixtures Westbrook (1981) found the quenching distance to be \( d_Q = 68. P^{-0.44} \) and Labuda (2011) proposed a different expression given by \( d_Q = 88. P^{-0.48} \). Thus, for a comprehensive formulation of the quenching distance, more work is required.

In general, the value of the Peclet number at quenching is approximately about 3.5 for single wall quenching of stoichiometric air fuel mixtures. This has been largely verified both experimentally and numerically by Poinset et al. (1993) and Westbrook (1981). However, it is a weakly dependent function of the fuel type, pressure and temperature but strongly affected by the equivalence ratio. Based on the Lavoie’s expression, Peclet numbers calculated for Foucher & Rousselle’s (2005) data are given below in Table 5.3.

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>( P(\text{bar}) )</th>
<th>( \delta_l(\mu\text{m}) )</th>
<th>( d_{cr}(\mu\text{m}) )</th>
<th>( Pe )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>10.4</td>
<td>27</td>
<td>106.65</td>
<td>3.95</td>
</tr>
<tr>
<td>0.9</td>
<td>9.8</td>
<td>18</td>
<td>55.548</td>
<td>3.086</td>
</tr>
<tr>
<td>1.0</td>
<td>9</td>
<td>16.4</td>
<td>38.54</td>
<td>2.53</td>
</tr>
</tbody>
</table>

At stoichiometric conditions, the calculated value is slightly different from the universal trend; but, within the range of acceptable limits. This may obviously be a discrepancy of neglecting the effects of temperature on quenching distance. However, due to the unavailability of a proper expression, Lavoie’s (1978) expression is used in this study to determine the quenching (critical) Peclet number. The sensitivity of the proposed correlation for the quenching Peclet number is plotted in the Figure 5.13. Note that, the maximum Peclet number was taken to be 120 in this case. Indeed, the error induced in the burning rate evaluation can be assumed small even for a relatively large error in the estimated quenching Peclet number.
5.7.2 Maximum Peclet Number

Only a hand few of investigations have been carried out to study the limits of maximum quenching distance. Among those, Foucher & Rousselle (2005) and Fouchet & Rousselle (2002) are the only experimental evidence for quenching distances in engine combustion. As the aim of the present study is to model premixed spark ignition combustion engines, the maximum Peclet number is taken to be 40 times the quenching Peclet number as recommended by Foucher et al. (2002). However, this only an approximate value and in reality, its value is a function of local thermodynamic and mixture properties; particularly the equivalence ratio. The sensitivity of the maximum Peclet number on the calculated quenching rates is shown Figure 5.14. In this case, the quenching Peclet number is assumed to be 3.0 and three values: 90, 120 and 150, for the maximum Peclet number were considered. As it is evident in this figure, the effect of the maximum quenching number is important in evaluating the quenching rates at the outer boundary of the influenced zone. Hence, further experimental studies on this matter are strongly suggested.
Chapter 5: Modeling Turbulent Premixed Combustion in SI Engines

5.8 Chemical Reactions in Fuel Oxidisation

Turbulent combustion in IC engines is characterised by a multistep chain reaction process involving thousands of intermediate species. The exact nature of the coupling between intermediate reactions is unknown, thus usually a simplified reduced set of reactions are considered in modelling. Accordingly, Jia et al. (2006) has used 38 species and 69 reactions for modelling the combustion in homogeneous charged gasoline fuelled compression ignition engines. Several other mechanisms have also been proposed for the oxidisation of iso-octane. Lu & Law (2008) and references therein provide a detailed description about such mechanisms. One of the major difficulties of using this type of mechanisms in practical CFD calculations is the associated excessively high computational cost. Mainly, these equations have to be iteratively solved and much finer time steps with refined meshes have to be used for better results. However, the use of such a detailed mechanism is important, only if the emission modelling is a primary task. The aim of the present work is only to predict in-cylinder pressure rise and the mass burn rate. Therefore, a vastly simplified set of reactions, shown in Table 5.4, are used. They are treated under two categories: kinetic reactions and equilibrium reactions. Source terms of the species balance equations are appropriately modified according to the molar ratios defined by these reactions.

Figure 5.14: Sensitivity of the maximum Peclet number on the calculated quenching rate

\[ Pe_{\text{max}} = 90 \]
\[ Pe_{\text{max}} = 120 \]
\[ Pe_{\text{max}} = 150 \]
\[ Pe_{r} = 3.0 \]
Table 5.4  Classification of chemical reactions

<table>
<thead>
<tr>
<th>Fuel Oxidisation</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>propane: C₃H₈ + O₂ → 3 CO₂ + 4 H₂O</td>
<td></td>
</tr>
<tr>
<td>iso-octane: 2 C₈H₁₈ + 25 O₂ → 16 CO₂ + 18 H₂O</td>
<td></td>
</tr>
</tbody>
</table>

Extended Zeldovich mechanism: kinetic reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂ + N₂</td>
<td>2 NO + 2N</td>
</tr>
<tr>
<td>N₂ + O₂</td>
<td>2 NO + 2O</td>
</tr>
<tr>
<td>N₂ + OH</td>
<td>2 NO + 2H</td>
</tr>
</tbody>
</table>

Chemical equilibrium

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>2H</td>
</tr>
<tr>
<td>O₂</td>
<td>2O</td>
</tr>
<tr>
<td>N₂</td>
<td>2N</td>
</tr>
<tr>
<td>2 OH</td>
<td>O₂ + H₂</td>
</tr>
<tr>
<td>4 OH</td>
<td>O₂ + 2 H₂O</td>
</tr>
<tr>
<td>2 CO₂</td>
<td>O₂ + 2 CO</td>
</tr>
</tbody>
</table>

Fuel oxidation is considered to be a simple one-step reaction and the reaction rate is calculated using the main combustion model. Propane and iso-octane were used as fuels in the present study. This reaction is initiated with the spark onset and continued until all the fuel is consumed. Other kinetic dissociation reactions and equilibrium reactions are locally calculated if the mass averaged cell temperature exceeds 1800 K as suggested by Amsden et al. (1989). For kinetically proceeded reactions, instantaneous reaction rate of rᵗʰ reaction $\bar{\omega}_r$ is evaluated by the following expression:

$$\bar{\omega}_r = k_{fr} \prod_m \left( \frac{\rho_m}{W_m} \right)^{a_{mr}} - k_{br} \prod_m \left( \frac{\rho_m}{W_m} \right)^{b_{mr}}$$  \hspace{1cm} (5.72)

$k_{fr}$ and $k_{br}$ respectively denote the forward and backward rate coefficients and General Arrhenius form is assumed. $a_{mr}$ and $b_{mr}$ are reaction orders. It is possible to use the stoichiometric coefficients $a_{mr}$ and $b_{mr}$ or experimental values appropriately for $a_{mr}^v$ and $b_{mr}^v$.

$$k_{fr} = A_{fr} T^{\xi_{fr}} \exp \left( - \frac{E_{fr}}{RT} \right)$$  \hspace{1cm} (5.73)

$$k_{br} = A_{br} T^{\xi_{br}} \exp \left( - \frac{E_{br}}{RT} \right)$$  \hspace{1cm} (5.74)
Arrhenius expressions for $k_{fr}$ and $k_{br}$ are provided by the above two equations. $A_{fr}$ and $B_{fr}$ are the pre exponential factors; $\zeta_{fr}$ are $\zeta_{br}$ are the temperature exponents and, $E_{fr}$ and $E_{br}$ are activation energies of the forward and backward reactions respectively. A database of required reaction coefficients and exponential factors when using the above equations can be found in Amsden (1993).

For equilibrium stage reactions, the reaction rate $\bar{\omega}_r$ is determined using an iterative procedure based on the following implicit requirement in Eq. (5.75). More details on the method can be found in Amsden et al. (1989).

$$\prod_m \left( \frac{\rho_m}{W_m} \right)^{(b_{mr} - a_{mr})} = K^r_e(T) \tag{5.75}$$

where, $K^r_e(T)$ is the concentration equilibrium constant given by Eq. (5.76) with $T_A = T / 1000$:

$$K^r_e = \exp \left( A_r \ln T_A + \frac{B_r}{T_A} + C_r + D_r T_A + E_r T_A^2 \right) \tag{5.76}$$

Values of the model constants $A_r, \ldots, E_r$ can be found in Amsden et al. (1986).

### 5.9 Summary

- Theoretical and practical aspects of combustion modelling during the fully developed phase were discussed, with regard to their applications in premixed SI engines.
- The well-known BML formulation was used as the base model for the present work and several issues of this model were identified; particularly, when applied to wall bounded combustion modelling.
- Consequently, a Fractal geometry based model was proposed for flame wrinkling and flame surface density calculations, which has a self-scaling property according to the local level of turbulence.
- Present approach has made the estimation of most of the BML model constants dynamic, using the information from local flow properties. Only a single parameter is left for fine tuning purposes.
- Similarly, the estimation of the integral scale of turbulence and the flame wrinkling scale has also made dynamic.
- A novel empirical correlation was derived for estimating the near wall flame surface density and quenching rates by curve fitting experimentally obtained flame image data.
The accuracy of a computational model can only be justified by comparing the predictions with experimentally measured data. In the present study, the validity of the developed models was primarily assessed by comparing with experimentally obtained pressure and heat release rate data from a laboratory engine. Results are also compared with published literature for qualitative comparisons. In addition, simulations were carried out based on some of the published experimental test cases for benchmarking purposes. More information about these test cases is appropriately presented where they are used. The focus of this chapter is limited to explanation of present experimental programme.

In this work, data was acquired from the Ricardo E6 engine in the Loughborough University engine laboratory for a range of operating conditions. Section 6.1 and 6.2 provide a brief overview of the experimental set up of the engine test rig, data acquisition system and the operating procedure. The principles of analysing the pressure data are detailed in section 6.3. Procedures for accurate phasing and referencing of pressure data, and possible errors embedded in readings are also explained in this section. In addition, the quality of the present data set is thoroughly assessed with a series of checks. A quantitative measure of the data quality was obtained through a statistical analysis. Analytical methods to calculate mass burn rate and heat release rate data from the measured pressure values are explained in section 6.4. A brief summary of this chapter is presented in section 6.5.
6.1 Ricardo E6 Engine and Data Acquisition System

The Ricardo E6 is a single cylinder, variable compression and four stroke research engine. The experimental pressure and mass burn data obtained from this engine is the main source of data used in the validation of developed models during this work. The engine can be operated either in spark ignition mode or in the compression ignition mode by suitably changing the engine cylinder head. Only the spark ignition mode is used in the present investigation. The E6 has originally been built with a carburetted fuel supply and a distributor type ignition system. Recent modifications have upgraded the engine into port fuel injection with a transistorized electronic ignition systems and a motorized throttle controller. A photograph of the engine and the test rig is shown in Figure 6.1.

![Ricardo E6 Engine](image)

Figure 6.1: The Ricardo E6 test engine and the MOTEC engine control unit at Loughborough University engine laboratory

E6 engine has an adjustable cylinder head, so that compression ratio can be varied from 4.5 to 20. The position of the cylinder head assembly can be lowered or raised relative to the crankshaft by means of a worm gear. The traversed distance is measured using a micrometre gauge and the corresponding compression ratio can be determined from the calibration curve provided by the engine manufacturer. This facility provides a mean of testing for a range of compression ratios in different operating conditions of the engine, without any hardware
modification. Geometric and other related specifications of the E6 engine are given in Table 6.1.

### Table 6.1 Ricardo E6 engine specifications

<table>
<thead>
<tr>
<th>Richardson E6 Engine</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>76.20 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>111.1 mm</td>
</tr>
<tr>
<td>Compression ratio(CR)</td>
<td>Variable</td>
</tr>
<tr>
<td>Squish at 8.7 CR</td>
<td>1.4428 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>241.30 mm</td>
</tr>
<tr>
<td>Spark advance</td>
<td>Variable</td>
</tr>
</tbody>
</table>

**Valve timing**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake valve opens</td>
<td>9° BTDC</td>
</tr>
<tr>
<td>Intake valve closes</td>
<td>37° ABDC</td>
</tr>
<tr>
<td>Exhaust valve opens</td>
<td>41° BBDC</td>
</tr>
<tr>
<td>Exhaust valve closes</td>
<td>10° ATDC</td>
</tr>
</tbody>
</table>

**Valve lift**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum lift - intake valve</td>
<td>11.56 mm @ 85° ATDC</td>
</tr>
<tr>
<td>Maximum lift - exhaust valve</td>
<td>10.60 mm @ 52° ABDC</td>
</tr>
</tbody>
</table>

**Valve diameter**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake valve max. diameter</td>
<td>34.37 mm</td>
</tr>
<tr>
<td>Exhaust valve max. diameter</td>
<td>29.62 mm</td>
</tr>
</tbody>
</table>

The E6 engine used in experiments has a pancake or cylindrical combustion chamber with a flat piston face and a flat cylinder head. Two poppet valves are vertically positioned parallel to the cylinder axis. Valve lift is controlled by a horizontal overhead camshaft via rocker arms. Measured valve lift profiles of the two valves are shown in Figure 6.2. The spark plug is located towards the cylinder wall between the two valves. Engine controlling was performed by a MOTEC m400 engine controller unit. This allowed the adjustment of fuel quantity, injection timing and ignition advance via the control interface. The air fuel ratio was measured using a NTK AFR meter connected through a Universal Exhaust Gas Oxygen (UEGO) sensor. Horiba Maxa-584L exhaust gas analyser was also used to verify the readings of NTK AFR meter. In addition, a Ford 96FP12B579AA hotwire anemometer type flow meter was fitted into the intake port for air flow measurements. The flow meter was calibrated using a steady flow test bench. Fuel flow rate was estimated by measuring the time taken for 50 ml of fuel to flow though the fuel meter. This provided an alternative method for checking the validity of the air fuel ratio measurements of other instruments through manual computations using air and fuel flow readings.
Figure 6.2: Measured valve lift profiles of intake and exhaust valves of the E6 engine

The engine was coupled to a direct current dynamometer and the load was automatically adjusted to maintain the specified engine speed for a given throttle position. Data acquisition was made using a NI PCI 6123 module and a NI LabView user interface developed by the Loughborough University. A schematic diagram of the engine control unit and the data acquisition system is given in Figure 6.3. Engine speed was measured using a Leine and Linde RSI 503 incremental optical encoder fitted to the crank shaft, which produces 3600 pulses per revolution. Thus, a crank degree marker (CDM) signal was fed to the data acquisition unit every 0.1 crank degree. A separate synchronisation signal was also generated each time the piston reached the top dead centre position.

K-type thermocouples were fitted to measure the cooling water, intake and exhaust air temperatures. Intake manifold pressure was measured using a Druck DPI260 unit, which is capable of measuring negative gauge pressures. A Kistler 1167BFD piezoelectric pressure transducer with a sensitivity of 15 pC/bar was used to measure in-cylinder pressure. Pressure signal was first sent to the charge amplifier and then the amplified signal was fed into the data acquisition system through BNC cables. Specific measures are required in measuring and analysing the pressure data and they are discussed separately in a latter section.
Figure 6.3: Schematic diagram of the engine control unit and the data acquisition system of the E6 engine test rig. Shown in dashed lines are electrical signals and solid lines indicate air/fuel lines.

### 6.2 Operating Procedure and Test Conditions

The charge amplifier and the air fuel meters were kept on standby mode for approximately 30 minutes prior to measurements for warming up, as per the instructions of manufacturers. Having set the compression ratio to the desired value, the fuel supply, extraction system and the cooling water system were turned on. Before the engine is fired, the dynamometer was set to run on 600 rpm. After ensuring smooth operation, the ignition was activated to fire the engine. Subsequently, the engine speed, ignition timing and injection timing were set to the required values and the injected fuel mass was manually adjusted by trial and error basis to obtain the preferred air fuel ratio based on real time continuous readings from NTK AFR meter. The software interface of the engine controller unit provides the facility for on the fly modifications of the engine map. After achieving required operating conditions, the engine was kept running until it reached a steady state. This could be identified by the engine oil and
cooling water temperature readings, which become stable at steady state operation. Usually, it takes around 10-15 minutes for the engine to reach the steady state. Data acquisition system was kept connected and switched on throughout the engine operation and hence, real time operating data was available on the software user interface. Having confirmed the steady state operation, pressure, crank and air flow rate data were recorded over 100 consecutive engine cycles. Fuel flow rate, cooling water, oil, intake and exhaust gas temperatures were also recorded separately. A similar procedure was carried out for other operating points as well.

Testing was performed for several operating points of each parameter: compression ratio, equivalence ratio and engine speed, at both fully and 1/4 open throttle positions, using standard commercial gasoline as the fuel. However, only some of these data sets were used for validation purposes, due to time constraints. The primary aim of the present experiments was to obtain an accurate data set for engine pressure for a range of operating conditions. The measured cyclic pressure traces have to be further analysed and referenced appropriately in order to compensate any thermal drift in the measured pressure signal. The following section provides the analysing procedure used in the present study.

### 6.3 Analysis of Pressure Data

One of the very first steps of pressure analysis is to cycle average the obtained pressure data over a reasonable number of cycles to compute mean values. In the present study, over 100 consecutive cycles were recorded during the data acquisition, although relatively less number of cycles could be sufficient for a sensible result. Figure 6.4 shows the cycle by cycle variation of the pressure curves for 20 consecutive engine cycles. Figure 6.5 depicts the cycle averaged pressure curves by considering different number of consecutive engine cycles. The engine has been operated at 1500 \( rpm \) under full load conditions with an equivalence ratio of 0.94 and a compression ratio of 8.7. This operating point is used as the reference test case for the demonstration of this analysis, throughout this chapter. The higher the number of engine cycles, the cycle averaged pressure will be more accurate. However, due to the limitations in computing resources, a finite number of cycles have to be considered. Accordingly, the nature of the cycle averaged pressure curve of different number of cycles from 25 to 100 was compared. It was found that even with 25 cycles, the peak pressure can be calculated within 1% error margin and its location within 1.0 crank degree, assuming that averaging over 100 cycles would produce the actual averaged pressure curve. The averaged pressure curves in all other locations were almost identical. Thus, the pressure data was processed by averaging over 50 engine cycles during the present study.
Figure 6.4: In cylinder pressure trace for 20 consecutive engine cycles. Shown in dashed line is the averaged pressure curve at motored conditions.

Figure 6.5: Comparison of cycle averaged pressure curves considering different number of engine cycles.
6.3.1 Pressure Volume Phasing

The signal obtained by the pressure transducer is automatically phased with CDM signal by the Labview programme. Similarly, each engine cycle is distinguished by detecting the TDC signal. The TDC position is determined by identifying the top most piston position by using a dial gauge. The shaft encoder is mounted to the crankshaft by referencing this location. However, this static TDC location could differ from the dynamic TDC due to shift of main bearings and torsional vibrations of the crankshaft (Kim & Kim 1989). Therefore, correct phasing of the pressure with the engine volume (or crank) is essential as this could result in significant errors in subsequent calculations. As pointed out by Lancaster et al. (1975) a shift in one crank degree could lead to a 4% error in the calculated indicated mean effective pressure.

In order to ensure the pressure signal is correctly phased with the crank angle a series of checks was performed. One of the simplest checks is to investigate the peak pressure location under motored conditions. Due to heat transfer through engine walls and blow by gases, the maximum pressure should locate slightly before the TDC position. The difference between the dynamic TDC and the static TDC is called the thermodynamic loss angle (TLA) (Hohenberg 1979) and it becomes lower at higher engine speeds due to reduced blow by and heat losses (Kim & Kim 1989). In the present test cases, it was found to be located in between 0.1 to 0.5 degrees BTDC, with the general trend of a reduction at high speeds. These values are in accordance with the previously measured TLA values: 0.0 to 0.74, for the same E6 engine by Woolridge (2007).

Additionally, the pressure volume diagram at motored condition is also a good source for verifying the dynamic TDC location. In cases, where the measured peak pressure is located after the TDC, indicating a higher expansion pressure than the compression near TDC, a crossing over of the compression and expansion lines is resulted. However, as shown in Figure 6.6 and Figure 6.7 in linear and logarithmic scales respectively, there are no such crossover points in present test cases. Thus, it confirms that the pressure is correctly phased with respect the cylinder volume. The engine operating conditions correspond to 1500 rpm, wide open throttle at 8.7 compression ratio.
Figure 6.6: Pressure volume diagram for motored conditions of E6 engine plotted on linear scale. Enlarged view of the curve close to the TDC at compression is shown on the top right corner.

Figure 6.7: Pressure volume diagram for motored conditions of E6 engine plotted on logarithmic scale. Enlarged view of the curve close to the TDC at compression is shown on the top right corner.
6.3.2 Pressure Referencing

Piezoelectric transducers are popular due to their fast response time, small size and low sensitivity to environmental conditions. However, the very high temperatures present within the engine combustion chamber increases the temperature of transducer housing and the quartz sensing element, which could cause an offset of the transducer output voltage. The amount of output charge produced by the transducers is referenced to an arbitrary datum by default and only proportional to the change in measured pressure. Thus readings have to be correlated to a known reference point during the engine cycle, before the absolute pressure is determined (Lee et al. 2008). This referencing procedure is called pegging and is a mandatory correction in engine pressure analysis. Incorrectly referenced pressure data produces errors in subsequent estimation of polytropic index, mass burn rate and mixture temperature.

There are several pegging methods available, but each method has its own merits and demerits. Setting the in-cylinder pressure intake BDC equal to the intake manifold pressure is one of the simplest and widely used methods, and is found to be much accurate than many other complex techniques. Randolph (1990) confirmed this fact by comparing nine pegging methods with a range of complexity, by evaluating pressure data of a single cylinder research engine. Thus, the present study uses this method. In addition, pegging exhaust manifold back pressure to the averaged in-cylinder pressure during the exhaust stroke, forcing a polytropic compression with a constant ploytropic index or a variable polytropic index and least square methods are some of the other commonly used techniques. Further details on these methods and their relative accuracies can be found in Randolph (1990) and Lee et al. (2008).

Some of the possible errors associated with pressure referencing can be identified by investigating the motored pressure volume diagram in logarithmic scale. Figure 6.7 shows a pressure volume diagram corresponding to one of the present test cases. Lancaster et al. (1975) showed that, the presence of a curvature during the early part of the compression stroke is an indication of selecting a too low reference pressure. No such curvature is seen in Figure 6.7 confirming that a correct reference pressure has been selected. Similarly, the presence of a curvature close to the TDC and the mid of the compression is a sign of incorrect clearance volume estimation or faulty pressure transducer. However, the compression curve in the present case is shown to be almost linear, verifying the good quality of the data set.

Piezoelectric transducers may be subjected to thermal shocks i.e. the rapid increase of temperature, when the flame front is in close contact with the sensing element. Thus, transducer diaphragm gets deformed momentarily due to thermal stresses producing
erroneous pressure data. The induced error due to thermal shock can be as high as the pressure being measured. The transducer recovery period may last throughout the expansion stroke or possibly can extend beyond the intake stroke. Hence, such situations can be identified by the presence of crossover points in the pumping loop of logarithmic pressure volume diagram of a fired engine cycle. In recent years, significant improvements have been made by the transducer manufacturers to minimise thermal shocks, but this problem is still not completely eliminated (Puzinauskas 1998). Figure 6.8 and Figure 6.9 illustrate the pressure volume diagram for firing conditions of the E6 engine in linear and logarithmic scales. No indication can be seen on thermal shock effects in the pumping loop; thus, the present data set is of good quality.

Figure 6.8: Pressure volume diagram for firing conditions of E6 engine plotted on a linear scale
6.3.3 Statistical Analysis

Substantial variations in engine pressure curves on cycle by cycle and cylinder by cylinder basis are often observed. The degree of variability of pressure is a clear indication of the level of variations in the combustion process. Differences in in-cylinder turbulence and flow motion, air-fuel ratio and residual level are some of the main reasons for such variations. Figure 6.10 depicts the mean pressure and its standard deviation at the corresponding crank location. Deviations were prominent only during the combustion period, while it was relatively small elsewhere. A maximum of 4.7 bar is recorded for the standard deviation at 7 degrees before mean peak pressure location and its value at the peak pressure location was 4. The shift between the two points is due to the cyclic variations of the peak pressure location. Similar values were obtained for other test cases as well.
Figure 6.10: Cyclic pressure variations in E6 engine. Solid line indicated the mean cylinder pressure and its standard deviation at a given crank position is shown by Error bars.

A good measure of estimating the cyclic variability of an engine is the coefficient of variation of indicated mean effective pressure (IMEP) (Heywood 1988). IMEP is the mean pressure during the power stroke, which should be maintained to produce the same amount of power as the actual crank varying pressure. It could be defined by the ratio between the work done per engine cycle and the engine displacement volume per stroke $V_d$ as follows.

$$P_{IMEP} = \frac{\phi p dV}{V_d}$$  \hspace{1cm} (6.1)

The coefficient of variation is given by:

$$COV_{IMEP} = \frac{\text{Standard deviation of IMEP}}{P_{IMEP}} \times 100 \%$$  \hspace{1cm} (6.2)

Figure 6.11 shows the distribution of IMEP values over 100 engine cycles for the given test conditions. An averaged IMEP value of 10.056 $bar$ was recorded while the coefficient of variation of the IMEP is 2.95%. This value is well within 5-10% range, which was suggested...
to be the acceptable limit by Stone (1999). Similar values were obtained for $COV_{IMEP}$ in other test cases as well.

![Figure 6.11: Scatter of indicated mean effective pressure for 100 consecutive engine cycles. Solid line indicates the averaged IMEP](image)

These values are in the same range compared to the previously measured values by Woolridge (2007) for the same engine at similar operating conditions.

### 6.4 Heat Release Rate Calculation

Other than the in-cylinder pressure, the heat release rate due to combustion and the fuel burning rate are the most useful parameters for quantitative comparison of combustion model predictions with experimental data. Usually, the combustion process of an IC engine takes place during the period, in which all valves are closed separating the manifolds from combustion chamber. Combustion starts 20 to 30 degrees before TDC during the latter part of compression stroke and lasts around 100 degrees of crank angle. Hence, it is reasonable to assume the combustion volume as a closed system during the period of combustion, neglecting any blow by mass transfer. On this basis, the pressure rise in the cylinder is directly associated with mass burn rate. There are several thermodynamic models in the literature to relate the change in pressure to heat release rate (Heywood 1988). The simplest model is based on the assumption that, pressure difference between a motored cycle and a combustion cycle is due to the heat release of reacting chemical species. This model inherent
with the disadvantage of not accounting for heat losses through cylinder walls yet, it is the most widely used and proven to be capable of calculating reasonably accurate mass burn data. It could also be possible to extend this model with the provision to compensate heat losses and crevice volume effects.

Compression and expansion processes of an engine can be precisely approximated with a polytrophic relation with a constant ploytropic index \( n \):

\[
PV^n = \text{Constant} \tag{6.3}
\]

where, \( n = 1.3 \pm 0.05 \) for conventional fuels (Heywood 1988).

Hence, during this period, two straight line segments can be observed in the logarithmic pressure volume graph, as in Figure 6.7 and Figure 6.9. In these figures, the starting point of combustion can be identified by the deviation point from the straight line as the rate of pressure rise is increased due to heat release from combustion. Similarly, the end point of combustion can also be recognized by the location, beyond which the curve becomes straight again due to the cease of combustion heat addition.

If \( \Delta p_t \) is the total in-cylinder pressure rise during a period of \( \Delta \theta \) crank angle interval, \( \Delta p_t \) can be expressed as the summation of pressure rise due to volume change (\( \Delta p_v \)) and the pressure rise due to combustion (\( \Delta p_c \)) during the same crank duration.

\[
\Delta p_t = \Delta p_c + \Delta p_v \tag{6.4}
\]

Under the assumption of polytropic combustion in the absence of combustion, the following relation can be established.

\[
p_i V_i^n = p_j V_j^n \tag{6.5}
\]

The subscript \( i \) denotes the initial conditions at the start of interval \( \Delta \theta_i \) and \( j \) denotes the end conditions. Hence, pressure rise due to volume changed can be estimated by Eq. (6.5).

\[
\Delta p_v = p_j - p_i = p_i \left[ \left( \frac{V_i}{V_j} \right)^n - 1 \right] \tag{6.6}
\]

Since, the total pressure rise is available from experimental data, pressure rise due to combustion can be calculated by substituting this expression in Eq. (6.4).
Assuming that, the rate of mass burned is equal to the rate of pressure rise due to combustion during $\Delta \theta_i$ period, mass fraction burned may be evaluated by using Eq. (6.7):

$$\frac{m_{b(i)}}{m_{b(total)}} = \frac{\sum_0 \Delta p_c}{\sum_0 \Delta p_c}$$ (6.7)

where, $m_{b(i)}$ is the total mass burned during the $i^{th}$ interval and $m_{b(total)}$ is the total mass burned during all $N$ number of crank intervals. The major drawback of this model is the lack of provision for heat losses through the cylinder walls. Selection of an appropriate value for polytropic index is also bit difficult due to the fact that, it is a function of in-cylinder temperature and composition. However, reasonably accurate values can be obtained for the polytropic index by computing the gradient of the straight line segments in logarithmic pressure volume diagram.

An extended model with the allowance to incorporate heat losses and crevice volume effects together with variations of specific heat capacity with time is given in Eq. (6.8) (Heywood 1988). The equation evaluates heat release rate due to chemical reactions instead of the mass fraction burned. The effect of incorporation of crevice effects and heat losses can only be achieved through good estimation of crevice volume and average convective heat transfer coefficient of combustion chamber. In most cases, the effect of crevice volume is neglected and only the heat loss through walls is accounted. Brunt & Platts (1999) used this formulation in a comparison study of heat release models in diesel engine combustion and obtained reasonably good results. Crevice volume effects were neglected while a second order polynomial of temperature was used to calculate the specific heat ratio.

$$\frac{dQ_{ch}}{d\theta} = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\theta} + \frac{\gamma}{\gamma - 1} V \frac{dp}{d\theta} + V_c r \left[ \frac{T'}{T_w} + \frac{T}{T_w(\gamma - 1)} + \frac{1}{bT_w} \ln \left( \frac{\gamma - 1}{\gamma' - 1} \right) \right] \frac{dp}{d\theta} + \frac{dQ_{ht}}{d\theta}$$ (6.8)

and,

$$\frac{dQ_{ht}}{dt} = A h_c (T - T_w)$$ (6.9)

where,
Chapter 6: Experimental Data Acquisition and Analysis

- Heat release rate into the mixture due to chemical reactions
- Heat release rate from cylinder walls due to convection
- Specific heat ratio for in cylinder mixture
- Specific heat ratio for crevice gas
- Crevice volume
- Crevice gas temperature
- Mean gas temperature
- Mean cylinder wall temperature
- Crank angle
- Combustion chamber surface area
- Convective heat transfer coefficient averaged over the chamber surface area

Figure 6.12: Variation of mean heat release rate, burned fuel mass fraction and the in-cylinder pressure with the crank angle
Both the mass burn rate model and the heat release model were appropriately used in this study, during the validation process of the present combustion models. However, crevice and wall heat transfer effects were not considered. Computed cycle averaged mean heat release rate and the mass burned rate for the present reference test case are shown in Figure 6.12, as an example.

### 6.5 Summary

- A brief overview to the experimental data acquisition procedure and the apparatus was provided in this chapter.
- Possible errors, correction methods and their applicability to experimentally measured pressure data were also discussed.
- The experimental data set was subjected to a series of quality checks to quantify the accuracy.
- Accordingly, the pressure values were observed to be correctly phased with engine volume and properly referenced to a known datum.
- Derivation of heat release and mass burn data from the measured pressure values were also demonstrated.
RESULTS AND DISCUSSION: RANS APPLICATIONS

The emphasis of this chapter is directed towards the validation of ignition and combustion models developed in previous chapters. Accuracy of a CFD model is best confirmed by rigorous comparison with experimental data. Accordingly, the validity of various aspects of present model formulations is comprehensively assessed by making comparison against experimental measurements in a range of engine and non-engine applications.

Section 7.1 describes the validation process of the present ignition and flame kernel formation model. In which, the model predictions are both quantitatively and qualitatively assessed against experimentally obtained flame image data under high swirling conditions and local bulk flow convection effects. In section 7.2, predictability of the ignition model is compared with published literature in SI engines. Further, the performance of the present combustion model is also benchmarked against literature, applied to a number of engine test cases. The validation process is further extended in section 7.3, by employing both the ignition and combustion models in simulating full cycle combustion process in the variable compression Ricardo E6 engine. Experimental pressure data obtained from the same engine, as a part of this research, is used in the comparison. Flame propagation characteristics, mass burn and heat release rates and the behavior of the present ignition and combustion model parameters are also carefully examined. A brief summary of the present chapter is given in section 7.4.
7.1 Validation of the Extended DPIK Ignition Model

In this section, the present ignition model formulation is validated under both laminar and turbulent conditions. Effect of the presence of a mean convection flow field is also examined. Accordingly, the flame kernel formation process in a closed cubic vessel is simulated to investigate the predictability under laminar and homogeneous turbulent conditions, in the absence of bulk convection. Flame development in a cylindrical chamber with low to very high swirling flow fields is also modelled to verify the model performance under engine like conditions, where substantial convection effects present.

7.1.1 Flame Kernel Development in the Absence of Swirl

Here, the flame kernel growth under laminar and low to moderate levels of turbulence, without bulk flow convection is considered. The aim of modelling laminar flame kernel development is to verify the accuracy of present DPIK ignition model formulation, under known conditions. According to simple laminar flame theories, the flame kernel should grow spherically at a rate given by the following relation in laminar flows.

\[
\frac{dr_k}{dt} = \frac{\rho_u}{\rho_k} (S_l + S_{\text{plasma}})
\]  

(7.1)

This equation has been found to produce reasonably accurate results during the early stage of flame development (Colin & Truffin 2011). From turbulent simulations, it is expected to evaluate the sensitivity and the characteristics of model parameters ahead of varying flow conditions. In the absence of a mean convecting flow field, turbulent flame kernel should also exhibit nearly spherical propagation; at least at the very early stage. Consequently, the flame radius calculated using burned gas volume and the mean radius of the sphere formed by Lagrangian marker particles should have the same values as predicted by the Eq. (7.1). Hence, this analysis provides a prospect to identify possible modelling discrepancies. Note that, for turbulent flow calculations, the laminar flame speed \( S_l \) in Eq. (7.1) should be replaced with turbulent flame speed \( S_t \).

7.1.1.1 Numerical Setup

The simulation domain was taken to be a close cube of \( 5 \times 5 \times 5 \) cm consisting \( 50 \times 50 \times 50 \) structured, uniform hexahedral cell elements. The cube was assumed to be filled with a propane air mixture at stoichiometric air-fuel ratio. Three different test conditions were considered for simulations, for which \( \frac{u'}{S_l} = 0 \), \( \frac{u'}{S_l} = 1 \) and \( \frac{u'}{S_l} = 2 \). The laminar flame velocity was assigned a constant value of 95 cm s\(^{-1}\) for all test cases, which
approximately corresponds to the laminar burning velocity of a stoichiometric propane air mixture at a pressure and temperature of 5 bar and 660 K respectively. Ideally, for the laminar case, the turbulent intensity should be zero, but to avoid possible computational errors due to potential undefined mathematical operations, a value of 0.0001 m/s was assigned to $u'$. Compared to the laminar flame speed, this value is very small and the influence is expected to be insignificant. In other cases, turbulent intensity was appropriately initialised to obtain the desired $u'/S_l$ value, assuming homogeneous isotropic turbulence. The ignition point was located at the centre of the cube. The ignition energy and the spark duration were taken to be 60 mJ and 1.2 ms respectively. These values represent typical magnitudes of ignition parameters of a transistorized coil ignition system (TCI). Initial flame kernel radius was taken as 0.5 mm. All flame kernel modelling work, presented in this chapter was performed by using the improved DPIK model described in Chapter 4. The only model constant $C_{IGN}$ was set to 10, in order to ensure fully burned conditions within the flame kernel. Fully implicit numerical schemes were used with all combustion phase calculations aiming a higher accuracy and the stability. Solution time step was automatically controlled by the present code, but the maximum possible time step was limited to $10^6$ seconds.

7.1.1.2 Results and Discussion

![Diagram](image)

Figure 7.1: Computed flame radii of spherical flame propagation under laminar and turbulent conditions without bulk flow convection
Figure 7.1 shows the comparison of flame radii, estimated using three different methods under prescribed laminar and turbulent conditions. Symbols show the mean flame kernel radii computed by averaging the spatial position of Lagrangian marker particles. Solid lines represent $r_k$, the equivalent flame radii computed using burned gas volume and the chained lines show $r_{th}$ (theoretical radius), the flame radii computed using the formula given in Eq. (7.1). Note that, the mean convection velocity was set to zero in these simulations. For all three test cases, the flame radii calculated using Eq. (7.1) and by averaging spatial coordinates of marker particles are shown to be identical. This is due to the fact that, the equation which describes the particle motion (see section 4.3 in Chapter 4) reduces to Eq. (7.1), in the absence of a mean convection flow field. Thus, both relations should predict a same rate for particle displacement. Consequently, these results verify the accuracy of present numerical algorithms developed to calculate particle motion within the computational mesh.

$r_k$ is also shown to be in good agreement with the theoretical radius $r_{th}$. However, during the very early stage: within 0-0.5 ms, $r_k$ is found to be considerably over predicted, with respect to the absolute value of the $r_{th}$. In addition, $r_k$ tends to be subjected uneven fluctuations. The variation of percentage error of the estimated $r_k$ value, compared to $r_{th}$ is illustrated in Figure 7.2, for two different mesh configurations.

![Figure 7.2: Percentage error of calculated flame kernel radius in two different meshes for laminar spherical flame expansion](image-url)
The main reason for this deficiency is that, in the early stage, either the flame kernel remains much smaller than the computational cell size or its size is not large enough to be resolved using the computational mesh. Therefore, as a large value is used for the ignition model constant $C_{IGN}$ to ensure full combustion inside the kernel (in the present case $C_{IGN}=10$), most of the fuel within computational cells, in which the flame kernel resides, is rapidly burned out during the first few time steps after the onset of ignition, before $r_{th}$ grows to the cell dimension. As a result, the burned gas volume is higher than its theoretical value, so that the estimated $r_k$ is larger than $r_{th}$. For a coarser mesh this error could be well above 100% attributable to the small size of the kernel, whereas it can be significantly reduced by using a sufficiently fine mesh as evident from Figure 7.2. Note that in these simulations, the mesh 1 has a nominal cell dimension of 1 mm and the mesh 2 has a value of 0.5 mm. However, the overall impact of this error is insignificant in the present model, as the fuel burning rate is not controlled by the concentration of burned gases, but by the number of marker particles within a cell. On the other hand, with the increase of the flame radius, i.e. where, there is a sufficient number of cells to estimate the burned gas volume, this error reduces rapidly. For example, in the present laminar test case in mesh 1, the maximum error is about 55% and it occurs 150 μs after spark onset, when $r_{th}$ is about 1 mm. This error becomes less than 10% after about 1 ms, corresponding to a $r_{th}$ value of 5 mm. Also it is interesting to note that, in the mesh 2, which is finer than mesh 1, the peak error is only about 25 %, and it drastically reduces below 10 %, when $r_{th}$ is about 0.25 mm.

![Figure 7.3: Growth of the mean flame kernel surface represented by Lagrangian marker particles under laminar conditions](image)
Figure 7.3 shows the spherical propagation of Lagrangian marker particles under laminar conditions. Initial flame kernel diameter at 0.0 ms is 1.0 mm and its value at after 2.67 ms is about 2 cm. Since, there is no effect from bulk convection, the mean flame surface remains spherical throughout the simulation. Also, it is worth to note that, the particle density diminishes with increasing flame radius. Hence, the higher the total number of particles the computed flame surface area will be more accurate. However, the computational overhead will also be increased with increasing number of particles.

Variations of plasma expansion speed and the mean flame surface area for above test cases are plotted in Figure 7.4. Solid lines show particulars corresponding to the laminar test case, while dashed and chained lines indicate turbulent cases. Further, the lines with square symbol denote the mean flame surface area computed using the equivalent burned gas volume, and lines with circles show the total wrinkled flame surface area. The flame kernel wrinkling factor was taken to be the ratio between the turbulent flame speed and the unstrained laminar flame speed.

At the time of spark breakdown, plasma expansion has a very high velocity due to excess of ignition energy, compared to the required minimum ignition energy. In general, it has been noticed that, plasma speed reaches very close to zero approximately within 0.4 ms (Herweg et
This observation is well reflected by the present simulations, where this decaying period is about 0.3-0.4\,ms. No significant difference of plasma expansion speeds on case by case basis can be observed as the thermodynamic properties of the gas mixture remain the same for all test cases. As expected, the rate of increases of flame area rises with the increasing turbulence level. This is primarily caused by the increase of turbulent flame speed, as evident from Figure 7.5. Initially, at smaller radii, the turbulent speed is very much close to the laminar speed and then rapidly increases towards a saturated value with the increasing flame kernel radius. The saturated limit is higher for high turbulent intensities, while for the laminar case, it is equal to the unstrained laminar burning velocity due to the absence of turbulent flame wrinkling. Once this saturation level is reached, the flame kernel can be considered in the fully developed stage. The limiting flame speed can be expressed approximately as the summation of strained laminar burning velocity and the turbulent intensity or more precisely by using an equilibrium turbulent flame relation (Peters 1999).

The flame wrinkling factor is always unity for laminar expansion, so that the curves of wrinkled and mean flame area coincide with each other as seen in Figure 7.4. For turbulent cases, this remains close to unity only during the very early stage and rapidly increases with the growing flame area.

![Figure 7.5: Turbulent flame speed and the flame stretch factor during the flame kernel development](image)

\( u' = 0 \)
\( u'/S_l = 1 \)
\( u'/S_l = 2 \)
Lines with symbols show turbulent flame speed
A similar behaviour is also shown by the flame stretch factor $I_0$, where a lower value is observed for smaller radii attributable to higher curvature stresses and it gradually increases towards the unity. However, the value always remains less than unity due to the presence of turbulent stresses. The higher the turbulence, the lower the saturated value of the stretch factor. These predictions are in well accordance with experimentally observed trends during the flame kernel development stage (Herweg et al. 1988) and it verifies the good predictability of the present formulation.

### 7.1.2 Flame Kernel Development in a Swirl Chamber

In this section, the validity of the present ignition and flame kernel model formulation is further tested by assessing its predictions with respect to published experimental literature. Here, the flame kernel growth in an engine swirl chamber is simulated and compared with experimentally measured flame kernel data by Herweg & Maly (1992). A schematic diagram of the swirl chamber and the engine configuration used for this purpose is shown in Figure 7.6.

![Schematic diagram of the swirl chamber and the engine configuration used for flame kernel imaging work of Herweg & Maly (1992)](image)

Figure 7.6: Schematic diagram of the swirl chamber and the engine configuration used for flame kernel imaging work of Herweg & Maly (1992)

The swirl chamber is connected to the engine cylinder head through a circular channel, which is tangentially attached to the chamber periphery. Thus, a strong swirl field is produced within the chamber, each time the piston reaches to its compression TDC. Optical access to swirl chamber was available from two orthogonal directions through quartz windows. Formation of the flame kernel and its development were continuously photographed using high-speed schlieren imaging. Total wrinkled flame surface area was calculated by evaluating the two
dimensional area in flame images assuming rotational symmetry about a suitable. In order to completely flush out residual gasses, the engine was skip-fired every sixteenth cycle.

Some of the major specifications of this engine are given in Table 7.1. The engine was fuelled with propane. Thin wire electrodes with an inter electrode gap of one millimetre were used connected to a TCI system for spark ignition. The ignition point was located towards the chamber wall at a radius of 12.5 mm measured from the centre axis. TCI systems show fundamentally different characteristics compared to traditional capacitive discharge ignition systems (CDI). TCI delivers most of the spark energy during the glow discharge phase, which last around 0.6 to 1.2 ms. In CDI systems most of the electrical energy is liberated during the spark breakdown phase (Herweg et al. 1988), which lasts only about 0.1 to 0.2 ms.

<table>
<thead>
<tr>
<th>Engine, swirl chamber and the ignition system parameters</th>
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<tbody>
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<td>Engine parameters</td>
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<tr>
<td>Bore</td>
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<tr>
<td>Stroke</td>
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<tr>
<td>Connecting rod</td>
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<tr>
<td>Compression ratio</td>
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<tr>
<td>Fuel</td>
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<tr>
<td>Skip cycle ratio</td>
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<td>Swirl chamber</td>
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<td>Diameter of connecting throat</td>
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<td>Diameter of swirl chamber</td>
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<tr>
<td>Clearance of side chamber</td>
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<tr>
<td>Ignition system</td>
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<tr>
<td>Type of the ignition system</td>
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<td>Spark location</td>
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<td>Spark electrode gap</td>
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<td>Ignition timing</td>
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Simulations were performed for three engine speeds: 300, 500 and 750 rpm, and two air-fuel ratios representing lean and stoichiometric conditions. Table 7.2 provides information about operating conditions and mean turbulent parameters. Pressure, mean flow velocity, turbulent data and the parameters of the ignition system were obtained from experimental measurements for all test cases (Herweg et al. 1988). Temperature at ignition was computed
using simple thermodynamic analysis based on inlet mixture temperature and measured crank
resolved in-cylinder pressure trace (Falfari & Bianchi 2007).

Table 7.2 Operating conditions and turbulence parameters of the simulated test cases

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<thead>
<tr>
<th>Operating conditions for the simulated test cases</th>
<th>Test case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine RPM</td>
<td>300</td>
</tr>
<tr>
<td>Fuel-air equivalence ratios</td>
<td>1.0 &amp; 0.77</td>
</tr>
<tr>
<td>Pressure at ignition (bar)</td>
<td>5</td>
</tr>
<tr>
<td>Temperature at ignition</td>
<td>660</td>
</tr>
<tr>
<td>Turbulent intensity (cms⁻¹)</td>
<td>44</td>
</tr>
<tr>
<td>Integral length scale (cm)</td>
<td>0.4</td>
</tr>
<tr>
<td>Mean flow velocity at peripheral spark location (cms⁻¹)</td>
<td>750</td>
</tr>
<tr>
<td>Ignition energy supplied (mJ)</td>
<td>60</td>
</tr>
<tr>
<td>Ignition duration (ms)</td>
<td>1.2</td>
</tr>
</tbody>
</table>

7.1.2.1 Numerical Setup

Simulation of the complete engine geometry and the swirl chamber requires significant
amount of computational time. In addition, some of the essential engine parameters required
in computations, such as valve lift profile and manifold pressure data were not available.
Therefore, only the swirl chamber was modelled in this study. The computational mesh
comprised of nearly 87,000 unstructured hexahedral cells with a nominal cell size of 0.7 mm.
Figure 7.7 (a) shows an image of the computational mesh. Simulations were started few
microseconds before the ignition and the chamber swirling flow field was initialised to follow
the profile of a Bessel function (Amsden et al. 1989). Swirl velocity was adjusted to match
the measured mean velocity at the spark location. Standard $k-\varepsilon$ turbulence model was
employed and the initial kinetic energy was set to obtain the measured turbulent intensity
value. Shown in Figure 7.7 (b) is the initialized flow field across the spark plane of the swirl
chamber. Arrows indicates the direction and relative magnitude of the tangential velocity
components on the section plane. SPK is the location of spark electrodes. The entire process
of ignition and the flame kernel lasts only a few milliseconds. Since the piston is closer to the
TDC, there is no significant displacement of piston face during this period. Accordingly, a
frozen turbulent field was assumed during the analysis. Therefore, all the turbulent parameters
in unburned gases are considered to remain unchanged. Turbulent intensity and the turbulent
integral length scales were directly used from measurements. Rest of the parameters were
numerically computed by the model. Simulations were carried out for 2.0 \( ms^{-1} \) and transition to main combustion model was not considered.

Figure 7.7: (a) Computational mesh of the swirl chamber
(b) Initial swirl velocity profile across the centre plane of the chamber for test case 2

7.1.2.2 Results & Discussion

Evolution of the total flame area during the flame kernel development stage for all six test cases is shown from Figure 7.8 to Figure 7.10. Symbols show the experimentally measured flame area as reported in Herweg & Maly (1992). Simulated results are shown in solid and chained lines. In general, measured and predicted flame areas were found to be in very good agreement for all engine speeds and air-fuel ratios. As it was already verified in the previous simulations in the closed cubic vessel, the model has been able to successfully respond to the changes in turbulence intensity and the mixture composition in these simulations as well.
Figure 7.8: Evolution of flame surface area during flame kernel formation at 300 rpm

Figure 7.9: Evolution of flame surface area during flame kernel formation at 500 rpm
Variations of ignition model parameters are shown from Figure 7.11 to Figure 7.16. Each graph shows the changes in laminar flame speed, flame stretch factor, turbulent speed, flame radius, plasma expansion speed and the effective flame propagation speed during the ignition period for a given engine speed and a fuel-air equivalence ratio. The effective flame speed $S_{eff}$ is given by the summation of turbulent flame speed and the plasma expansion speed. It should be noted that, the third axis of these graphs shows the plasma expansion speed. Initially plasma speed has a high value and drops towards zero within about 0.4 ms as often experimentally observed. It is seen that, this time delay is somewhat larger for the lean mixture compared to the stoichiometric conditions in all cases. This trend has also been experimentally observed by Herweg et al. (1988). As a result, the effective speed of flame propagation and the total reaction rate become very high at the beginning but, exponentially decay with the decreasing plasma speed.
Figure 7.11: Variation of computed ignition model parameters during ignition for stoichiometric air-fuel mixture at an engine speed of 300 rpm

Figure 7.12: Variation of computed ignition model parameters during ignition for an equivalence ratio of 0.77 at an engine speed of 300 rpm
Figure 7.13: Variation of computed ignition model parameters during ignition for stoichiometric air-fuel mixture at an engine speed of 500 rpm

Figure 7.14: Variation of computed ignition model parameters during ignition for an equivalence ratio of 0.77 at an engine speed of 500 rpm
Figure 7.15: Variation of computed ignition model parameters during ignition for stoichiometric air-fuel mixture at an engine speed of 750 rpm

Figure 7.16: Variation of computed ignition model parameters during ignition for an equivalence ratio of 0.77 at an engine speed of 750 rpm
Influence of turbulence on the flame propagation is evident even from the very early stage. Turbulence speed remains close to the corresponding laminar speed only during the very early stage of kernel formation. It rapidly becomes much larger than the laminar speed and saturates at the equilibrium turbulent flame speed. It can be noticed in Figure 7.11 to Figure 7.16 that the deviation point of the turbulent flame speed from its laminar velocity remains close to 0.1 $ms^{-1}$. This is where the turbulent effects start to appear for the first time in the course of kernel formation. These predictions are further supported by the findings in Herweg et al. (1988), as it was reported that in swirl chamber experiments, turbulent effects became apparent after 0.1 $ms^{-1}$ from the spark breakdown.

In general, the variation of other parameters, such as the stretch factor, laminar flame speed and the flame radius show a similar trend as observed in the simulations in the closed cubic vessel. However, significant differences of the flame kernel shape and its location were noted. In addition, initial stage fluctuations in the flame kernel radii are minimal in these simulations, as the computational mesh used here is relatively finer than the mesh of the cubic vessel.

Shown in Figure 7.17 are contour plots of reaction progress variable across the centre plane of the swirl chamber and the distribution of flame kernel particles, during the flame kernel formation in the stoichiometric air-fuel mixture at an engine speed of 750 $rpm$. The intersection point of the dashed lines shows the spark location. An enlarged view of these contours is shown in Figure 7.20. In this case, the conditions in the vicinity of the spark location correspond to a mean swirl speed of 18.7 $ms^{-1}$ and a laminar flame speed of 95 $cms^{-1}$. Due to high swirl, the flame kernel gets stretched and the shape of the flame kernel becomes ellipsoidal. This phenomenon is often observed in SI engines and therefore, Pischinger & Heywood (1990) modelled the flame kernel as an ellipsoid in their ignition model. Also, the location of the centre of the flame kernel is found to be displaced significantly from the spark location. In the present case, this distance is about 1.0 $cm$ after 0.625 $ms^{-1}$ from breakdown and is very much comparable to both the flame dimension and the chamber dimension which is also about 1.0 $cm$ and 4.5 $cm$ respectively.
Accordingly, these observations confirm that, the apparent flame kernel elongation and mean flow convection effects have to be essentially incorporated in an accurate formulation. It should also be noted that, the original form of the DPIK model, in which the spherical flame kernel expansion centred on the spark location is assumed, it cannot account for such effects.

### 7.1.3 A Qualitative Comparison with Schlieren Flame Images

In this section, a qualitative comparison between simulated and experimentally photographed images of the flame kernel is made. First rows of Figure 7.18 to Figure 7.20 show contour plots of the reaction progress variable on flame front. Corresponding time elapsed after the spark breakdown also shown. These contours represent the mean shape and the location of the flame kernel. The second row shows analogous experimental schlieren images taken at the specified time. Note that, these schlieren images have been modified from their original form in Herweg & Maly (1992) and Herweg et al. (1988) to enhance the picture quality, but without any loss of major flame details. The circular sections in schlieren images represent the flame kernel, while the straight segment attached to it, is the thin wire electrode. It should also be noted that, both contour plots and schlieren images have been scaled up from their actual size with two different arbitrary scales, thus only the relative dimensions should be compared.

Figure 7.17: Flame kernel formation represented by reaction progress variable contours and Lagrangian marker particles at stoichiometric air-fuel ratio and 750 rpm under swirling conditions
Figure 7.18: Comparison of simulated and schlieren imaged flame kernel formation at stoichiometric air-fuel ratio and 300 rpm

A representative case of formation of the flame kernel under low levels of turbulence and swirl conditions is shown in Figure 7.18. The mean turbulent intensity is about 44 $cms^{-1}$ and the laminar flame speed is 95 $cms^{-1}$; thus $u'/S_l < 1$. The mean convection velocity is also measured to be around 7.5 $ms^{-1}$. Consequently, the flame kernel remains nearly spherical throughout the development phase as revealed by both the present simulations and experimental images. It is interesting to note that, even with this low level of bulk flow convection velocity, the flame kernel centre seems to displace from the spark location. In this case, the flame radius is approximately about 0.4 cm after 0.625 ms from breakdown and the displacement of the kernel centre is of the same order. These experimental observations have been very well predicted by the present simulations.

Figure 7.19 shows the results corresponding to $u'/S_l ≈ 1$; where, $u' = 73$ $cms^{-1}$ and $S_l = 95$ $cms^{-1}$. The mean convection velocity is close to 12.4 $ms^{-1}$. It is clear that, no longer the spherical nature of the kernel expansion can be observed from both simulations and experimental images. The flame is spherical only during the first 250 $\mu$s and later it gradually becomes ellipsoidal. As in the previous case, a comparable displacement of the flame kernel centre, in the order of the flame radius is apparent. The relative size of the flame kernel is also found to be larger than that of 300 rpm cases due to the enhanced flame propagation by the increased turbulent intensity. Interestingly, these variations have also been successfully captured by the present model.
Figure 7.19: Comparison of simulated and schlieren imaged flame kernel formation at stoichiometric air-fuel ratio and 500 rpm

Figure 7.20: Comparison of simulated and schlieren imaged flame kernel formation at stoichiometric air-fuel ratio and 750 rpm

Figure 7.20 shows the flame kernel images corresponding to 750 rpm. The mean convection velocity is around $18.7 \, ms^{-1}$. The laminar flame speed is $95 \, cms^{-1}$ and the turbulent intensity is $109 \, cms^{-1}$. In this case also, it can be considered as $u'/S_l \approx 1$ but, $u' > S_l$. Compared to the two other cases previously discussed, this has the highest flame growth rate and the largest displacement of the kernel centre from the spark location, due to the presence
of the highest turbulent and mean convection speed levels. Remarkably, these effects have also been well recovered by the present flame kernel model.

With the increase of the convection velocity, the flame kernel tends to show a cornucopia shape, deviating from the ellipsoidal shape as clearly seen in Figure 7.20. This effect is caused by the curvature of the chamber walls which makes the mean flow to follow a curved path. In addition, two other global trends can also be observed. As it is evidence from all the experimental images, the flame remains attached to the spark electrode as a result of electrical energy discharge from the ignition system. This is called the flame holder effect and is predominant only in the TCI ignition systems with longer discharge duration. In general, conventional CDI ignition systems do not exhibit significant flame holder effects. Also, there is a noticeable tendency to burn into the centre of the chamber due to the large centrifugal acceleration field within the chamber as discussed in Groff and Sinnamon (1982). No special model was introduced in the present formulation to account for these effects. However, the tendency of flame kernel to propagate into the chamber has been reasonably captured by the present model. In a Lagrangian type model, simulation of an attached flame requires incorporation of some form of ad-hoc modelling assumptions. For example, Herweg and Maly (1992) in their zero dimensional ignition model, simulated this phenomenon by a set of continuously emerging flame kernels at the end of every time step, similar to re-striking (re-ignition). Pischinger & Heywood (1990) fixed one end of the ellipsoidal flame kernel at the spark location. Similarly, Duclos & Colin (2001) maintained a set of Lagrangian particles across the spark channel in the Arc and Kernel Tracking Ignition Model (AKTIM). However, in some cases, particularly in lean mixtures and CDI systems, the flame kernel get detached from electrodes and blown away by the flow field. It has not yet been identified a definite criterion to distinguish between these two situations. Hence, in the current formulation, these effects were neglected. However, present simulations have been able to successfully recover the size and the position of the core region of the flame kernel with a better accuracy.

Figure 7.21 shows the simulation and experimental results of ignition in a lean mixture at 500 rpm. The growth rate of the flame kernel is slower than that of stoichiometric mixture under similar turbulent conditions due the reduced laminar flame speed. However, the displacement of the kernel centre is comparable as the mean convection speed remains the same. These characteristics have been well predicted by the flame kernel model with good qualitative and quantitative agreements.
Simulation results for other two lean cases corresponding to 300 rpm and 750 rpm are shown in Figure 7.22 and Figure 7.23. However, no experimental images of these two cases were available for comparison. As, in the previous cases, the flame tend to propagate slowly, but the kernel displacement is in the similar order as stoichiometric conditions due to the changes in laminar flame speed and the unchanged mean swirl velocity.
7.2 Validation of the FBML Combustion Model

The focus of this section is to benchmark the FBML model, developed in Chapter 5, using published literature. Performance of the present ignition and flame kernel model is also verified as a secondary objective. In this test case, propane combustion in the General Motor (GM) research engine published in Kuo and Reitz (1989) was modelled. This engine has a pancake combustion chamber with a centrally located spark plug. In-cylinder pressure trace, mass burn data and relevant operating conditions have been unambiguously specified in Kuo and Reitz (1989). This data set has also made the foundation for several previous validation studies as reported in Groff & Sinnamon (1981) and Abraham et al. (1985). Specifications and geometric details of the of the GM research engine are given in Table 7.3.

<table>
<thead>
<tr>
<th>Specification</th>
<th>GM research engine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (cm)</td>
<td>10.50</td>
</tr>
<tr>
<td>Stroke (cm)</td>
<td>9.525</td>
</tr>
<tr>
<td>Squish (cm)</td>
<td>1.260</td>
</tr>
<tr>
<td>Connecting rod length (cm)</td>
<td>15.80</td>
</tr>
<tr>
<td>Intake valve opening</td>
<td>30° BTDC</td>
</tr>
<tr>
<td>Intake valve closing</td>
<td>243° BTDC</td>
</tr>
<tr>
<td>Maximum intake valve lift (cm)</td>
<td>1.0</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>8.56</td>
</tr>
<tr>
<td>Fuel</td>
<td>Propane</td>
</tr>
</tbody>
</table>

*Squish height - distance between piston crown surface and the cylinder head at piston TDC position*

Figure 7.23: Simulated images of flame kernel formation at equivalence ratio of 0.77 and 750 rpm
7.2.1 Numerical Setup and Test Conditions

Computational mesh used in this simulation is shown in Figure 7.24 and it comprises of 320,000 unstructured hexahedral cells. The squish region comprises around 100,000 computational cells, which corresponds to a nominal cell dimension of 1.0 mm. Operating conditions of the engine for each case considered are summarized in Table 7.4. Test conditions were chosen to investigate the model behaviour in changing equivalence ratio, engine speed, spark advance and different load conditions. For example, case 2 represents wide open throttle conditions under full load while, case 1 represents part load conditions.

![Computational mesh for the GM research engine at 110° before TDC](image)

Table 7.4 Operating conditions of GM research engine

<table>
<thead>
<tr>
<th>Case</th>
<th>$\phi$</th>
<th>RPM</th>
<th>Spark advance (BTDC)</th>
<th>$T_w$ (K)</th>
<th>$T_{IVC}$ (K)</th>
<th>$u'_{IVC}$ (cm/s)</th>
<th>$L_{IVC}$ (cm)</th>
<th>Residual mass fraction (%)</th>
<th>Trapped mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.87</td>
<td>1500</td>
<td>27°</td>
<td>420</td>
<td>453</td>
<td>46</td>
<td>0.403</td>
<td>12.0</td>
<td>0.486</td>
</tr>
<tr>
<td>2</td>
<td>0.87</td>
<td>1500</td>
<td>27°</td>
<td>440</td>
<td>429</td>
<td>46</td>
<td>0.403</td>
<td>9.8</td>
<td>0.710</td>
</tr>
<tr>
<td>3</td>
<td>0.98</td>
<td>1500</td>
<td>27°</td>
<td>425</td>
<td>453</td>
<td>46</td>
<td>0.403</td>
<td>14.0</td>
<td>0.499</td>
</tr>
<tr>
<td>4</td>
<td>0.87</td>
<td>1000</td>
<td>29°</td>
<td>405</td>
<td>436</td>
<td>31</td>
<td>0.403</td>
<td>13.8</td>
<td>0.496</td>
</tr>
</tbody>
</table>
Simulations were started at intake valve closure during the compression stroke. Initial properties and mass fractions were calculated using a thermodynamic analysis. In cylinder, fluid and turbulent properties were homogeneously initialized except the dissipation rate of turbulent kinetic energy, which was taken to be inversely proportional to the distance from the cylinder wall. For all the calculations, a swirl ratio of 0.67 was used as recommended by Kuo et al. (1989). The improved DPIK model was used for ignition and flame kernel modelling and the fully developed phase was simulated using the FBML model.

### 7.2.2 Application of the Ignition Model in the GM Engine

![Graphs showing variations of flame speed components and flame radius during the ignition period for different operating conditions of the GM research engine.

**Case 1**
- Spark advance = 27 BTDC
- Engine speed = 1500 rpm
- Trapped mass = 0.486 g
- $\phi = 0.87$

**Case 2**
- Spark advance = 27 BTDC
- Engine speed = 1500 rpm
- Trapped mass = 0.710 g
- $\phi = 0.87$

**Case 3**
- Spark advance = 29 BTDC
- Engine speed = 1000 rpm
- Trapped mass = 0.496 g
- $\phi = 0.98$

**Case 4**
- Spark advance = 29 BTDC
- Engine speed = 1000 rpm
- Trapped mass = 0.496 g
- $\phi = 0.87$

Figure 7.25: Variations of flame speed components and flame radius during the ignition period for different operating conditions of the GM research engine.
Shown in Figure 7.25 are the predictions of the ignition model for the above test cases in the GM research engine. The major differences between case 1 and case 2 are the intake mixture temperature, wall temperature and the trapped mass within the engine cylinder. Compared to case 1, case 2 has a higher charge mass but, its inlet temperature is lower by 24 K. Consequently, by the time of ignition, the case 1 has a lower pressure and a higher temperature so that, it gains a slightly higher laminar flame speed. The plasma expansion speeds remain approximately the same as the relative increase in unburned enthalpy of case 1 is much less compared to the burned gas internal energy and the mean pressure is somewhat similar. Plasma speed has dropped closer to zero within 3 – 4 crank degrees or within 0.3 – 0.4 ms after breakdown as often observed in engine applications.

Case 3 is close to stoichiometric conditions than other test cases, thus it has the highest laminar flame speed. Case 4 has a lower engine speed and thus, lowest in turbulence intensity. Therefore in case 4, the resultant turbulence flame propagation speed is also lower than other cases. In all cases, the transition from the ignition model to the main combustion model occurs around 7 crank degrees. By this time, the flame kernel has a mean radius of 5-6 mm. These results are well in agreement with the observations of Heywood (1994) and Herweg & Maly (1992), who reported approximate transition radii of 5 mm and 10 mm respectively. Moreover, Heywood (1994) observed that it takes around 5 – 10 crank degrees at 1500 to 3000 rpm engine speeds for the flame kernel to reach the fully developed stage. Accordingly, these observations have been further verified by the results of present simulations, as the predicted values of these parameters are well within the experimental limits.

### 7.2.3 Application of the FBML model in the GM engine

One of the main objectives of the present study is to investigate the suitability of the present improved BML model (or the FBML model) in predicting wall-bounded combustion. Thus, the flame propagation characteristics in the vicinity of solid walls in GM engine were examined with the aim of assessing the effects of each of the suggested improvements. Consequently, the complete model form of the FBML model used to evaluate the unburned species consumption rate can be recast as follows:

\[
\dot{\omega} = \frac{C_{FBML} \rho_u I_0 S^0}{\sigma_f} \left( 1 + 2\bar{c} \right) \bar{c} \left( 1 - \bar{c} \right) I_{QR} \left( 1 + \frac{a}{Re^*_a} + \frac{b}{Re^*_a} \right) \frac{u'^3}{\varepsilon} \left( \frac{S_i}{u'} \right)^{6D-12}
\]  

(7.2)
where, \( C_{FBML} \) is the integrated model constant. As a reference case, the standard BML model (identified as MF1) with classical definition for the integral scale and constant \( n = 1 \) was used and the resultant flame evolution is shown in the first column in Figure 7.26. The second column depicts the predictions of the new BML model but with no wall-quenching model (MF2). Illustrated in column three are the results of the complete model, which comprises of the dynamic calculation of model constants and the quenching model (MF3).

![Figure 7.26: Propagation of the turbulent flame front represented by reaction progress variable in the GM research engine](image)

Figure 7.26 shows the variation of reaction progress variable across an axial cross sectional plane in the engine cylinder with the crank angle. Reacting zone may be identified as the region between zero and 1.0 values of the progress variable. Zero represents the unburned zone and unity is for the fully burned zone. The excessive flame acceleration with the standard BML (MF1) model is apparent even from the very early stage of the combustion process. This is more noticeable in the figure corresponding to -5 ATDC, where the burned fuel fraction reaches unity much faster on the piston surface even before the core area reaches...
its maximum. As a result, the propagating flame front is seen to be concave in the inner region and nearly flat in the leading front, where in reality both these regions are observed to be convex.

It can be seen from column 2 that, the introduction of the dynamic calculation of model constants (MF2) has made a considerable improvement over the standard model and has resulted in a more physical convex and outward flame front. However, in the vicinity of the walls a comparatively higher rate of reaction can still be seen. Dynamic evaluation of model constants with the allowance for local anisotropy has made a marked improvement over MF1, but at walls \( u' \) becomes so small such that, it overcomes the damping effects of dynamically calculated \( C_L \) and \( n \). As can be seen in the third column, employment of the novel quenching correlation (MF3) has been able to successfully inhibit the flame wall acceleration and has made the flame front agreeably convex. In addition, the resulting flame brush thickness is also thinner than the other model forms, which is more acceptable in this type of low turbulence engines. These observations are in good agreement with the optical imaging results of Weller et al. (1994) as well.

Not only the flame front evolution, but also the accurate prediction of pressure rise and the fuel burning rate is also equally important, particularly in engine combustion. Hence, the performances of the FBML model are compared against the pressure and mass burn data of the GM engine. Case 1 was chosen as the reference case and integrated model constant \( C_{FBML} \), which is the only adjustable constant was tuned to 1.23, in order to match with the measured peak pressure. The same value was used for all other computations in the GM engine. Computed results are very much encouraging and they are in close agreement for all the considered test cases as shown in Figure 7.27 and Figure 7.28.

Both the rate of pressure rise and the mass burned rate in the initial and middle stages of combustion has been very well predicted by the present model formulation for all cases. However in general, a slight over prediction of the peak cylinder pressure value is seen. This effect is predominant in the lower speed case; i.e. case 4, and the overshoot of the peak pressure is approximately 3.5 \( \text{bar} \). The common trend in peak pressure is to increase, when the engine speed is reduced as more time is available for combustion process, if all other conditions are kept unchanged (see Tan & Reitz 2006). However, if the effect of reduced turbulent intensity on the turbulent flame propagation is large enough to overcome other influences, a lower peak pressure may be obtained. In case 4, compared to case 1, all the conditions (including equivalence ratio and trapped mass) are similar, except the charge gas
temperature, wall temperatures and spark advance. The spark timing has been advanced by 2.0 crank degrees and in practice, this should contribute to an increase in peak pressure under normal circumstances. However, the reduction in wall and gas temperatures results in comparably lower temperatures at ignition and thus, a lower laminar flame propagation speed is expected. Therefore, the present over prediction in pressure in case 4 may probably be due to shortcomings associated with the estimation of laminar burning velocity or inaccuracies in the wall heat transfer calculations. On the other hand, this could be a result of incorrect estimation of flame wrinkling scale or turbulence level. However, further work is suggested to properly understand the causes and remedies in this regard.

![Graphs showing comparison of measured incylinder pressure with calculated values using the FBML model for different operating conditions of the GM research engine](image)

Figure 7.27: Comparison of measured incylinder pressure with calculated values using the FBML model for different operating conditions of the GM research engine
Calculated mass burn rates are in excellent agreement with the experimentally derived values, up until the cumulative mass burned is about 80%. It is difficult to draw a precise conclusion about the prediction during the very late stage of combustion, as experimental data was not available in Kuo et al (1989). However, beyond this point, an over prediction of mass burn rate is seen from the calculated results.
7.3 Full Cycle Simulation of Ricardo E6 Engine

The validation process is further extended here, by modelling the full cycle combustion process of Ricardo E6 engine at Loughborough University. Simulation of full cycle of an engine has a number of advantages over simulating only compression and combustion. Mainly, the in-cylinder mixture composition, species mixing and residual fractions at the time of combustion can be accurately simulated via a full cycle simulation without ad-hoc assumptions. In addition, the impact of spatial variations of turbulence, swirl and tumble motions on flame propagation and heat transfer is more realistically introduced. Moreover, precise estimation of localized turbulence effects is crucial, especially in the early stage of combustion during the flame kernel development, as excessive turbulence can hinder the flame development while, an adequate turbulence would accelerates its propagation.

A detailed description on the geometric details of the E6 engine, experimental setup, data acquisition system and the data analysing procedures can be found in Chapter 6. Therefore only, the numerical setup and the test conditions relevant to the chosen validation test cases are described here.

7.3.1 Numerical Setup and Test Conditions

Four different test cases were considered for validation, where each case is set to investigate the model response to changes in equivalence ratio, engine speed, spark advance, compression ratio and load conditions. These operating conditions are summarized in Table 7.5. Case 1, running under full load conditions, is considered to be the reference test case and case 2 is set to investigate the effect of variation in equivalence ratio. In case 3, the engine rpm and the spark advance is altered under part load conditions, whereas in case 4, the compression ratio is altered.

Table 7.5 Operating conditions of Ricardo E6 engine

<table>
<thead>
<tr>
<th>Case</th>
<th>( \phi )</th>
<th>RPM (BTDC)</th>
<th>Spark advance</th>
<th>Comp. ratio</th>
<th>( T_{in} (K) )</th>
<th>( T_{w} (K) )</th>
<th>Injected fuel mass (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.089</td>
<td>1500</td>
<td>16</td>
<td>8.7</td>
<td>298</td>
<td>360</td>
<td>425</td>
</tr>
<tr>
<td>2</td>
<td>0.936</td>
<td>1500</td>
<td>16</td>
<td>8.7</td>
<td>298</td>
<td>360</td>
<td>368</td>
</tr>
<tr>
<td>3</td>
<td>0.967</td>
<td>1800</td>
<td>20</td>
<td>8.7</td>
<td>300</td>
<td>365</td>
<td>317</td>
</tr>
<tr>
<td>4</td>
<td>0.953</td>
<td>1500</td>
<td>16</td>
<td>7.5</td>
<td>298</td>
<td>360</td>
<td>404</td>
</tr>
</tbody>
</table>

Ricardo E6 engine : Fuel - Gasoline
Figure 7.29 shows the computational mesh of the E6 engine used in these simulations. It comprises nearly 400,000 unstructured hexahedron cells at BDC. The mesh was created using the in-house mesh conversion software developed as a part of this research. More details on this software tool and the meshing procedure of the E6 geometry can be found in Chapter 2. The squish region comprises around 100,000 computational cells, which corresponds to a cell dimension in the order of 1.0 mm. Fully implicit solution algorithms with automatic time step controlling were used and the maximum time step was limited to 0.2 crank degrees.

![Computational mesh of Ricardo E6 engine](image)

Figure 7.29: Computational mesh of Ricardo E6 engine

Simulations were started 20° before TDC on the exhaust stroke. Initial properties and mass fractions were calculated using a thermodynamic analysis. In-cylinder and exhaust gas mixture was considered to be in fully burned conditions with negligible amounts of fuel residuals and intermediate combustion products. Based on measurements, burned gas temperature was set to be 750 K. Other in-cylinder fluid and turbulent properties were homogeneously initialized, except the dissipation rate of turbulent kinetic energy, which was taken to be inversely proportional to the distance from the cylinder wall. Initial turbulent kinetic energy in port regions was assumed to be 10% of the square of the initial mean flow velocity, following the recommendations of Amsden et al. (1989). In-cylinder turbulent intensity was initialized using the procedures suggested in Tabaczynski et al. (1980), assuming angular momentum conservation during rapid distortion. Mean temperatures on
combustion chamber surfaces were approximated using the thermal maps in Zhao et al. (1991, 1994) for a similar sized engine. Following Stewart (2006), cylinder wall temperature was taken to be $10 K$ greater than measured coolant temperature. The piston surface temperature is usually somewhat hotter than cylinder walls, so that it was considered to be $50 K$ higher than the cylinder wall temperature. The highest temperature, which is about $100 K$ above the wall temperature, is assigned for the cylinder head. Usually, the mean intake is slightly cooler and the exhaust valve is slightly hotter than the mean cylinder head. Therefore, it was assumed that, the exhaust valve temperature is $20 K$ higher and the intake valve is $20 K$ lower than the cylinder head temperature. However, given the fact that, the surface temperatures depend on many factors such as materials, cooling system design, engine speed and spark timing the actual values may differ as much as $20 \%$ or more; but in general, these errors has only a minor influence on the overall result (Henson 1998).

Intake plenum pressure was set to the measured intake port pressure and the exhaust plenum pressure was set to the measured averaged in-cylinder pressure during the mid-stage of the exhaust stroke. Note that, often in-cylinder pressure falls below atmospheric towards the end of the exhaust stroke (see Chapter 6). This is caused by the effects of complex wave action and usually, the exhaust manifold is intentionally designed to achieve such conditions, as it boosts the intake charge flow rate. Hence, the in-cylinder pressure towards the end of the exhaust stroke is not an appropriate value to be used as the exhaust port pressure. These wave action effects, particularly during with exhaust blow down and valve overlap period, can be substantial. However, for the time being, such effects were neglected in the present study. These effects may be explicitly considered in a future study by using experimentally measured pressure data at the exhaust plenum with a suitable wave action sub model or by simulating the entire engine breathing system. All turbulence and wall models remained the same as described in Chapter 3.

### 7.3.2 Predicted Flow Characteristics during Intake and Compression Strokes

Figure 7.30 to Figure 7.34 illustrate the evolution of in-cylinder flow field of the E6 engine during intake and exhaust strokes under the conditions specified for case 1. Images on the left side show the computed magnitude of the velocity across the intake valve plane. Shown on right are the two dimensional velocity vectors interpolated onto the same plane. The actual nature of the flow field is strongly three dimensional, which can only be represented by a dynamic multiple plane visualisation. However, these figures provide an insight into some of the key flow features.
Figure 7.30: Ricardo E6: Computed velocities at the intake valve plane—valve overlap and early intake
Figure 7.31: Ricardo E6: Computed velocities at the intake valve plane – mid intake
Figure 7.32: Ricardo E6: Computed velocities at the intake valve plane – late intake
Figure 7.33: Ricardo E6: Computed velocities at the intake valve plane – early compression
Figure 7.34: Ricardo E6: Computed velocities at the intake valve plane – mid/late compression
Figure 7.30 depicts the flow pattern during the valve overlap and early intake. The valve overlap period starts with the opening of intake valve at $9^0$ BTDC and lasts until the exhaust valve closure at $10^0$ ATDC. Following the opening of the intake valve, high pressure burned gases within the cylinder, flow into the intake manifold with a very high speed inducing a reverse flow. With the start of the intake stroke, the strength of the reverse flow diminishes, drawing fresh gases into the cylinder through the intake valve. The most complex flow structures are evolved during the intake. The high speed conical jet through the valve passage generates a three dimensional toroid structure below the intake valve. The right centre (as viewed) of this structure remains below the valve face throughout the intake, while the left center follows the piston descend. Interaction of the jet stream with cylinder wall, piston face and the valve skirt results in formation of several tumbling eddies, by the time of mid intake as shown in Figure 7.31. When the piston has reached to BDC, a distinct large tumbling motion is evident, with smaller eddies in-between. On the other hand, as illustrated in Figure 7.35, a strong swirling motion has also been formed. Combination of both the tumbling and swirling motions produces a large vortex structure, whose central axis lies diagonally across the cylinder.

![Figure 7.35: Computed in-cylinder velocities at intake BDC on three radial planes](image)

- $z = 11 \text{ cm}$
- $z = 07 \text{ cm}$
- $z = 03 \text{ cm}$

Vel. mag. ($\text{cms}^{-1}$)

- 2000
- 1500
- 1000
- 500
- 0

2000 $\text{cms}^{-1}$
Note that the vectors have been scaled up by a factor of two from Figure 7.32 to Figure 7.34. Intake valve closes $37^0$ after the start of the compression stroke and by this time, flow structures have significantly dissipated vortex energy making mean flow velocity relatively lower. Rising piston face forms an ordered upward motion of the flow, inducing a weak eddy structure close to the cylinder head, which still exhibits a swirling motion as shown in Figure 7.34.

Illustrated in Figure 7.36 (a) is the in-cylinder flow structure of the Ricardo E6 engine just before ignition. Flow field in the vicinity of the spark plug appears relatively less intense. Although, an apparent convection field directed towards the centre of the cylinder is present across the spark plug location, its absolute magnitude is not that strong enough to make a distinct influence. Consequently, the flame kernel is more likely to show a spherical progression. The turbulent intensity is also shown to be relatively small in the spark region. One of the main characteristics of turbulence: decaying towards solid boundaries, can clearly be identified from the Figure 7.36 (b). The near wall intensity of the turbulent kinetic energy is within the range $0-5000 \text{ cm}^2\text{s}^{-2}$, which is approximately about 50 times lower than its magnitude in the core region. Hence, the conventional approach of BML model should result in flame-wall acceleration, when applied to this test case.

Figure 7.36: Computed (a) velocity field (b) turbulent kinetic energy, in Ricardo E6 engine for case 1, on the spark location plane, just before ignition
### 7.3.3 Flame Kernel Formation in the E6 Engine

![Case 1](image1.png) ![Case 2](image2.png) ![Case 3](image3.png) ![Case 4](image4.png)

**Figure 7.37:** Variations of flame speed components and flame radius during the ignition period for different operating conditions of the E6 engine

Results of the present improved DPIK model, applied to the E6 engine are plotted in Figure 7.37. Basic characteristics of the flame kernel formation largely show common trends as explained in earlier sections. The average evolution period up to the transition, is about 5 crank degrees, except in the case 1, where it is slightly lower. The longest duration has been predicted for case 3, which has a lower compression ratio. Averaged transition radius of the flame kernel is approximately 0.5 cm and the highest of 0.58 cm has been predicted for case 4. The difference in transition flame kernel radius in case 4 is primarily due to the transition criteria used the present model formulation. The transition takes place when the flame radius
is greater than the integral scale of turbulence. When the piston is close to TDC, the integral scale of turbulence is proportional to the squish height. As the compression ratio in case 4 is lower, its squish height is larger by 3 mm compared to the other test cases. Thus, case 4 has a larger integral scale (provided that, other turbulent conditions are similar) and the longest kernel evolution period. Since, no experimental data is available on the flame kernel formation in the E6 engine, it is difficult to make an exact comparison. However, based on published literature, it could be concluded that, the present predictions are quite agreeable with commonly observed trends during flame kernel formation in similar sized SI engines operating in similar conditions (see Tan & Reitz 2003).

Figure 7.38: Flame kernel formation in case 1, represented by the iso-surface of the progress variable \( \tilde{c} = 0.5 \)

Figure 7.38 shows flame kernel surface represented by the iso-progress variable surface \( \tilde{c} = 0.5 \) for case 1. As expected, the evolution of the flame kernel in the E6 engine is shown to be more spherical due to the absence of a strong convection field. However, by the transition time is reached, the kernel has been pronouncedly convected towards the centre of the cylinder, with respect to the spark location.
7.3.4 Prediction of Fully Developed Combustion in E6 Engine

In this section, results of the combustion simulations in E6 engine using the new formulation of BML model are discussed. The only adjustable model constant $C_{FBML}$ was optimised to 2.15 to obtain the peak pressure of the case 1, and used unchanged for all the other cases. All other sub models were kept unchanged as in previous cases. Pressure trace of the predictions are compared with the experimentally measured values and plotted in Figure 7.39 to Figure 7.42. In general, the predicted and simulated traces of in cylinder pressure are in good agreement, except in case 4, where a slight over prediction is observed. Importantly, the model has precisely captured the trends in in-cylinder pressure variations under different operating conditions. Estimation of the peak pressure was reasonably accurate. Predicted peak pressure locations are slightly deviated by few crank degrees within the range of 0-4 degrees.

![Comparison of measured and predicted pressure traces for full cycle engine simulation in Ricardo E6 engine – case 1](image)

Figure 7.39: Comparison of measured and predicted pressure traces for full cycle engine simulation in Ricardo E6 engine – case 1
Figure 7.40: Comparison of measured and predicted pressure traces for full cycle engine simulation in Ricardo E6 engine – case 2

Figure 7.41: Comparison of measured and predicted pressure traces for full cycle engine simulation in Ricardo E6 engine – case 3
It is noted that the present model over predicts the pressure drop during the latter stage of the power stroke. This may probably be due to the absence of a blow by model in these simulations. In case 1, where there is a higher peak pressure and a lower engine speed, the difference is much noticeable compared to case 3, where engine speed is higher and the peak pressure is low. In case 3, as less time (due to high \textit{rpm}) and a lower peak pressure is available, less blow by mass is expected, so that the predictions closely follow the experimental trace. Correspondingly, the blow-by mass should be higher in case 1, so that there is a slight difference in two pressure traces. In general, the overall agreement in the pressure predictions during the early and middle stage of the engine cycle is quite satisfactory for all cases proving the capability of present model formulation in turbulent combustion predictions in SI engines.

Comparison of experimentally determined heat release data with the predicted heat release rates are shown in Figure 7.43. Heat release rate is a direct function of the time derivative of in-cylinder pressure. Even though the simulated and measured pressure curves seem to match closely, there can be a significant mismatch in heat release rate curves. Therefore, only a well formulated model can predict both pressure and heat release curves with a good success. Heat release from the measured pressure curve is derived following the method explained in
Chapter 6. A value for the specific heat ratios was estimated by curve fitting the log P-V diagram during the compression period. For simplicity, this value was assumed unchanged during the combustion as well. Heat release curves represent the net heat release i.e. the wall heat flux has been subtracted from the heat release rate due to combustion.

![Graphs showing heat release rate and cumulative heat release rate](image)

Figure 7.43: Comparison of heat release rate and cumulative heat release rate predicted by FBML model with the values calculated for experimental data

The model has well predicted the peak value of heat release within a 10% error margin and the global trend is likely to over predict. As it was noted in pressure curves, location of the peak heat release rate has a slight shift of 0-4 crank degree. In first two cases, the peak heat release location occurs after the measured location, whilst in the other two cases, it occurs few
degrees before the measured point. However, the resultant cumulative heat release has been calculated with a much better accuracy and the overall error is well within 5%. For case 1 and case 2, the predicted rate of increase of heat release rate during the early stage is slightly lower than that of experimental values. In other two cases, they follow the experimental rate quite closely. In general, a distinct early start of the heat release can be identified. This could be an indication of the incorrect estimation of the onset kernel volume. Predicted heat release in the last stage of combustion is found to be acceptable in the first two cases, while a drift towards right is seen for the other two cases. However, for all cases the rate of change of heat release rate during the latter stage are shown to agree well.

Spatial variations of some of the FBML model parameters across the flame region are illustrated in Figure 7.44 to Figure 7.46. The flame and the burned gas region can be identified by the enclosed region of the reaction progress variable in Figure 7.44 (a). The iso-contour of $\bar{c} = 0.5$ approximately represents the mean flame front. Comparison of Figure 7.45 (a) and Figure 7.46 (a) indicates that, the computed mean flame wrinkling scale $L_y$ does not seem to follow the exact distribution of integral scale of turbulence $L_i$. In fact, as already noted, it is a complex function of laminar flame speed, turbulent intensity and the integral length scale. In this illustrated case, the value of $u'/S_i$ is approximately around 2.0. Thus, according to Eq. (7.2), $L_y$ always has a lesser value than $L_i$. However, both $L_y$ and $L_i$ have comparatively higher values within the flame front. Similarly, they have minimum values near the wall in fresh gas and gradually increase across the flame front towards burned gases. Due to the inverse relationship with turbulent intensity, $L_y$ reaches to local maximums in low turbulence regions.

As shown in Figure 7.45(b), the dynamic integral scale constant $C_L$ varies from a minimum of 1.0 to slightly higher than 1.3 in this case. For the bulk of the flow, $C_L$ has value close to the unity. The higher the turbulent intensity it is much closer to this limit. The maximum value is reached close to walls in the burned gas region. On the other hand, as depicted in Figure 7.46 (b), the wrinkling scale exponent $n$ has a minimum of slightly less than 0.8 at low turbulence burned gas region. It gradually increases across the flame front, until it achieves a maximum of 2.1 in fresh gas region. Also note that, its value is relatively small near walls.
Figure 7.44: Variation of FBML combustion model parameters at 19$^0$ ATDC for case 1. Ignition is at 16$^0$ BTDC: Reaction progress variable and turbulent kinetic energy

Figure 7.45: Variation of FBML combustion model parameters at 19$^0$ ATDC for case 1. Ignition is at 16$^0$ BTDC: Integral scale and dynamic integral scale constant
Figure 7.46: Variation of FBML combustion model parameters at 190 ATDC for case 1. Ignition is at 160 BTDC: Mean flame wrinkling scale and wrinkling scale exponent

Figure 7.47 shows the propagation of the flame front for case 1. The flame front was approximated as the iso-surface of the progress variable $\tilde{c} = 0.5$. Spherical behaviour of flame propagation during the early stage of flame development is apparent from the figure at 349 CAD, which is just after 5 degrees from ignition. By 354 CAD, the flame front is sufficiently large enough to be wrinkled by turbulence and by 364 CAD the flame can no longer be seen with a laminar like flame front. Figures corresponding to 373 CAD and 382 CAD clearly show the features of fully developed flame propagation and 390 CAD shows the quenching of flamelets due to wall flame interaction. Flame at intake valve side reaches the wall slightly faster compared to the exhaust side as its propagation is delayed by the recirculating fresh gases on XZ plane near the exhaust valve side (see Figure 7.36). However, the global mean flame propagation is shown to be approximately symmetric across vertical spark plug plane. This is obviously typical for these types of flat piston, flat head engines running at low speeds.
7.4 Summary

- Newly developed ignition and flame kernel formation model was comprehensively validated against experimental measurements and schlieren images.
- Flame kernel surface area, displacement of the kernel centre and the physical shape of the kernel volume were assessed during the comparison and shown to be in good agreement with measured values.
- Introduction of special measures would be needed to simulate flame holder effects with the present model.
- FBML turbulent combustion model was applied to simulate the premixed wall bounded combustion in spark engine applications. The benchmark calculations were performed using the published data on the GM research engine.
- Predicted pressure and mass burn rates results were in very good agreement with the experimental data for a range of operating conditions of the engine and model has been able to successfully eliminate the wall flame acceleration problem.
- Validation was extended by simulating the full cycle simulation of Ricardo E6 engine.
• Predicted and measured profiles for pressure and heat release were found to be in good agreement and also the predicted flame front profile was found to be in par with the experimental observations.

• Implementation of a blow-by model and a wave action sub model may have the potential of improving the predictability of the present formalism.

• In general, the present model developments have been very successful for the applications of RANS, which is still extensively used by many engine developers for modelling and design work.
Use of the LES techniques has become increasingly popular for engineering simulations. LES results are more accurate, less model dependent and provide detailed information. In addition, LES is very much appropriate for engine simulations as it provides the opportunity to simulate inherent unsteady phenomena such as cycle-to-cycle variations and combustion instabilities. Therefore, the use of LES in engine modelling provides a more reliable way of investigating operational and geometric refinements. LES techniques have been widely used in non-reacting flow modelling. Its application to combustion simulation is still in a preliminary stage. In particular, studies devoted to IC engine simulations using LES are very limited. In this chapter, an attempt has been made to develop an LES engine code based on the well-known KIVA 4 - RANS code, to be used in combustion simulations.

A brief introduction to the filtering concepts of LES is provided in section 8.1. Derivation of filtered balance equations for species, momentum and energy transport is explained in section 8.2. Closure of these balance equations requires developing a sub-grid scale turbulence model, which is somewhat similar to the closure problem in RANS. The present approach to solve this issue and possible alternative methods are also discussed in detail in section 8.3. An in depth discussion on one of the most powerful features of LES: the ability to calculate model constants dynamically, based on resolved scale information, is presented in section 0. In sections 8.5-8.7, filtered governing equations are further refined specifically to suite for the easier implementation in the present code. Limitations of LES in wall layer modeling and possible solutions are explained in section 8.8 and a concluding summary is provided in section 8.9.
8.1 LES Filtering Procedure

In LES, the flow field is spatially filtered; i.e. a flow property \( \phi(x, y, z, t) \) is decomposed in to resolved and unresolved components given by \( \bar{\phi}(x, y, z, t) \) and \( \phi'(x, y, z, t) \) respectively. In LES context, over bar is used to indicate the spatially filtered or resolved quantities and prime shows unresolved quantities. Resolved terms are commonly named as super-grid or grid filtered terms and unresolved terms are called sub-grid scale (SGS) components. Super-grid terms can be directly calculated by solving filtered governing equations, whereas SGS terms need modelling. The two components are related to each other as follows:

\[
\phi = \bar{\phi} + \phi'
\]  

(8.1)

Filtration of a function \( f(x, y, z, t) \) by a given filter kernel \( G(x, y, z, \Delta) \) can be mathematically interpreted as shown in Eq. (8.2). An integral of this form is termed as the convolution. The Filter kernel \( G(x, y, z, \Delta) \) should be a rapidly decaying function in space with the normalisation property given in Eq. (8.3).

\[
\tilde{f}(x_i, t) = \int_\Omega G(x_i, x'_i, \Delta) f(x'_i, t)dx'_i
\]  

(8.2)

\[
\int_\Omega G(x_i, x'_i, \Delta) dx'_i = 1
\]  

(8.3)

\( x_i \equiv (x, y, z) \) is a spatial location on which the filtering is performed and the cut-off width \( \Delta \) defines the size of the local filter stencil. \( \Omega \) represents the global filter domain. \( x'_i \) is the spatial coordinates of neighbouring points and thus \( |x_i - x'_i| \) is the distance measured from \( x_i \).

In particular, the filter width determines the lower cut-off limit of fluctuations. Also, it is an indicative measure of the resolved and rejected eddy sizes. Eddies larger than the cut-off scale are directly computed within the computational mesh while smaller ones are rejected. If the same filtering function is used throughout the computational domain (as usually done in practical LES calculations), filter kernel can be further simplified to \( G(x_i, x'_i, \Delta) = G(x_i - x'_i, \Delta) \). Even though it is possible to define various filter kernels, the most commonly used filter kernels in finite volume based CFD modelling are the Box filter and the Gaussian filter. Some LES calculations have also been performed using spectral cut-off filters in time domain as detailed in Lesieur & Métais (1996). However, spectral methods present fundamental difficulties when adapting to general purpose CFD problems (Versteeg & Malalasekera 2007).
Box or top hat filter

\[ G(x_i - x'_i, \bar{\Delta}) = \begin{cases} 
\frac{1}{\bar{\Delta}^3} |x_i - x'_i| \leq \bar{\Delta}/2 \\
0 & |x_i - x'_i| > \bar{\Delta}/2
\end{cases} \]

(8.4)

Gaussian filter

\[ G(x_i - x'_i, \bar{\Delta}) = \left(\frac{\xi}{\pi \bar{\Delta}^2}\right)^{3/2} \exp \left[ -\frac{\xi |x_i - x'_i|^2}{\bar{\Delta}^2} \right] \]

(8.5)

Choice of a filter type has only a minor influence on results (McMillan 1979), but top hat filtering is preferred in LES modelling of engineering systems due to the simplicity. Gaussian filtering is also occasionally applied and in such cases, it is customary to take \( \xi = 6 \) (Calaf et al. 2010).

In theory, it is possible to select any size for the filter cut-off width, but use of a smaller value than the computational cell size has no advantage as only a single value is left in the cell centre at the end of the computation. Therefore, traditionally, the cut-off scale is taken to be in the same order of cell dimension and may be given by:

\[ \bar{\Delta} = (\Delta x \Delta y \Delta z)^{1/3} \]

(8.6)

where, \( \Delta x \), \( \Delta y \) and \( \Delta z \) are length, width and height of the computational cell respectively and hence, the cut-off scale is often taken equivalent to the cubic root of the cell volume.

If the filter width is independent of time, it is possible to establish the commutative property of filtering of time derivatives as given in Eq. (8.7). However, care must be taken when the filter width in a given location is varying with time such as in IC engine simulations with moving boundaries. Thus, adequate measures should be taken to account for temporal commutative errors in such situations.

\[ \frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial t} \]

(8.7)

According to Moureau et al. (2004b), this error can be neglected up to the first order, if both the flow field and mesh motion is generated by the movement of the same boundary surface. This is often the case in conventional SI engine simulations. However, if adaptive local mesh refinement techniques are used, no longer the temporal commutative errors can be disregarded.
Commutation property may not be valid for spatial derivatives in general, except if the filter width is also spatially uniform. A detailed study on this aspect can be found in Goshal and Moin (1995). However, in general, uncertainties associated with the spatial commutation errors are neglected and corrective measures are assumed to be incorporated in the SGS model. In fact, this assumption may be wrong for IC engine like complex geometries, where the spatial variance of the grid size is considerable. Spatial commutation of a property $\phi$ may be approximated as follows.

$$\frac{\partial \overline{\phi}}{\partial x} \sim \frac{\partial \tilde{\phi}}{\partial x} \quad (8.8)$$

### 8.1.1 Favre Filtering

In variable density flows, density weighted filtering or Favre filtering is always preferred.

$$\tilde{\rho} \tilde{f}(x_i, t) = \int_{\Omega} \rho G(x_i, x'_i, \Delta) f(x'_i, t) dx'_i \quad (8.9)$$

In this section, tilde indicates the Favre filtered quantities defined by the following relations.

$$\tilde{\phi} = \frac{\overline{\rho \phi}}{\overline{\rho}} \quad (8.10)$$

$$\phi = \tilde{\phi} + \phi'' \quad (8.11)$$

In the present study, filtered governing equations have been derived by applying the Favre filtering on unsteady Navier-Stokes equations. The filter kernel was taken to be of the form of top hat, with a cut-off width equal to cubic root of the cell volume.

In addition to commutative properties, LES filtered variables should satisfy the following properties under general circumstances.

$$(\overline{\phi + \psi}) = \tilde{\phi} + \tilde{\psi}, \quad \overline{\phi''} \neq 0 \quad \text{and} \quad \overline{\phi} = \overline{\phi} \quad (8.12)$$

Here, $\approx$ denotes double Favre filtered variables. Contrary to RANS, it should be noted that the filtered SGS fluctuations are not zero. $\psi$ is an another flow property similar to $\phi$. 

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8.2 Filtered Balance Equation for Momentum

Given in Eq. (8.13) is the unsteady Navier-Stokes equation for momentum transport in the $x$ direction. LES balance equation for momentum is derived by filtering this equation.

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u U) + \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial \tau_{yx}}{\partial y} - \frac{\partial \tau_{zx}}{\partial z} = \vec{F}_B
\]

(8.13)

Using the definition of Favre filtering and temporal commutative property, the rate of change of momentum can be written as:

\[
\frac{\partial (\rho u)}{\partial t} = \frac{\partial (\rho u)}{\partial t} = \frac{\partial (\rho u)}{\partial t}
\]

(8.14)

The convection term can also be written in the following form by assuming the spatial commutation.

\[
\nabla \cdot (\rho u U) = \nabla \cdot (\rho u U) = \nabla \cdot (\rho u U)
\]

(8.15)

In order to evaluate the resultant term $\nabla \cdot (\rho u U)$, it is required to compute the filtered quantity $\tilde{u} \tilde{U}$. There is no simple mathematical technique to directly compute this term. Hence, to accomplish this task, a new term $\nabla \cdot (\rho u \tilde{U})$ is introduced as shown by Eq. (8.16).

\[
\nabla \cdot (\rho u \tilde{U}) = \nabla \cdot (\rho u \tilde{U}) + [\nabla \cdot (\rho u \tilde{U}) - \nabla \cdot (\rho u \tilde{U})]
\]

(8.16)

If the term within the square brackets is taken to be equal to $\tau_{sgs,x}$ as given by Eq. (8.17):

\[
\tau_{sgs,x} = \tilde{\rho}(\tilde{u} \tilde{U} - \tilde{u} \tilde{U})
\]

(8.17)

the resultant convection term becomes

\[
\nabla \cdot (\rho u \tilde{U}) = \nabla \cdot (\rho u \tilde{U}) + \nabla \cdot \tau_{sgs,x}
\]

(8.18)

The first term on the right hand side, which was introduced externally, can be directly computed from the resolved variables. However, the term $\tilde{u} \tilde{U}$ is still embedded in $\tau_{sgs,x}$ and requires some form of modelling approximation in order to close the equation. $\tau_{sgs,x}$ represents the SGS stresses in $x$ direction. It is worth to highlight the importance of the externally introduced term $\nabla \cdot (\rho u \tilde{U})$, at this juncture. It forms the definition of SGS stress.
tensor and modelling the SGS stress tensor is the fundamental problem in LES. This is similar to finding a closure for Reynolds stresses in RANS. An alternative definition has also been suggested by Germano (1989) and a brief discussion on this formulation is made in the context of test filtering in section in Appendix B.

SGS stress tensor comprises of nine stress components. A general component $\tau_{sgs_{xy}}$, may be written as:

$$\tau_{sgs_{xy}} = \bar{\rho}(\bar{u}\bar{v} - \bar{u}\bar{v})$$

(8.19)

The complete filtered momentum equation in $x$ direction can be recast as:

$$\frac{\partial}{\partial t} (\bar{\rho}\bar{u}) + \nabla. (\bar{\rho}\bar{u}\bar{U}) + \nabla. \tau_{sgs,x} = -\frac{\partial \bar{\rho}}{\partial x} + \frac{\partial \bar{\tau}_{xx}}{\partial x} + \frac{\partial \bar{\tau}_{yx}}{\partial y} + \frac{\partial \bar{\tau}_{zx}}{\partial z} + \bar{\rho} \bar{g}_x$$

(8.20)

$\tau$, the resolved stress tensor, is obtained by filtering the Newtonian viscous stress tensor.

$$\tau_{xy} = \mu \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right) - \frac{2}{3} \mu \left( \frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} \right) \delta_{xy}$$

(8.21)

$$\tau = \mu \left[ (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^T \right] - \frac{2}{3} \mu (\nabla \cdot \bar{U}) I$$

(8.22)

Eq. (8.21) shows a general component of the resolved stress tensor and Eq. (8.22) shows the assembled form in compact tensor notation.

### 8.3 Sub-Grid Closure Methodology

One of the fundamental problems in LES modelling is to find an expression for the SGS stress tensor. This has been an active topic of research for many decades. The traditional way of modelling the SGS stress tensor is to follow the Leonardo decomposition (Leonard 1974). The SGS model used in this study is somewhat different from the Leonardo’s approach, as much advanced strategies are needed to accurately estimate complex flow features in IC engines. However, for the completeness and the historical perspective, the conventional approach is briefly discussed at this point. In fact, many of the current advanced formulations are still established upon the basic ideas suggested in Leonardo decomposition.

According to Leonard (1974), the stress tensor may be decomposed into three terms. If the SGS stress tensor in Eq. (8.19) is expanded by using the definition given in Eq. (8.11), a general component of the SGS tensor can be written as:
where, $L_{xy}$ is the Leonard term and it can be explicitly calculated from the resolved velocity field. However, $C_{xy}$, the cross stress terms and $R_{xy}$, the SGS Reynolds stresses need to be modelled. Leonard stresses are due to the interaction of resolved scale eddies and cross stresses are formed by interacting resolved and unsolved eddies. An approximate expression to calculate cross stress terms can be found in Ferziger (1977). Reynolds stresses are the result of convective momentum transfer between unresolved eddies and closed by using a SGS turbulence model. Smagorinsky (1963) suggested the following model for the calculation of Reynolds stresses.

### 8.3.1 Smagorinsky SGS Model

Since the SGS scale eddies are believed to be almost isotropic and the production and dissipation of turbulence is in equilibrium, Smagorinsky suggested that they can be modelled using a similar formulation as the Boussinesq’s eddy viscosity hypothesis. Accordingly, the local SGS Reynolds stresses are taken to be proportional to the local strain rate of the resolved flow field as given in Eq. (8.25) to Eq. (8.27). The constant of proportionality is the sub-grid dynamic viscosity given by $\mu_{sgs}$.

$$R_{xy} = -2\mu_{sgs} \left[ \tilde{S}_{xy} - \frac{1}{3} (\nabla, \bar{U}) \delta_{xy} \right] + \frac{1}{3} R_{kk} \delta_{xy}$$  \hspace{1cm} (8.25)

$$R_{kk} = R_{xx} + R_{yy} + R_{zz}$$ \hspace{1cm} (8.26)

$$\tilde{S}_{xy} = \frac{1}{2} \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right)$$ \hspace{1cm} (8.27)

The term $1/3 R_{kk} \delta_{xy}$ is to recover the correct expression for SGS kinetic energy and $1/3 (\nabla, \bar{U}) \delta_{xy}$ ensures the same in variable density flows.

If a suitable expression for cross stresses is used, it is possible to use the Smagorinsky model in practice. In fact, this has been the basis for several early LES investigations. However, later it was found that, the three stress terms could be lumped together (Versteeg & Malalasekera 2007) despite their different nature and the whole SGS stress can be modelled as a single entity given by:
\[ \tau_{sgs, xy} = -2\mu_{sgs} \left[ \delta_{xy} - \frac{1}{3} (\nabla \cdot \mathbf{U}) \delta_{xy} \right] + \frac{1}{3} \tau_{sgs, kk} \delta_{xy} \]  \hspace{1cm} (8.28)

\[ \tau_{sgs, kk} = \tau_{sgs, xx} + \tau_{sgs, yy} + \tau_{sgs, zz} = 2k_{sgs} \]  \hspace{1cm} (8.29)

where, \( k_{sgs} \) is the unresolved kinetic energy. Based on the Prandtl’s mixing length model, the SGS viscosity is estimated as:

\[ \mu_{sgs} = \tilde{\rho} C_{sgs}^2 \tilde{\Delta} \sqrt{2 \delta_{xy} \delta_{xy}} \]  \hspace{1cm} (8.30)

It should be noted that \( \mu_{sgs} \) is a local property, which varies spatially with the flow field. The mixing length scale is taken to be same as the filter cut-off width. \( C_{sgs} \) is a model constant to be evaluated experimentally. A range of values for \( C_{sgs} \) has been suggested from 0.1 to 0.24 by Lilly (1966, 1967) and Rogallo & Moin (1984). Usually the application of Smagorinsky model required fine-tuning of \( C_{sgs} \) for the particular flow configuration. This may probably be an indication that the sub-grid eddies are not that isotropic as expected in the derivation (Versteeg & Malalasekera 2007). Further, this model has been found to be excessively dissipative, especially near walls. However, Smagorinsky model is still widely used in both reactive and non-reactive LES modelling in engine and non-engine applications (see Moureau et al. 2004a, Richard et al. 2007 & Goryntsev et al. 2010 for example).

One of main aims of LES turbulence modelling is to accurately solve more flow structures. This could be accomplished only by providing sufficient allowance for non-linear terms (Rutland 2011). There are two possibilities to meet this requirement. One is to use a less dissipative turbulence model and the other is to use a denser grid. Both these methods improve non-linear interactions by increasing the percentage of resolved kinetic energy. In this regard, the quality of the SGS turbulence model plays a major role. The higher the accuracy of the turbulence model the lesser the grid resolution requirement for a satisfactory solution. The Smagorinsky model is simple, but much dissipative, so that it demands higher grid densities. An alternative is to use a more accurate higher order SGS model. Because of this reason, the feasibility of couple of sub-grid scale kinetic energy based models: \( k_{sgs} - \Delta \) and \( k_{sgs} - k_{sgs} l \) models, has been assessed in the present study. The basic form of these models has been originally developed for atmospheric flows by Yshizawa & Horiuti (1985) and later modified for engineering flows by Kim & Menon (1995). These models are still based on SGS viscosity but, solve a separate transport equation for SGS kinetic energy \( k_{sgs} \), providing enhanced provision to account for more physical processes such as production,
convection and dissipation of $k_{sgs}$. Hence, the effect of dissipation term of $k_{sgs}$ is not that important as in the Smagorinsky model. Recently, a non-viscosity based model called dynamic structure model has been proposed by Pomraning & Rutland (2002) and found to produce promising results. However, this model needs further research to be applied to engine like practical engineering applications.

### 8.3.2 $k_{sgs} - \Delta$ SGS Model

It is possible to define the sub-grid kinetic energy in the following manner.

$$
k_{sgs} = \frac{1}{2} [((u\bar{u} - \bar{u}\bar{u}) + (v\bar{v} - \bar{v}\bar{v}) + (w\bar{w} - \bar{w}\bar{w})] \tag{8.31}
$$

$$
k_{sgs} = \frac{1}{2} [((u^2 - \bar{u}^2) + (v^2 - \bar{v}^2) + (w^2 - \bar{w}^2)] \tag{8.32}
$$

$$
U''_{sgs} = \sqrt{u''^2 + v''^2 + w''^2} = \sqrt{\frac{2}{3} k_{sgs}} \tag{8.33}
$$

Now, a general component in the SGS stress tensor given in Eq. (8.28) can be re-written as:

$$
\tau_{sgs_{xy}} = -\mu_{sgs} \left( \frac{\partial \bar{u}}{\partial y} + \frac{\partial \bar{v}}{\partial x} \right) + \frac{2}{3} \left[ (\nabla.\bar{U}) + \bar{\rho} k_{sgs} \right] \delta_{xy} \tag{8.34}
$$

The assembled SGS stress tensor in compact vector notation can be given by:

$$
\tau_{sgs} = -\mu_{sgs} \left[ (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^T \right] + \frac{2}{3} \left[ (\nabla.\bar{U}) + \bar{\rho} k_{sgs} \right] \mathbb{I} \tag{8.35}
$$

In this model, the sub-grid viscosity is evaluated by the following expression.

$$
\mu_{sgs} = C_v \bar{\rho} k_{sgs}^{1/2} \bar{\Delta} \tag{8.36}
$$

where, $C_v$ is a model constant and usually taken to be 0.067 for engine configurations (Calhoon 1996, Sone et al. 2000a and Hori et al. 2007). SGS kinetic energy is obtained by solving the following transport equation.

$$
\frac{\partial}{\partial t} (\bar{\rho} k_{sgs}) + \nabla. (\bar{\rho} k_{sgs} \bar{U}) = -P_{sgs} - D_{sgs} + \nabla. \left( \frac{\mu_{sgs}}{S_{Ck}} \nabla k \right) + \bar{W}^{s\text{p}a\text{r}y} \tag{8.37}
$$

$P_{sgs}$ represents the production rate of $k_{sgs}$ due to sub-grid stresses and may be closed by using the following expression (Sone et al. 2000a).
\[ P_{sgs} = \tau_{sgs_{xx}} \frac{\partial \tilde{u}}{\partial x} + \tau_{sgs_{xy}} \frac{\partial \tilde{u}}{\partial y} + \tau_{sgs_{xz}} \frac{\partial \tilde{v}}{\partial x} + \tau_{sgs_{yx}} \frac{\partial \tilde{v}}{\partial y} + \tau_{sgs_{yz}} \frac{\partial \tilde{w}}{\partial z} \]
\[ + \tau_{sgs_{zx}} \frac{\partial \tilde{w}}{\partial x} + \tau_{sgs_{zy}} \frac{\partial \tilde{w}}{\partial y} + \tau_{sgs_{zz}} \frac{\partial \tilde{w}}{\partial z} \]  
\[ (8.38) \]

\[ D_{sgs} = (\nabla \otimes \tilde{U}) : \tilde{\tau}_{sgs} \]  
\[ (8.39) \]

The model constant \( C_e \) is often taken to be 0.916.

### 8.3.3 \( k_{sgs} - k_{sgs}l \) SGS Model

For the purpose of comparison, a two equation model proposed by Arunajatesan & Sinha (2000) has also been implemented. This type of closure was initially introduced for RANS modelling, and further developed to suite LES. In this model, in addition to the transport equation for the sub-grid kinetic energy, a secondary transport equation is solved for the product of length scale and the sub-grid kinetic energy. Further details on this approach can be found in Arunajatesan & Sinha (2000) and Speziale (1998).

The transport equation for the product of SGS kinetic energy and the length scale is given by:
\[ \frac{\partial}{\partial t} (\bar{\rho}k_{sgs} l) + \nabla \cdot (\bar{\rho}k_{sgs} l \tilde{u}) \]
\[ = P_{sgs, kl} - D_{sgs, kl} + \nabla \left[ \bar{\rho}C_{kI} \left( k_{sgs}^{1/2} \right) \nabla k_{sgs} l + \bar{\rho}C_{kI} \left( k_{sgs}^{3/2} \right) l \nabla l \right] \]  
\[ (8.41) \]

It should be noted that, an alternative definition is used to compute the sub-grid viscosity in this model given by:
\[ \mu_{sgs} = C_v \bar{\rho}^{1/2} k_{sgs} l \]  
\[ (8.42) \]
8.4 Dynamic Evaluation of SGS Model Constants

One of the major problems of SGS modelling is the calibration of SGS model constant to suite a particular application. In order to avoid this tedious task, Germano et al. (1991) suggested a procedure, which allows automatic calculation of SGS model constant accounting for both spatial and temporal variations, using information from smallest resolved scales. This is considered to be one of the revolutionary breakthroughs in LES modelling. Later this procedure was extended for compressible flows by Moin et al. (1991). Most importantly, this approach can be equally applied not only for SGS turbulence modelling but also for the dynamic determination of other SGS scalar fluxes and combustion model constants in reacting flows.

However, it is somewhat unclear whether to use this dynamic approach for turbulence modelling of IC engine, as even the static models are not yet adequately tested (Rutland 2011). Therefore, the implementation of the dynamic $k_{sgs} - \Delta$ or any other dynamic turbulence model was not considered in this study. For the completeness, a comprehensive discussion on dynamic SGS modelling, the major equations involving in such an implementation and required explicit test filtering procedures in both structured and unstructured grids are described in Appendix B.

8.5 Mass Conservation

Filtered balance equation for the conservation of species mass can be expressed as:

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{U}) + \nabla \cdot (\bar{\rho} \bar{Y}_m \bar{V}_m) + \nabla \cdot \Phi_{sgs} + \nabla \cdot \Theta_{sgs} = \bar{\omega}_{m,\text{spray}} + \bar{\omega}_{m,\text{chem}}$$

(8.43)

$\Phi_{sgs}$ is the SGS convective mass (a scalar) fluxes given by:

$$\Phi_{sgs} = \bar{\rho} (\bar{u} \bar{Y}_m - \bar{U} \bar{Y}_m)$$

(8.44)

and $\Theta_{sgs}$ is the SGS scale molecular diffusion fluxes specified in the following form.

$$\Theta_{sgs} = \bar{\rho} (\bar{V}_m \bar{Y}_m - \bar{V}_m \bar{Y}_m)$$

(8.45)

Compared to the SGS convection, $\Theta_{sgs}$ is quite small and often neglected in LES modelling. Contribution of $\Phi_{sgs}$ is rather important and precise modelling in a reacting flow field with very high heat release rates is a challenging task. This is similar to turbulent mass flux.
modelling in RANS and the complexity associated with this term has been previously discussed in Chapter 3.

Several modelling strategies are available in the literature for SGS scalar flux modelling. Simple gradient transport hypothesis, linear eddy model (Kerstein 1991), scale similarity model (Fureby & Möller, 1995) and dynamic structure function model (Chumakov & Rutland 2004) are among some of the popular methods. However, simple gradient transport also seems to produce very good results in the LES context. Borger and Veynante (2000) observed that, the simple gradient model alone has been able to produce the effects of complex counter gradient transport phenomenon in premixed combustion in a V-shaped flame holder. This finding is highly encouraging and still a vast majority of LES simulations are based on this method. Therefore, in the present study, simple gradient hypothesis is used.

\[
\nabla \cdot \Phi_{sgs} = -\nabla \cdot (\overline{D}_{sgs} \nabla \bar{Y}_m) \tag{8.46}
\]

\[
\overline{D}_{sgs} = \frac{\mu_{sgs}}{\overline{S}c_{sgs}} \tag{8.47}
\]

Using Fick’s law of diffusion, super-grid diffusion fluxes are closed.

\[
\nabla \cdot (\rho \bar{Y}_m \bar{V}_m) = -\nabla \cdot (\rho \overline{D}_m \nabla \bar{Y}_m) \tag{8.48}
\]

\[
\overline{D}_m = \frac{\mu}{\overline{S}c} \tag{8.49}
\]

\(\mu\) and \(\overline{S}c\) are respectively the molecular viscosity and the Schmidt number.

Adding up all the species mass conservation equations, the global mass continuity equation is derived.

\[
\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{U}) = \bar{\omega}_{spray} \tag{8.50}
\]

### 8.6 Internal Energy Equation

Filtered balance equation for the transport of internal energy can be expressed as follows:

\[
\frac{\partial}{\partial t} (\bar{\rho} \bar{I}) + \nabla \cdot (\bar{\rho} \bar{I} \bar{U}) + \bar{p} \nabla \cdot \bar{U} + \nabla \cdot \bar{q} - (\nabla \otimes \bar{U})^T \cdot \tau = \bar{Q}_{1,spray} + \bar{Q}_{1,chem} \tag{8.51}
\]
Convection term \( \nabla \cdot \rho \tilde{I} \tilde{U} \) is rearranged as shown below so that, the new term \( h_{sgs} \) has to be modelled.

\[
\nabla \cdot \rho \tilde{I} \tilde{U} = \nabla \cdot \rho \tilde{I} \tilde{U} + (\nabla \cdot \rho \tilde{I} U - \nabla \cdot \tilde{I} U) \tag{8.52}
\]

\[
h_{sgs} = \tilde{p}(\tilde{I} U - \tilde{I} \bar{U}) \tag{8.53}
\]

As in the SGS mass flux modelling, classical gradient assumption is used to close the SGS internal energy fluxes.

\[
h_{sgs} = -\frac{\mu_{sgs} c_p}{\rho_{sgs}} \nabla \tilde{T} \tag{8.54}
\]

SGS viscous energy dissipation can be modelled in the following manner.

\[
(\nabla \otimes \bar{U})^\pi \cdot \tau = (\nabla \otimes \bar{U})^\pi \cdot \tilde{\tau} + \Theta_{sgs} \tag{8.55}
\]

\[
\Theta_{sgs} = (\nabla \otimes \bar{U})^\pi \cdot \tau - (\nabla \otimes \bar{U})^\pi \cdot \tilde{\tau} \tag{8.56}
\]

\( \Theta_{sgs} \) has to be calculated using a suitable model. However, this can be modelled using the dissipation rate of the SGS kinetic energy following the RANS approach in original KIVA version (Amsden et al. 1989). Hence, \( \Theta_{sgs} \) was taken to be equal to \( D_{sgs} \). The heat flux vector is expressed by:

\[
\bar{q} = -\mathcal{K}(\nabla \tilde{T}) - \tilde{\rho} \sum_m D_m \tilde{h}_m (\nabla \tilde{Y}_m) \tag{8.57}
\]

The remaining super-grid term \( (\nabla \otimes \bar{U})^\pi \cdot \tilde{\tau} \) was explicitly modelled. Note that, the original RANS approach does not treat laminar and turbulent parts of viscous energy dissipation separately. Instead, the overall effect is lumped together through the rate of dissipation of turbulent kinetic energy. As in the case of SGS mass flux modelling, it is possible to use aforementioned alternative approaches for SGS energy fluxes as well. However, they were not considered here for implementation, due to the reasons explained above.
8.7 The Working Set of Equation for LES

The set of governing equations derived in the above sections are summarised here for the completeness.

**Momentum Equation**

\[
\frac{\partial (\bar{\rho} \bar{U})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{U} \bar{U}) + \nabla \cdot \bar{\rho} \vec{v} + \nabla \cdot \left( \frac{2}{3} \bar{\rho} \bar{k}_{sgs} \right) - \nabla \cdot \bar{\tau}_{eff} = \bar{\rho} \ddot{g}
\]  

(8.58)

\[
\tau_{eff} = \mu_{eff} \left[ (\nabla \otimes \bar{U}) + (\nabla \otimes \bar{U})^T \right] - \frac{2}{3} \mu_{eff} (\nabla . \bar{U}) I
\]  

(8.59)

\[
\mu_{eff} = \mu + \mu_{sgs}
\]  

(8.60)

**Species and Global Mass Conservation**

\[
\frac{\partial (\bar{\rho} \bar{\gamma}_m)}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\gamma}_m \bar{U}) = \bar{\omega}_{spray}
\]  

(8.61)

\[
\frac{\partial (\bar{\rho} \bar{\gamma}_m)}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\gamma}_m \bar{U}) - \nabla \cdot (\bar{\rho} D_m \nabla \bar{v}_m) + \nabla \cdot \phi_{sgs} = \bar{\omega}_{m,spray} + \bar{\omega}_{m,chem}
\]  

(8.62)

\[
\phi_{sgs} = - \left( \frac{\mu_{sgs}}{S_{\gamma_{sgs}}} \nabla \bar{v}_m \right)
\]  

(8.63)

**Internal Energy Conservation**

\[
\frac{\partial (\bar{\rho} \bar{\zeta})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\zeta} \bar{U}) + \bar{\rho} \bar{\zeta} (\nabla \cdot \bar{U}) - (\nabla \otimes \bar{U})^T : \bar{\tau} + \nabla \cdot \bar{h}_{sgs} - \bar{D}_{sgs}
\]  

(8.64)

\[
= \bar{Q}_{l,spray} + \bar{Q}_{l,chem}
\]

\[
\bar{h}_{sgs} = - \frac{\mu_{sgs} \bar{c}_p}{\bar{p}_{sgs}} \nabla \cdot \bar{\zeta}
\]  

(8.65)

\[
\bar{D}_{sgs} = C_\varepsilon \bar{p} \frac{\bar{k}_{sgs}^{3/2}}{\bar{\Lambda}}
\]  

(8.66)
SGS Kinetic Energy

\[
\frac{\partial}{\partial t}(\bar{\rho}k_{sgs}) + \nabla \cdot (\bar{\rho}k_{sgs} \bar{U}) = -P_{sgs} - D_{sgs} + \nabla \cdot \left( \frac{\mu_{sgs}}{Sc_k} \nabla k \right) + \bar{W}^{spary}
\]  \hspace{1cm} (8.67)

\[
P_{sgs} = (\nabla \otimes \bar{U}) : \bar{\tau}_{sgs}
\]  \hspace{1cm} (8.68)

\[
\mu_{sgs} = C_v \bar{\rho} \bar{k}_{sgs}^{1/2} \bar{\Delta}
\]  \hspace{1cm} (8.69)

\(k_{sgs}\) is separated from the SGS tensor and treated explicitly. Then, both laminar and SGS tensors are formally similar and can be assemble to a single tensor via effective viscosity. Now the momentum equation is exactly the same as KIVA-RANS momentum equation and no modification required in implementation. Species and global mass conservation equations are also similar in form. If the gradient hypothesis is used to close the SGS mass fluxes, it is possible to assemble the SGS and super-grid fluxes via effective viscosity. However, the SGS mass fluxes are required in the energy equation to model the SGS heat fluxes. Hence, the two quantities are explicitly calculated. Thus, compared to the analogues RANS equation, \(\nabla \cdot \Phi_{sgs}\) presents an additional term and \(\bar{\rho}D_m \nabla \Phi_m\) characterises resolved scale diffusive fluxes. Contrary to the RANS equation, \(h_{sgs}\) is the only additional term which needs explicit modelling in the LES internal energy. The LES heat flux vector now represents the resolved part.

Previously derived LES governing equations are formally similar to the original RANS equations used in the KIVA code. Therefore, the code can be modified to perform LES calculation without a significant difficulty. RANS version uses the effective viscosity: the summation of laminar and turbulent viscosities, in all terms. However for LES, all three viscosities: SGS, laminar and effective viscosities, are appropriately used. Therefore, care must be taken to use the relevant viscosity depending on the term being modeled. Unlike previous versions, where viscosity terms are explicitly used in computations, now in KIVA-4, the viscosity terms have been embedded into the geometric coefficients of cell faces. Hence, not only the procedures for viscosity calculations but also the geometric coefficients have also to be suitably modified. Moreover, the additional SGS terms arising due to filtering are also required to introduce appropriately.
8.8 Boundary Conditions and Wall Treatment

Similar to RANS, present LES mesh resolutions are not small enough to resolve the boundary layer (Piomelli 2008, Sagaut 2006). Hence, a suitable wall model has to be employed for better results. LES wall models can be broadly classified into three groups (Gungor 2010): equilibrium stress models, zonal approach and the hybrid approach. In equilibrium wall stress models; first proposed by Deardorff (1970) and later refined by Schumann (1975), no slip velocity boundary conditions are replaced with a suitable algebraic formulation for wall shear stresses and the tangential velocity component at the first node point assuming a log law distribution. However in these formulations, it was needed to prescribe the mean wall stresses as a priory from either experimental, RANS or high fidelity simulations. Reasonably accurate results have been reported using these models in simple channel flow problems but, extension for complex flow configurations was impractical due to the need of prior knowledge on wall shear stresses (Piomelli & Balars 2002). Further work of Grötzbach (1987) and Werner & Wengle (1993) has been successful in eliminating this limitation; consequently, these models are frequently used in today’s LES simulations. Recent advances and applications of these models and many other similar formulations can be found in the review of Piomelli (2008).

In the zonal approach; also known as two layer model (TLM) (Balaras & Benocci 1994), filtered LES equations are solved in the core region and simplified three dimensional LES transport equations are solved in the inner layer of the boundary region, within an embedded secondary mesh, which is highly refined in the wall normal direction. The hybrid approach, which is also called the detached eddy simulation (DES) (Spalart et al. 1997), uses only a single mesh, but the core region is resolved with LES equations and the boundary layer is modeled with RANS. In this case, the boundary region mesh has to be smoothed enough to be computed by RANS equations. Significantly improved results can be obtained with DES and TLM, even in engine like complex engineering problems as demonstrated in Hasse et al. (2010). On the other hand, a significant increase of the computational cost also to be expected with this method. Recent progress of these two methods can be found in Gungor & Menon (2010) and Spalart (2009).

Accordingly at present, the only possible solution for boundary layer modeling in complex geometries is to use an algebraic equilibrium log-law wall function formulation. For example, Enaux et al. (2011) and Vermorel et al. (2010) used the log-law model proposed in Schmitt et al. (2007) in engine applications with a reasonable success. However, the IC engine simulations of Goryntsev et al. (2011), Hori et al. (2007), Sone & Menon (2003) and Haworth
& Jansen (2000) have used no-slip boundary conditions, without using any form of wall model in relatively coarser meshes. Remarkably, the results are much superior and excellent agreements have been achieved with experimental measurements. Accordingly, no wall model was used in the present simulations other than the no-slip condition. Following the same work, temperature wall functions were also ignored. Other boundary conditions were kept unchanged as used in RANS modeling, described in Chapter 3. However, the investigation on the requirement of a suitable wall model for present LES formulation is highly recommended.

### 8.9 Summary

- Development of LES governing equations and their adaptation procedures were described in this chapter.
- Instantaneous Navier-Stokes equations were top-hat filtered and the SGS turbulence was modeled using the $k_{sgs} - \Delta$ model.
- Expecting to study the feasibility and for the comparison purposes, $k_{sgs} - k_{sgs}l$ model: an alternative SGS model, was also implemented.
- Both these models are based on the eddy viscosity concept and solve transport equations for SGS kinetic energy.
- Internal energy and species mass fluxes at SGS level were closed using the classical gradient hypothesis.
- Dynamic evolution procedures for SGS model constants were not employed in this work, but a comprehensive guideline was provided for a future implementation.
- Use of an appropriate wall layer model is essential, however as a first step, no slip boundary conditions were used.
- Other boundary conditions were kept unchanged as used in RANS simulations.
Turbulent combustion modelling is well established in RANS, but it is relatively new in LES. As a result, so called best practices are yet to be developed. Fundamental concepts in turbulent combustion, developed in the context of RANS are also valid in LES; however, cannot be applicable in the exact form. Combustion modelling in LES is particularly attractive, as it provides an insight into the associated unsteady effects. In addition, LES dynamic procedures allow automatic computation of combustion model constants as temporally and spatially varying functions of resolved scale information. To date, only a very few studies have been carried out to model SI engine combustion in LES. In fact, no attempt has been made at all, with a dynamic formulation. Therefore, in this chapter, a dynamic combustion model and a new ignition and flame kernel formation model have been developed to simulate the premixed combustion process in spark ignition engines.

In section 9.1, a brief introduction is provided on current concepts and challenges of combustion modelling in LES. An in depth description for the present approach has been provided in section 9.2. Procedures developed for dynamic evaluation of combustion model constants are explained in section 9.3. The development process of a new ignition and flame kernel formation model, to simulate the early stage of combustion is presented in section 9.5. A concluding summary of this chapter is provided in section 9.6.
9.1 LES Techniques for Modelling Premixed Flames

Premixed combustion modelling with LES is particularly a challenging task due to a number of difficulties. Usually, the premixed laminar flame thickness $\delta_l$, is very thin and it cannot be resolved on a computational mesh with typical LES mesh sizes. For example, the flame thickness in SI engine applications is about 0.1 mm (Heywood 1988). In order to adequately describe the flame front, a minimum of 5-10 grid points are needed with a common finite volume based CFD code (Vermorel et al. 2009). Therefore, this resolution requirement is prohibitively expensive, compared to the mesh resolution possible with current computing power, which is typically about 0.5 mm.

A possible solution is to neglect this physical consideration and model the combustion process using an eddy break-up (EBU) type formulation (Spalding 1971, 1977, Magnussen & Hjertager 1976). In such an approach, any modelling discrepancy may be absorbed by an adjustable model constant. The required turbulent time scale may be estimated in terms of the SGS kinetic energy and the LES filter width. The EBU model has two major shortcomings: negligence of the chemistry interaction with combustion and poor predictions in highly strained regions such as near walls. Moreover, the EBU model constant seems to be strongly dependent on the flow conditions and mesh configuration. However, there is only a very little work has been carried out to investigate the applicability of this type of a formulation (Poinsot & Veynante 2005) and some initial applications of the LES-EBU model can be found in Fureby & Löfström (1994) and Fureby and Möller (1995).

The $G$-equation (level-set) approach is also an alternative solution, where the flame front is described as a zero thickness surface. The propagation of the flame brush may be tracked by the field variable $\tilde{G}$ and the flame front is taken as the iso-level $\tilde{G} = G^*$; where, $G^*$ is often defined to be zero. The interesting fact is that, the resolved $\tilde{G}$ field does not have to follow the progress variable gradient. It can be smoothed out in space as broad as several mesh elements, so that it may be resolved on the LES mesh. Simulation of $\tilde{G}$ field requires the solution of a transport equation, where the displacement speed is modelled using the turbulent flame speed (Pitsch & Duchamp 2002, Moureaua et al. 2009). The major difficulty is that the turbulent flame speed is not yet a well-defined quantity and no universal model form is available. Usually, the simulations are relied on empirical or simple theoretical turbulent flame speed relations, wherein the RANS based turbulent velocity is directly replaced by the SGS velocity without a further justification (Poinsot & Veynante 2005).
Several geometrical assumptions have also to be imposed to maintain the adequate simplicity of the model, while artificial diffusivity should be added to avoid numerical difficulties, arising due to the formation of flame cusps (Piana et al. 1997, Janicka & Sadiki 2005). Consequently, significant further research is required to identify effective methods for the integration of level-set formulation with the turbulent flow field. Simulation of the full scale gas turbine combustor by Kim et al. (1999) is one of the successful engineering applications of this technique.

The thicken flame model (Butler and O’Rourke 1977) artificially enhances the flame front thickness, so that it can be sufficiently resolved in the computational mesh. Thickening of the flame front could be achieved by multiplying the thermal diffusivity by a user defined factor $F$, as the flame thickness $\delta_f$ is given by the ratio between the thermal diffusivity and the laminar flame speed. However, it is required to maintain the true laminar flame propagation speed, so that a correction for the reaction rate is mandatory. Simple laminar flame theories suggest that, the laminar flame speed is proportional to the product of thermal diffusivity and the pre-exponential factor of the Arrhenius reaction rate equation. Hence, correct reaction rate is achieved by dividing the pre-exponential factor by the same factor $F$.

The major advantage of this formulation is that, it can be used to study various phenomena such as ignition and wall flame interaction, without the use of ad-hoc sub models, as the reaction rate is modelled using the Arrhenius law (Colin et al. 2000). However, due the thickening of the flame front, interaction between chemistry and the turbulence is modified. To overcome this problem, an efficiency factor for SGS wrinkling has to be introduced (Colin et al. 2000).

Since the use of this method is combined with an Arrhenius type reaction model, not only the flame region but also the preheat region has also to be accurately resolved for a reasonable solution. On the other hand, the thicken flame model requires the use of a combustion filter width, which is at least larger than 10 times the cell dimension (the classical LES filter width). For better results, this can be up to 50 times (Colin et al. 2000). Use of a coarser mesh would result in a highly expanded flame front; perhaps, filling the entire combustion chamber. Therefore, much finer meshes are required to maintain an acceptable flame thickness. Hence, compared to the other methods, thicken flame approach is more demanding in terms of the mesh resolution requirement (Wang et al. 2012). Applications of this model for gas turbine combustion analysis (Selle et al. 2004, Franzelli et al. 2012) and SI engines (Enaux et al. 2011) have been reported. Extension of this study to analyse cyclic variations of combustion instabilities in SI engines has also been demonstrated by Granet et al. (2012).
Another interesting approach to solve the flame thickness problem is to filter the progress variable (or species mass fraction) by a larger filter size than the classical LES filter width, which is often taken to be equal to the cell dimension (Boger et al. 1998). The present study is based on this technique, combined with the flame surface density (FSD) model, as explained in the following sections.

9.2 Flame Surface Density Modelling in LES

In the FSD approach; i.e. $\Sigma$: the available flame surface area for unit volume, the reaction zone within the flame is viewed as a collection of infinitely thin wrinkled layers between unburned and burned gases. These flame layers are known as flamelets and they locally propagate at the laminar flame speed, within the limits of high Damköhler number. A detail discussion of this concept is provided in Chapter 5 of this thesis. In conjunction with the filtered balance equation of progress variable or species mass fractions, it is possible to extend the theories developed in RANS, to perform combustion calculations in LES. However, as already pointed out, the stiffness associated with the spatial distribution in progress variable has to be eliminated in order this method to be successful.

9.2.1 Combustion Filter Width

![Progress variable gradient](image)

Figure 9.1: Progress variable gradient resolved by using a combustion filter larger than the mesh width (adapted from Boger et al. 1998)

It has been demonstrated that, if the flame front is filtered with a larger filter size, than the classical LES filter width, a similar effect can be seen as the thicken flame model (Boger et al. 1998). For example, if the combustion filter width $\Delta_c$ is taken to be 4 times the grid filter width $\Delta_x$.
width $\bar{\Delta}$, the progress variable gradient is dispersed over $2\bar{\Delta}_c/\bar{\Delta}$ grid points ($2\bar{\Delta}_c/\bar{\Delta} = 8$ in this case) as shown in Figure 9.1. In practice, the flame front is thickened by a factor in the order of $\bar{\Delta}_c/\delta_l$ (Wang et al. 2012), making it possible to resolve with a practically viable computational grid. The resolution parameter $\eta_{res}$ is defined by relating the combustion and grid filter widths as:

$$\bar{\Delta}_c = \eta_{res} \bar{\Delta}$$  \hspace{1cm} (9.1)

It has also been highlighted in Boger et al. (1998) that, there should be at least eight grid points for the accurate solution of the flame front. Therefore in practice, $\eta_{res}$ is chosen such that $5 < \eta_{res} < 10$ (Vermorel et al. 2009). It should be noted here that, the filter width $\bar{\Delta}_c$ is applied only to the flame region. For the rest of the domain, the classical filter width $\bar{\Delta}$ must be used. In addition, $\bar{\Delta}_c$ is used only with the species (or progress variable) and enthalpy transport equations. In the momentum equation, $\bar{\Delta}$ is used all over the domain, including the flame brush. However, in a practical CFD simulation, it is difficult to exactly identify a flame region. Thus, the combustion filter width may be used only in a prescribed region, where the filtered progress variable $\bar{\varepsilon} \leq \bar{c} \leq 1 - \varepsilon$ as recommended in Vermorel et al. (2009). $\varepsilon$ is an appropriate small value, taken to be $10^{-4}$ in this work.

Use of the filter width in governing equations is associated with the calculation of the SGS viscosity. Hence, the SGS viscosity in the flame region $\mu_{sgs-c}$, has to be calculated as follows assuming Kolmogorov energy cascade in the inertial sub range:

$$\mu_{sgs-c} = C_v \bar{\rho} \varepsilon_{sgs-c}^{1/2} \bar{\Delta}_c$$  \hspace{1cm} (9.2)

where, $k_{sgs-c}$ is taken as:

$$k_{sgs-c} = k_{sgs} \left( \frac{\bar{\Delta}_c}{\bar{\Delta}} \right)^{2/3}$$  \hspace{1cm} (9.3)

Consequently, the balance equations for mass fraction, enthalpy or progress variable have to be modified to incorporate the combustion filter scale viscosity, as given in Eq. (9.4), for a general scalar $\phi$.

$$\frac{\partial \bar{\rho} \bar{\phi}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\phi} \bar{U}) - \nabla \cdot \left[ \sigma_c \left( \frac{\mu}{Sc} + \frac{\mu_{sgs-c}}{Sc_{sgs}} \right) \nabla \bar{\phi} \right] = S_\phi(\bar{\Delta}_c)$$  \hspace{1cm} (9.4)
\( \sigma_c \) is a user defined parameter introduced by Richard et al. (2007), in order to maintain the flame brush thickness approximately equal to \( \tilde{\Delta}_c \). The effect of this parameter in practical engine combustion calculations is of minor importance, as it remains close to the unity. Also, it is worth mentioning that the combustion source term in the above equation is a function of the combustion filter width \( \tilde{\Delta}_c \).

### 9.2.2 Transport of the Progress Variable

The balance equation for the progress variable in LES context is also formally similar to the scalar equation given in Eq. (9.4). However, in the LES FSD approach, it requires some rearrangements in order to facilitate the calculation of combustion source term. Therefore, the equation is rewritten in unfiltered form as given below.

\[
\frac{\partial (\rho c)}{\partial t} + \nabla \cdot (\rho c \mathbf{U}) = \nabla \cdot (\mathcal{D} \nabla c) + \dot{\omega}
\]  

(9.5)

\( \dot{\omega} \) represents the source term due to combustion and \( \mathcal{D} \) is the molecular diffusivity. Eq. (9.5) could be further manipulated to obtain the following form:

\[
\frac{\partial (\rho c)}{\partial t} + \nabla \cdot (\rho c \mathbf{U}) = \left[ \frac{\nabla \cdot (\mathcal{D} \nabla c) + \dot{\omega}}{|\nabla c|} \right] |\nabla c| 
\]  

(9.6)

\[
\frac{\partial (\rho c)}{\partial t} + \nabla \cdot (\rho c \mathbf{U}) = \rho S_D |\nabla c| 
\]  

(9.7)

where, \( S_D \) is the effective displacement speed of the flame front (taken as an iso-\( c \) surface), relative to the fresh gases. It represents the combined effect of the molecular diffusion normal to the flame surface, tangential diffusion due to curvature effects and the consumption speed due to combustion reactions. The balance equation of the Favre filtered progress variable \( \bar{c} \) can be obtained by density weighted filtering Eq. (9.7).

\[
\frac{\partial (\bar{\rho} \bar{c})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{c} \bar{U}) + \nabla \cdot (\bar{\rho} (\bar{c} \bar{U} - \tilde{c} \bar{U})) = \overline{\rho S_D |\nabla c|} 
\]  

(9.8)

The unresolved transport term is generally closed by the classical gradient assumption, while the displacement term in the right hand side has to be modelled. The latter can be written due to Boger et al. (1998) as:

\[
\overline{\rho S_D |\nabla c|} = \langle \rho S_D \rangle \bar{S} \bar{c} 
\]  

(9.9)
where, $\bar{\Sigma} = |\nabla c|$ denotes a generalized filtered flame surface density and it is a measure of total flame surface area contained within the filtered volume. The density weighted surface averaged displacement speed $\langle \rho S_D \rangle_S$ is usually approximated in terms of the unburned gas density and laminar flame speed.

$$\langle \rho S_D \rangle_S = \rho_u S_l \quad (9.10)$$

As in RANS, the laminar flame speed in LES is also often estimated using empirical correlations. Hence, the relation proposed in Gülder (1984) is used in the present study.

### 9.3 A Dynamic FSD Model for SI Engine Simulations

Closure of the combustion source term now requires modelling the generalized flame surface density. It is possible to solve a balance equation for the transport of FSD, making necessary allowances for the unresolved contribution. Usually, the forms of $\bar{\Sigma}$ balance equation in LES and RANS are similar; but, with some additional terms to address LES specific aspects (see Hawkes & Cant (2001) and Candel & Poinsot (1990)). However, these models often involve several model constants, which need to be specified on case by case basis. For example, the FSD formulation of Hawkes & Cant (2001) involves five unknown model constants; each corresponds to the resolved strain source, heat release strain source, residual strain source, resolved propagation term and the SGS destruction term respectively. Moreover, use of such an approach in IC engine simulations, often results in significant increase in computational cost; thus, often solved in massively parallel CFD codes such as AVBP (Richard et al. 2007 and Vermorel et al. 2009).

Alternatively, a simpler but an attractive approach is to use an algebraic formulation, which may only have either one or two calibration constants. Moreover, with the present advancement in LES combustion modelling, it is now possible to dynamically estimate the values of model constants as a function of both space and time, using the resolved scale information. The potential of such dynamic algebraic formulations in predicting reacting SI engine flows have never been tested. On the contrary, the use of a complex transport equation does not always guarantee better results (Zhao et al. 1994); instead, that may increase the associated modelling uncertainty. Consequently, with the aim of gaining confidence in premixed turbulent combustion in SI engines, the present work adopts an algebraic FSD formulation.
9.3.1 Modelling Generalised Flame Surface Density

In LES, the resolved part of the FSD can be directly computed from the resolved flow properties and the SGS part has to be modelled. Boger et al. (1998) was the first to come up with an algebraic expression for $\bar{\Sigma}$, after an extensive analysis of DNS flames data. The analysis is based on filtering the balance equation of progress variable with a Gaussian filter having a cut off width $\bar{\Delta}_c$, which is large than the mesh size $\bar{\Delta}$. The deduced expression is of the parabolic form given by:

$$\bar{\Sigma} = 4\beta \bar{\Delta} \frac{c(1-c)}{\bar{\Delta}_c}$$  \quad (9.11)

where, $\beta$ is a model constant, estimated to be $\sqrt{6/\pi}$ via analytical derivation. Interestingly, the above equation is formally similar to the well-known BML model for FSD in RANS (see Chapter 5 for more details), if $\bar{\Delta}_c/\bar{\Sigma}$ is viewed as the length scale of flame surface wrinkling. It is worth to emphasise that, this model assumes the combustion filter width $\bar{\Delta}_c$ is larger than the classical LES filter width $\bar{\Delta}$; so that, the filtered progress variable gradient can be adequately resolved with $\bar{\Delta}_c/\bar{\Delta}$ grid points.

However, the above formulation only provides an approximation for the resolved FSD. The factor $\bar{\Sigma}$ accounts for the SGS flame wrinkling effects. It may also be defined as the ratio of the generalised FSD to the projected FSD normal to the propagating direction.

$$\bar{\Sigma} = \frac{\int_{\gamma c} |\nabla c| G(x_i - x'_i) dx'_i}{\mathbf{N}. \int_{\gamma c} |\nabla c| G(x_i - x'_i) ndx'_i} = \frac{|\nabla c|}{|\nabla \bar{c}|} = \frac{|\bar{\Sigma}|}{|\nabla \bar{c}|} \quad (9.12)$$

where, $\mathbf{n} = -\nabla c/|\nabla c|$ and $\mathbf{N} = -\nabla \bar{c}/|\nabla \bar{c}|$ are respectively the normal unit vectors to the instantaneous iso-$c$ surface and the resolved iso-$\bar{c}$ surface pointing towards unburned gas direction. A suitable modelling expression is needed to evaluate the flame wrinkling factor.

In Eq. (9.8), the effects of molecular diffusion on flame propagation is implicitly embedded within the generalised FSD. Therefore, the unresolved scalar flux term $\nabla \rho (\bar{c} \bar{U} - \bar{c} \bar{U})$ is the only other unknown term to be modelled. The classical gradient approximation is used here for this purpose. However, Boger & Veynante (2000) noticed that, this combination under predicts the laminar flame propagation and the following correction is made as shown in Eq. (9.13). Accordingly, this improved formulation is retained in the present work.
\[
\frac{\partial (\bar{\rho} \bar{c})}{\partial t} + \nabla \cdot (\bar{\rho} \bar{c} \bar{U}) + \nabla \left[ \left( \rho_u \frac{S_t \bar{\Delta}_c}{16 \sqrt{6/\pi}} + \mu_{sgs-c} \right) \nabla \bar{c} \right] = 4 \rho_u S_t \bar{c} \sqrt{\frac{6 \bar{c} (1 - \bar{c})}{\bar{\Delta}_c}} \tag{9.13}
\]

The combustion filter width \( \bar{\Delta}_c \) was taken as five times the classical LES filter width (i.e. the cubic root of the local cell volume in the present case).

### 9.3.2 SGS Wrinkling Factor and Its Dynamic Evaluation

The wrinkling factor \( \Xi \) may be used as a tuning constant or estimated using a suitable formalism. A promising approach is to solve a transport equation for the wrinkling factor following Tabor and Weller (2004). However, similar to the FSD balance equation, the necessity of modelling several unknown terms, the presence of a number of tuning constants and the associated computational overhead remain as some of the disadvantages of this approach. Conversely, the algebraic models for computing \( \Xi \) are much superior, as they can be formulated as a dynamic model using a Germano like identity, eliminating all the tuning parameters. The Germano identity for the reaction rate is expressed by the following relation.

\[
\bar{\Xi} \bar{\Delta}_c = \bar{\eta} \Xi \bar{\Delta}_c \tag{9.14}
\]

The left hand side of this expression can be interpreted as the reaction rate computed at combustion filter scale \( \bar{\Delta}_c \), which has been, subsequently, test filtered at a scale \( \Xi \bar{\Delta}_c \). The parameter \( \Xi > 1 \) and the symbol \( \bar{\Xi} \) denotes the test filtering operation. The right hand side denotes the reaction rate computed with a combustion filter of \( \Xi \bar{\Delta}_c \).

Angelberger et al. (1998) suggested the following linear formulation to estimate the SGS wrinkling factor.

\[
\Xi_{\Delta_c} = 1 + \alpha \Gamma_{\Delta_c} \left( u'_{\Delta_c}, S_t \right) \frac{u'_{\Delta_c}}{S_t} \tag{9.15}
\]

Note that, the subscript \( \Delta_c \) denotes the filter scale at which the corresponding parameter is evaluated. \( \Delta_c \) may be either the combustion filter width, classical LES filter width or any other scale to be appropriately chosen (see Colin et al. 2000). \( \alpha \) is a model constant and \( \Gamma_{\Delta_c} \left( u'_{\Delta_c}, S_t \right) \) is an efficiency function to account for the straining effects of all turbulent scales smaller than \( \Delta_c \). Very good results have been obtained with this formulation in coupled radiative heat transfer calculations by Santos et al. (2008). However, this type of linear models cannot be made dynamic, as the Germano identity becomes ineffective (see Charlette
et al. 2002b). Therefore, the power law wrinkling model in Eq. (9.16) was proposed by Charlette et al. (2002a).

\[ \Xi_{\Delta e} = \left(1 + \frac{\Delta_e}{\delta_c}\right)^\xi \]  

(9.16)

In this model, \( \Delta_e \) is the outer and \( \delta_c \) is the inner cut off scales respectively. These two parameters represent the maximum and minimum possible flame wrinkling length scales at sub-grid level. It is assumed that, scales larger than \( \Delta_e \) are resolved by LES. For example, when \( \Delta_e = \bar{\Delta}_c \), the outer cut-off scale becomes \( \bar{\Delta}_c \) as all the scale above the combustion filter width are resolved. The unity is added to ensure that \( \Xi_{\Delta e} \) is reached to unity for \( \delta_c \gg \Delta_e \). The wrinkling exponent \( \xi \) could be spatially and temporally dependent on \( \delta_c, \Delta_e \) and other relevant parameters such as the Reynolds number and the turbulent velocity. However, if \( \xi \) is assumed to be independent of the cut off scales and \( 0 < \beta < 1 \), the fractal flame wrinkling model (Gouldin 1987) can be recovered with \( \xi = D - 2 \), where \( D \) is the fractal dimension. Postulating the equilibrium between production and destruction of SGS flame surface density and further DNS analysis of interaction of turbulent eddies with the flame front lead to the following extension of above model (Charlette et al. 2002a).

\[ \Xi_{\Delta e} = \left(1 + \min \left[\frac{\Delta_e}{\delta_l}, \Gamma_{\Delta e} \left(\frac{\Delta_e}{\delta_l} \cdot \frac{u'_{\Delta e}}{S_l} \cdot Re_{\Delta e} \right) \frac{u'_{\Delta e}}{S_l}\right]\right)^\xi \]  

(9.17)

\( \Gamma_{\Delta e} \) was added to account for the reduced ability of smaller eddies to wrinkle the flame surface. Note that, the efficiency function \( \Gamma_{\Delta e} \) has been modified from Eq. (9.15) and \( Re_{\Delta e} \) is the SGS Reynolds number at scale \( \Delta_e \).

In order to progress for the dynamic evaluation of \( \xi \), it is taken that the reaction rate is given by the following equation:

\[ \bar{\omega}_{\Delta e} = \Xi_{\Delta e} \frac{\bar{W}_{\Delta e}}{\Delta e} \]  

(9.18)

Subsequently, a dynamic expression for the model constant \( \xi \) can be obtained by applying the Germano identity on Eq. (9.16). For notational convenience, take \( \gamma \bar{\Delta}_c = \bar{\Delta} \).

\[ \langle \Xi_{\Delta e} \frac{\bar{W}_{\Delta e}}{\Delta e} \rangle = \langle \Xi \frac{\bar{W}_{\bar{\Delta}}}{\bar{\Delta}} \rangle \]  

(9.19)
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Note that, the Germano identity is true in both globally and locally in all points in space and time; but in practice, the reaction rate is meaningful only in the averaged sense (Charlette et al. 2002b). In addition, volume averaging eliminates unphysical fluctuations of the computed value of $\xi$. Therefore, the angle brackets in the Eq. (9.19), indicates some form of averaging.

To proceed further, some assumptions are needed. It is assumed that $u_{ \Delta e}'$ is uncorrelated from the local value of $\tilde{W}_{ \Delta e}$ within the averaging control volume, which is taken to be larger than the test filter width $\hat{\Delta}$. As a result, $\langle u_{ \Delta e}' \rangle$ becomes independent of the filtering operation. The flame thickness and the laminar flame speed are also independent of the filtering operation. Consequently, the Eq. (9.20) is recast as follows.

\[
\left[ 1 + \min \left( \frac{\Delta_c}{\delta_t}, \Gamma_{\Delta e} \frac{\langle u_{ \Delta e}' \rangle}{S_t} \right) \right]^\xi \tilde{W}_{ \Delta e} = \left[ 1 + \min \left( \frac{\hat{\Delta}}{\delta_t}, \Gamma_{\hat{\Delta}} \frac{\langle u_{ \hat{\Delta}}' \rangle}{S_t} \right) \right]^\xi \tilde{W}_{ \hat{\Delta}} \quad (9.21)
\]

\[
\xi = \log \left( \frac{\langle \tilde{W}_{ \Delta e} \rangle}{\langle \tilde{W}_{ \hat{\Delta}} \rangle} \right) / \log \left[ 1 + \min \left( \frac{\Delta_c}{\delta_t}, \Gamma_{\Delta e} \frac{\langle u_{ \Delta e}' \rangle}{S_t} \right) \right] \left( 1 + \min \left( \frac{\hat{\Delta}}{\delta_t}, \Gamma_{\hat{\Delta}} \frac{\langle u_{ \hat{\Delta}}' \rangle}{S_t} \right) \right) \quad (9.22)
\]

Hence, the value of $\xi$ can now be evaluated from the known resolved field. Charlette et al. (2002b) successfully tested the validity of this formulation, combined with the thicken flame model, for freely propagating flames in homogeneous and decaying isotropic turbulence. However, in modelling turbulent jet flames, Wang et al. (2011) noticed that, this formulation suffers from some practical deficiencies. Mainly, it requires estimating the turbulent intensity at both combustion and testing filter levels. The simple linear relation $u_{ \Gamma_{\Delta}} = \gamma^{1/3} u_{\Delta}'$ based on homogenous isotropic turbulence assumptions or the fairly complex expression in Colin et al. (2000) may be used for this purpose. However, it was found by Wang et al. (2011) that, both these relations make the dynamic procedure numerically unstable due to modelling uncertainties. As a result, it was suggested to eliminate the requirement of estimating the turbulence intensity at different scales by computing the wrinkling factor at the limiting case of large turbulent intensities as given by:
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\[
\lim_{u'_e \to \infty} \Xi_{\Delta_e} = \left( \frac{\Delta_e}{\delta_l} \right)^\xi
\]  

(9.23)

This would result in the following reduced form for \( \xi \).

\[
\xi = 1 + \frac{\log \left( \frac{\overline{W_{\Delta_e}}}{\overline{W_\Delta}} \right)}{\log(Y)}
\]  

(9.24)

Unfortunately, Wang et al. (2011) further noticed that this expression produces incorrect results for laminar flat flames where, \( \Xi_{\Delta_e} = \Xi_{Y\Delta_e} = 1 \). As a corrective measure, the laminar flame thickness was replaced by an *equivalent flame thickness* equal to \( 2.2\delta_l \). However, this modification is somewhat similar to the use of an inner cut off scale of flame wrinkling, which is often in the order of 2-3 times the laminar flame thickness (Knikker et al. 2002). Accordingly, the model has been reduced back to the simple fractal flame wrinkling model given by Eq. (9.25) for \( \Delta_e \gg \delta_e \).

\[
\Xi_{\Delta_e} = \left( \frac{\Delta_e}{\delta_e} \right)^\xi
\]  

(9.25)

Use of this formulation in turbulent jet flames has produced very good results as reported in Wang et al. (2011). Further, the applications of these formulations in modelling early stage flame development under homogeneous isotropic decaying turbulence with encouraging success has been reported in Wang et al. (2012). Therefore, this approach is retained in the present study.

Based on similarity concept, another promising method to account for the SGS contribution has been suggested by Knikker et al. (2002, 2004), where the SGS FSD is explicitly and dynamically estimated from the resolved scale information. Gubba et al. (2008) and Ibrahim et al. (2009) employed this formalism in deflagration flame modelling in explosions with very good success. This model has not yet been applied in the context of IC engines like complex engineering problems and should be tested in a future study. In addition, priory DNS assessments of a number of other SGS FSD models have been reported in Chakraborty and Klein (2008). This provides a good reference for the comparison of each of the model forms.

### 9.3.3 Dynamic Fractal Flame Wrinkling Model

In this work, following the work of Charlette et al. (2002a) and Wang et al. (2011, 2012), \( \Xi \) is modelled by the simple fractal model in Eq. (9.25) and the reaction rate is evaluated from
Eq. (9.13). Accordingly, for combustion ($\bar{\Delta}_c$) and test filter ($\hat{\Delta}$) levels the reaction rates are expressed as follows.

$$\tilde{\omega}_{\bar{\Delta}_c} = \rho_u S_l 4\beta \left( \frac{\bar{\Delta}_c}{\delta_c} \right)^\xi \hat{c}(1 - \hat{c}) \frac{\hat{\Delta}}{\bar{\Delta}_c}$$

(9.26)

$$\tilde{\omega}_{\hat{\Delta}} = \rho_u S_l 4\beta \left( \frac{\hat{\Delta}}{\delta_c} \right)^\xi \hat{c}(1 - \hat{c}) \frac{\hat{\Delta}}{\hat{\Delta}}$$

(9.27)

Note that, in Eq. (9.27), the reaction rate at test filter level has been evaluated by using the test filtered progress variable $\hat{c}$. However, $\hat{c}$ is not computed via governing equations, so that it should be obtained by explicit test filtering of the $\hat{c}$ field. Hence, $\hat{c}$ would be replaced with $\hat{\hat{c}}$ in forthcoming equations to symbolise the required test filtering operation. In the case of a fully fractal flame, $\xi$ may reduce to $D - 2$ where $D$ is the fractal dimension. However, $\xi$ is herein dynamically determined from resolved scale information considering as an exponential factor in general. Hence, $\xi$ varies in both space and time, making it different from a classical fractal model, where a given fractal dimension is prescribed.

The Eq. (9.28) has been obtained by applying the Germano like identity for Eq. (9.26) and Eq. (9.27).

$$\langle \rho_u S_l 4\beta \left( \frac{\bar{\Delta}_c}{\delta_c} \right)^\xi \hat{c}(1 - \hat{c}) \rangle = \langle \rho_u S_l 4\beta \left( \frac{\hat{\Delta}}{\delta_c} \right)^\xi \hat{c}(1 - \hat{c}) \rangle$$

(9.28)

By definition, the unburned gas density and the laminar flame speed are independent from the filtering operation. Assuming the inner cut off scale also to be independent of the filter width, it can further be rearranged as:

$$\xi = 1 + \log \frac{\langle \hat{c}(1 - \hat{c}) \rangle}{\langle \hat{c}(1 - \hat{c}) \rangle} \log (Y)$$

(9.29)

where, the test filter width has been replaced with $\hat{\Delta} = Y \bar{\Delta}_c$ and angle brackets indicates some form of averaging over a volume larger than the test filter width.

It has been mentioned that the use of this expression in practice might result in incorrect estimation of the wrinkling factor for laminar or nearly laminar like flames, as $\xi$ does not reach to zero under such conditions (Wang et al. 2012). However, the effect of this formulation has never been practically investigated in LES. Thus, as a first step the above
expression is retained here. The gradient based method suggested in Wang et al. (2012), where \( \tilde{c}(1 - \tilde{c}) \) term is replaced with \( |\nabla \tilde{c}| \) (similarly the test filtered terms as well), would possibly be more accurate. However, the current approach is particularly attractive, because of less computational time involved; whereas, it needs a significant computational time to evaluate gradients in unstructured grids.

Finally, to complete the model, an expression for the inner cut-off scale should be specified. Number of expressions can be found in the literature for this purpose (see Gülder & Smallwood (1995) and Chakraborty and Klein (2008)). A more detailed discussion on this aspect can also be found in Chapter 5. In the present study, the inner cut-off scale is taken as three times the thermal flame thickness following Wang et al. (2012), Knikker et al. (2002, 2004), Gubba et al. (2008) and Ibrahim et al. (2009).

### 9.3.4 Test Filtering Procedure

The Gaussian test filter defined by Eq. (9.30) is used in the present study,

\[
G(x_i - x'_i, \hat{\Delta}) = \left(\frac{6}{\pi \Delta^2}\right)^{3/2} \exp \left[ -\frac{6}{\Delta^2} \left( (x-x')^2 + (y-y')^2 + (z-z')^2 \right) \right] \tag{9.30}
\]

where, \( x_i \equiv (x, y, z) \) is the centre of the filter kernel and \( x'_i \equiv (x', y', z') \) is the coordinate of a neighbouring point on which the value of the Gaussian coefficient is calculated. The test filter width is taken to be two times the combustion filter width. Consequently, the effective Gaussian filter width becomes \( \hat{\Delta} = Y\bar{\Delta}_c \), where \( Y \) is given by the following relation (Knikker et al. 2004).

\[
Y = \frac{\hat{\Delta}_c^2 + (2\hat{\Delta}_c)^2}{\hat{\Delta}_c} = \sqrt{5} \tag{9.31}
\]

Therefore, care must be taken to use the appropriate value \( \sqrt{5} \) for \( Y \) in Eq. (9.29) for the dynamic expression of the wrinkling exponent.

Combustion test filtering is somewhat different from the usual 3 or 5 points filters discussed in Appendix B under dynamic SGS turbulence modelling in non-reaction flows. As it was already mentioned, the test filter width is taken to be twice the combustion filter width and the combustion filter width is taken as five times the cell size in the present work. Hence, the test filtering volume of a given cell is a sphere with a radius of \( 5\sqrt{5} \) times the cell dimension. Thus, test filtering domain involves nearly a thousand \( (\approx 2 \times 5)^3 \) of neighbour cells per
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each test filtering cell. Therefore, simple averaging techniques introduced in Appendix B cannot be used in combustion test filtering.

The discrete convolution operation on a cell centred mass averaged flow property $\tilde{\phi}$ is defined by the following relation.

$$\tilde{\phi}_i = \frac{\sum_{j \in \Omega_i} G_{ij} \tilde{\phi}_j V_j}{\sum_{j \in \Omega_i} G_{ij} V_j} \quad (9.32)$$

$\tilde{\phi}_i$ is the test filtered value of $\tilde{\phi}$ in $i^{th}$ cell. $\tilde{\phi}_j$ is the value of the same flow property in the $j^{th}$ neighbouring cell, which resides within the test filtering volume $\Omega_i$. The Gaussian weight $G_{ij}$ at the cell centre of $j^{th}$ cell, with respect to $i^{th}$ test filtering cell, is calculated from the Eq. (9.30). $V_j$ is the volume of the of $j^{th}$ neighbouring cell.

Storage of this information for each of the cell in combustion chamber requires a huge amount of memory, which is unaffordable at present stage. Similarly, real time calculation also needs a very large computational time. In the work of Wang et al. (2011, 2012), a separate parallelized computer code has been run in conjunction with the combustion code, just for test filtering purposes. An alternative strategy was adapted in the present study, particularly suited for serial computation. In this method, the neighbour cell data and Gaussian weights were pre-calculated and stored in two direct access binary files. Records were appropriately read from these files as required. This procedure was found to be extremely faster than the real time calculation of Gaussian weights. However, use of this procedure required to maintain a fixed mesh in both the space and time, where the vertex locations do not move. To facilitate this constrain, piston motion was simulated only by adding and removing of cell layers, but avoiding being compressed or expanded.

Test filtering near solid boundaries require special measures. It is assumed that there exists an imaginary mesh outside the boundary, which has a similar mesh density as the actual computational mesh. For a reasonably uniform mesh, average number of test filtering cells per each cell and the summation of the Gaussian weights should also be nearly uniform. Thus, averaged values of the Gaussian weights were used, when test filtering the cells close to the boundary. A zero value for the progress variable is assumed in the imaginary mesh, similar to the popular zero padding technique, often used in image processing (Gonzalez and Woods 2002).
9.4 Modelling Flame Kernel Formation in LES

The simplest way to model the ignition process is to impose a predefined burned gas volume, in the vicinity of the spark position, at the time of ignition. The shape of this initial burned gas volume may be assumed spherical and its diameter, in the order of inter-electrode distance, i.e. 1.0 mm. However, as the nominal cell size of a present LES computational mesh is also of the same order, the flame front cannot be resolved (Richard et al. 2007). Therefore, specific measures have to be used to model the early flame kernel formation and the reaction rate until the flame kernel is large enough to be resolved in the computational mesh.

Combustion characteristics during the early stage of kernel formation, is fundamentally different from its fully developed phase (Heywood 1988). Flame has not achieved equilibrium and flame propagation is mainly affected by volumetric expansion. A detailed discussion on the considerations has been made in Chapter 4. As it was noted, the turbulent combustion models developed to simulate fully developed phase, cannot be used to predict the early stage flame behaviour, without necessary modifications. In this section, a new ignition model is developed to model the ignition and flame kernel growth in spark ignition engines to be used with LES calculations.

It is possible to use the Lagrangian particle tracking techniques used in the DPIK ignition model for LES calculations as well. However, particle tracking is normally a time consuming task and especially, this method is unattractive in LES, as more refined meshes with relatively smaller time steps are used. Therefore, if implemented, it will results in a considerable increase in computational time. For this reason, an Eulerian based ignition models are preferred.

To date, only a very limited amount of work has been carried out in the LES context, on ignition and flame kernel formation in SI engines. Use of the Euler version of the AKTIM model has been reported by Richard et al. (2007) and Vermol et al. (2009). Colin & Truffin (2011) further developed the AKTIM model to be used in conjunction with the FSD transport equation. One of the limitations of the AKTIM model is that it requires a considerable amount of experimental inputs from the ignition system for accurate functioning. Usually, these parameters are not readily available and also difficult to measure in practical situations. On the other hand, the effect of plasma expansion during the glow discharge is not considered. Herweg and Maly (1992) have reported that it is crucial to account for the initial plasma phase for accurate simulations. In the present development, it is expected to address these difficulties in a simplified manner. Recently, an experimentally based comprehensive
formulation combined with the $G$-equation approach has also been proposed in Dahms et al. (2009) for RANS simulations. This would, probably be easily extended in to LES, in a $G$-equation formulation. However, in the present work, a simple model, but effectively capable of producing global results of ignition and early stage of flame propagation is proposed.

### 9.5 A New Flame Kernel Growth Model for LES in SI Engine

The ultimate aim of an ignition and flame kernel model should be to find an accurate expression to describe the flame surface area distribution during early stage of flame development. The unburned gas consumption rate during this period $\bar{\omega}_k$ can be expressed in the usual manner given by:

$$\bar{\omega}_k = \rho_u \bar{\Sigma} S_D$$  \hspace{1cm} (9.33)

where, $S_D$ is the displacement speed, which is equivalent to the traverse speed of the flame surface, with respect to the unburned gases. Under the thin flame front assumption, this may be taken equal to the mean consumption speed $S_C$. At the initial stage the flame traverse speed is enhanced by the effect of the plasma expansion. Hence, the effective consumption speed is the summation of laminar and plasma expansion speeds (Ewald & Peters 2007).

$$S_C = S_{\text{plasma}} + S_l$$  \hspace{1cm} (9.34)

$S_l$ is the strained laminar flame speed influenced by the curvature and aerodynamic straining effects. $S_{\text{plasma}}$ is the mean expansion speed of the high temperature plasma kernel. $\bar{\Sigma}$ is the total SGS flame surface density which can be related to the available mean SGS flame surface area $\delta A$ in an infinitesimal volume $\delta V$ (volume of a computational cell) as:

$$\bar{\Sigma} \delta V = \delta A$$  \hspace{1cm} (9.35)

### 9.5.1 Initiation of Ignition

The most accurate method to initiate the ignition is to impose a plasma channel based on the electrical system and in-cylinder mixture properties (Sher et al. 1992). However, modelling the electrical system requires a number of measured inputs, such as breakdown energy and the secondary circuit voltage (Duclos & Colin 2001), which in practise needs a significant effort to measure. On the other hand, initial kernel is formed by high temperature ionized plasma well above 60,000 $K$. Conventional thermodynamic relations are not valid in this stage and
solving for the complex plasma physics is usually a formidable task. A detail discussion on this topic has been made in the Chapter 5 of this thesis.

In the present approach, the flame kernel is initiated by depositing a burned gas mass of $m_{ign}$ at the spark location. Breakdown and arc discharge periods are simply neglected as the total duration of these events is of few microseconds. If, the necessary data from the ignition system is available, $m_{ign}$ can directly be estimated from the relations given in Duclos & Colin (2001). A simplified approach is adopted in the present study, as no data was available on the present ignition system. Onset kernel is assumed to be spherical with a diameter of $d_e$: the spark electrode gap, and the burned gases at adiabatic temperature. Consequently, $m_{ign}$ can be calculated from the following expression:

$$m_{ign} = \frac{\pi}{6} \rho u d_e^3$$

(9.36)

Then, this burned gas volume is filtered by the combustion filter width $\tilde{\Delta}_c$ by adopting the following Gaussian relation proposed by Cobl and Truffin (2011).

$$\tilde{c} = c_0 \exp \left[ -\frac{|x - x_{spk}|^2}{0.6^2 \tilde{\Delta}_c^2} \right]$$

(9.37)

$x - x_{spk}$ is the distance measured from the spark location. The constant $c_0$ is estimated such that,

$$\int \tilde{\rho} \tilde{c} dV = m_{ign}$$

(9.38)

where, $\tilde{c}$ is the Favre filtered progress variable. Figure 9.2 shows the Gaussian distribution of initial progress variable with the distance from the ignition point location, for different combustion filter width ratios. The maximum of the progress variable is located at ignition point with a value of $c_0$. The curve corresponding to $\tilde{\Delta}_c/\tilde{\Delta} = 5$ represents present distribution of initial progress variable.
9.5.2 Mean Flame Kernel Surface Area

In order to find the unburned gas consumption rate, an expression is needed for the total SGS flame surface density $\bar{\Sigma}$. During the early stage of flame development the flame kernel size is smaller than the combustion filter width, so that the flame details are naturally filtered out. As a result, $\bar{\Sigma}$ has to be estimated with physical arguments. It is assumed that, the early flame kernel is roughly spherical, so that the volume of the flame kernel can be approximated equal to the total volume occupied by burned gas $V_k$. Consequently, the mean flame kernel radius $r_k$ and the flame area corresponding to the burned gas volume $A_k$ are defined respectively as:

$$r_k = \left( \frac{3V_k}{4\pi} \right)^{1/3} \quad (9.39)$$

$$A_k = 4\pi r_k^2 \quad (9.40)$$

The flame wrinkling factor $\Xi$ is now defined as the ratio between the total flame surface area $A$ and the surface area of the burned gas volume $A_k$. Accordingly, $\Xi$ and flame surface densities can also be related by:
\[ \Xi = \frac{A}{A_k} = \frac{\bar{\Sigma}}{\bar{\Sigma}_k} \]  
(9.41)

where, \( \bar{\Sigma}_k \) is the FSD corresponding to the burned gas volume and the reaction rate expression is now modified as:

\[ \bar{\omega}_k = \rho_u \Xi \bar{\Sigma}_k S_c \]  
(9.42)

A relation for the flame area evolution of a thin flame kernel can be formulated following Boudier et al. (1992) as:

\[ \frac{1}{A} \frac{dA}{dt} = \frac{1}{A_k} \frac{dA_k}{dt} + K_W \]  
(9.43)

For nearly spherical flames, under the absence of plasma expansion, the evolution of burned gas volume can be given by (Herweg & Maly 1992):

\[ \frac{dA_k}{dt} = 8\pi r_k \frac{\rho_u}{\rho_b} S_t \]  
(9.44)

The flame wrinkling factor can be related to the turbulent and laminar flame speeds as:

\[ \Xi = \frac{S_t}{S_l} \]  
(9.45)

Therefore, by combining Eq. (9.41), (9.43) and Eq. (9.44) the following relation is obtained.

\[ \frac{dA}{dt} = 8\pi r_k \frac{\rho_u}{\rho_b} S_c \Xi^2 + K_W A \]  
(9.46)

The two terms on the right hand side correspond to the strain rate due to volumetric expansion and turbulent flame wrinkling. Note that, in this equation, the laminar flame speed is \( S_l \) has been replaced with a more general consumption speed \( S_c \), which includes plasma expansion speeds as well. Volumetric strain may be neglected for fully developed flames, but has to be estimated properly in flame kernel modelling as it is in the same order or even higher than the turbulent strain. The validity of this evolution equation has been successfully tested in DNS by Echekki et al. (1996). The burned gas volume is computed by evaluating the following integral over the combustion chamber.
\[ V_k = \int \bar{c} \, dV \]  

(9.47)

### 9.5.3 Local Flame Surface Density

The local mean flame surface density is calculated assuming a parabolic profile similar to the expression given in Boger et al. (1998). Note that \( \alpha \) may be different from the original values proposed in Boger et al. (1998), as the flame has not yet reached the fully developed equilibrium phase. Nevertheless, \( \alpha \) was assumed to be a global time varying coefficient independent of the filter width.

\[ \Sigma = \alpha \frac{\bar{c}(1 - \bar{c})}{\Delta_c} \]  

(9.48)

\( A_c \), the Local mean flame surface area within a cell, is then approximated by integrating over the cell volume \( v_c \).

\[ A_c = \alpha \int_{v_c} \frac{\bar{c}(1 - \bar{c})}{\Delta_c} \, dV \]  

(9.49)

The total mean flame kernel area \( A_k \), can then be calculated by integrating the local values in the burned gas volume.

\[ A_k = \alpha \int_{V_b} \frac{\bar{c}(1 - \bar{c})}{\Delta_c} \, dV \]  

(9.50)

If the filter width is assumed to be uniform in space, local mean flame surface area can be related to the flame area calculated using the burned gas surface area as (Ricard et al. 2007):

\[ A_c = A_k \frac{\int_{v_c} \bar{c}(1 - \bar{c}) \, dV}{\int_{V_b} \bar{c}(1 - \bar{c}) \, dV} \]  

(9.51)

It is worth to note that, the use of this procedure has eliminated unknown parameter \( \alpha \) from the final expression.
9.5.4 SGS Flame Wrinkling Factor

The term $K_W$ in Eq. (9.46) is modelled as:

$$K_W = \Gamma_{\Delta_e} \frac{u_{\Delta_e}^e}{\Delta_e} \left( \Xi_{EQ} - \Xi_{t=0} \right)$$

(9.52)

where, the efficiency function $\Gamma_{\Delta_e}$ is taken to be the LES version of the ITNFS (Intermittent Turbulent Net Flame Stretch) function evaluated at scale $\Delta_e$. It was first, proposed by Meneveau & Poinsot (1991) for RANS modelling and later improved by Colin et al. (2000) and Charlette et al. (2002a) for LES. The curve fitted relation for $\Gamma_{\Delta_e}$ to match with DNS results is given by the following set of equations.

$$\Gamma \left( \frac{\Delta_e}{\delta_l}, \frac{u_{\Delta_e}^e}{S_l}, Re_{\Delta_e} \right) = \left[ \left( f_u^{-a} + f_\Delta^{-a} \right)^{-1/\alpha} \right]^{-1/b} + f_{Re_{\Delta_e}}^{-1/b}$$

(9.53)

$$f_u = 4 \left( \frac{27C_k}{110} \right)^{1/2} \left( \frac{18C_k}{55} \right)^2 \left( \frac{u_{\Delta_e}^e}{S_l} \right)^2$$

(9.54)

$$f_\Delta = \left[ \frac{27}{110} \frac{C_k \pi^{4/3}}{} \left[ \left( \frac{\Delta_e}{\delta_l} \right)^{4/3} - 1 \right] \right]^{1/2}$$

(9.55)

$$f_{Re_{\Delta_e}} = \left[ \frac{9}{55} Re_{\Delta_e} \exp \left( - \frac{3C_k \pi^{4/3}}{2Re_{\Delta_e}} \right) \right]^{1/2}$$

(9.56)

The constant $C_k \approx 1.5$ is often called the Kolmogorov constant. This function gives the total sub-grid scale flame stretch, produced by all eddies, which are smaller than the characteristic cut off width $\Delta_e$. For practical and conceptual reasons $\Delta_e$ should be selected such that $\eta < \Delta_e < L_i$ to comply with the assumption that Kolmogorov scale and integral scales correspond to the minimum and maximum scales of flame wrinkling. In fully developed combustion simulations, $\Delta_e$ is taken to be similar to the combustion filter width, as only the effects of the scales larger than $\Delta_e$ are resolved. As the flame at an early stage has not reached equilibrium, a linear evolution of $K_W$ is assumed. $K_W$ vanishes, when the equilibrium conditions are achieved. The initial value of the wrinkling factor is taken as $\Xi_{t=0} = 1$. The equilibrium wrinkling factor $\Xi_{EQ}$ is expressed according to the simple fractal model in Eq. (9.57).
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\[ D = 2.05 \frac{S_t}{S_t + u'_{A_e}} + 2.35 \frac{u'_{A_e}}{S_t + u'_{A_e}} \]  \hspace{1cm} (9.58)

The laminar flame thickness corresponds to the thermal flame thickness: 98% of the reaction zone width, and may be obtained using the fact that, flame Reynolds number \( Re_f \approx 4 \) (Vaynante & Vervisch 2002).

\[ Re_f = \frac{\delta_t S_t}{v} \approx 4 \]  \hspace{1cm} (9.59)

The angle brackets in Eq. (9.52) denote the flame averaging operation. This is different from the conventional mass averaging, and may be defined as follows in Eq. (9.60) for a scalar quantity \( \phi \). The integration is performed over the entire flame surface.

\[ \langle \phi \rangle_S = \frac{\int_S \Sigma \phi dV}{\int_S \Sigma dV} \]  \hspace{1cm} (9.60)

As already noted, the ITNFS function calculates the total stretch induced on the flame surface by all the eddies smaller than a given characteristic cut off size \( A_e \). During the early stage of flame kernel formation, flame dimension is smaller than both the size of the integral scale and the combustion filter width. Hence, the largest possible eddy size, which can wrinkle the flame, is in the order of the flame kernel diameter: \( d_k \). Consequently, the use of combustion filter width as the characteristic cut off diameter overestimates the wrinkling factor. Hence, \( A_e \) has to be replaced by the flame kernel diameter as long as the flame dimension remains smaller than the combustion filter width. Hence, the characteristic cut off width is defined as:

\[ \Delta_e = \text{min}(d_V, \bar{A}_e) \]  \hspace{1cm} (9.61)

Accordingly, \( u'_\Delta_e \) now corresponds to the velocity scale of eddies of the flame dimension. Assuming that SGS scales are in the inertial sub range following Kolmogorov energy cascade, the SGS velocity in the grid scale (\( \bar{A} \)) and the characteristic scale can be related by:
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\[ u'_{\Delta e} = \left[ \frac{\min(d_y, \Delta)}{\Delta} \right]^{1/3} u'_{\Delta} \]  

(9.62)

**9.5.5 Plasma Expansion Speed**

The expressions used in DPIK model as described in Chapter 5 is still valid in LES for plasma speed calculation. Nevertheless in LES, internal energy and enthalpy have to be replaced with appropriate filtered quantities as given below.

\[ S_{\text{plasma}} = \frac{\eta \bar{Q}_{\text{spark}}}{A_k \left[ \bar{\rho}_u \left( \bar{U}_k - \bar{h}_u \right) + p_k \frac{\bar{\rho}_u}{\bar{\rho}_k} \right]} \]  

(9.63)

**9.5.6 Transition to the Main Combustion Model**

Flame surface density approach assumes that, there exists fully burned gas behind the flame front. Therefore, ignition model is employed until a fully resolvable flame front is developed; so that, progress variable becomes unity somewhere in the combustion domain. Beyond this point, the combustion rate is calculated by the main combustion model. This approach has been successfully used in Richard et al. (2007) and Vermorel et al. (2009) and retained in this work. However, in practice, a slightly less value than the unity has to be used for the limiting progress variable, as in the present simulations, the combustion model is applied only in the flame region, in which \( \bar{c} \leq 1 - \varepsilon \), where \( \varepsilon \) is a small positive value. Hence, it is highly unlikely that, \( \bar{c} \) would reach the unity. On the other hand, it was noticed here that, \( \bar{c} \) reaches to its maximum value asymptotically. This is believed to be mainly a consequence of very low reaction rate at this stage and partly due to numerical diffusion and truncation errors. Accordingly in the present work, a value of 0.90 was used as the limiting maximum \( \bar{c} \) value at transition.

**9.6 Summary**

- A complete formulation to be used in LES for the calculation of species consumption rate due to combustion in SI engines was developed in the present chapter.
- Usual combustion models developed for fully developed combustion cannot be used to simulate the early stage of flame kernel propagation due to theoretical inconsistencies.
- Consequently, a novel model was developed considering particular aspects of flame kernel formation in the context of large eddy simulation.
• Specific procedures were described to be adopted during the flame surface density modelling in LES to overcome the numerical difficulties associated with the flame thickness.

• A FSD based SGS combustion model was developed for the simulation of fully developed premixed combustion in SI engines.

• In this model, the flame wrinkling factor is estimated using a fractal based formulation.

• The fractal dimension is dynamically calculated in both space and time using a test filtering procedure.

• A new test filtering procedure was adopted to be used in combustion simulations of wall bounded systems, based on the fundamentals of image processing.
This chapter reports the application of the developed LES code and combustion models in a variety of engineering problems. These include both reacting and non-reacting configurations operating in dynamic conditions. Experimental measurements obtained in each of those test cases are used to validate and assess the capability of the present formulation.

Accordingly, as described in section 10.1, multi-cycle non-reacting flow in a research engine was simulated with the aim of identifying LES performances of the present code in unstructured deforming meshes. Predictions are compared against experimentally measured velocity and turbulent data. A comprehensive discussion on these simulations is provided in section 10.1. Validation of the present ignition and flame kernel model is presented in 10.2, where the early stage of the flame kernel development in a swirl chamber is modelled. Section 10.3 is devoted to the validation of the dynamic flame surface density combustion model developed under this research. The applicability of this formulation in predicting premixed combustion and cyclic variability in SI engines is evaluated by simulating full cycle combustion in a Ricardo E6 engine. Results are compared with experimentally obtained cycle resolved pressure and heat release data for different test conditions. A concluding summary of this chapter is presented in section 10.4.
10.1 Cold Flow Simulation in a Motored Piston Engine

As the present interest is to simulate IC engines using LES, cold flow simulation of a simplified engine configuration was considered as the validation test case. This investigation provides an opportunity to study the behaviour of present LES implementation, in the presence of deforming and moving boundaries. A schematic diagram of the engine assembly considered is shown in Figure 10.1. The engine has an axisymmetric geometry and a pancake chamber, with a 75 mm bore, 60 mm stroke and a 30 mm squish clearance. The vertical overhead valve, located along the central axis of the cylinder, is fixed at the indicated position leaving 4 mm annular gaps between the valve and the cylinder head for air flow, at an angle of 30° with the vertical axis. Hence, no compression is taken place and the domain is open to the atmosphere at upstream near the valve stem. The piston is moved in simple harmonic motion by an especial mechanism, with an average speed of 200 rpm. The mean piston speed \( V_p \) is approximately about 40 \( cms^{-1} \). The Reynolds number based on the bore diameter is close to 2000.

![Schematic diagram of the motored piston engine](image)

**Figure 10.1:** Schematic view of the motored piston engine, its major dimensions and operating conditions.
This engine configuration has been the subject of many experimental and numerical studies. Ensemble averaged mean and turbulent velocity statistics of this engine, measured using Laser-Doppler anemometry, was reported in Morse et al. (1978, 1979). In their work, axial velocity data for different radial locations has been recorded for 100 engine cycles at crank positions of 36° and 144° after TDC for every 10 cm increments: measured along the cylinder axis starting from the cylinder head. Results of five different data sets have been compared to ensure the repeatability. Several experimental errors may present in these measurements. Uncertainty in the measurement location, flow asymmetry, variations of the piston speed and the limitations of measurement hardware are some of the error sources. A detailed discussion with some explanation to several other possible error sources can be found in Morse et al. (1979). However, it has been verified that the maximum error remains less than 3% in all locations, except where the maximum, mean and rms turbulence velocity occur.

Accordingly, the work of Morse et al. (1978, 1979) provides the validation data set for present simulations. Use of these experimental measurements in a number of RANS validation studies have been reviewed by Tahry & Haworth (1992). Haworth (1999), Haworth & Jansen (2000), Sone & Menon (2003) and Liu & Haworth (2010) have also used this data set for verification of LES results. In general, both these RANS and LES predictions were in good agreements with the mean measured velocities; however some discrepancies were noted in rns velocity predictions.

### 10.1.1 Numerical Setup

Figure 10.2 shows the computational mesh of the engine assembly used in present simulations, which comprises of 200,000 unstructured hexahedral elements. Relatively finer mesh distribution has been maintained around the valve and squish region as it was noted during initial simulations that, this would increase the agreement between predations and measurements. Simulations were conducted using $k - \Delta$, $k - kl$ and $k - \varepsilon$ turbulence models. The working fluid was taken as air and the ambient conditions were taken to be 300 K and 1 bar. All solid walls were considered isothermal at a temperature of 300 K. No slip conditions were set for both LES and RANS simulations. Intake was specified to be a pressure boundary at atmospheric conditions. Simulations were started 100° before TDC and the initial conditions were taken to be atmospheric, but with superimposed small random fluctuations on velocity. It has been noted that, without these fluctuations, the flow remain axisymmetric at least for three engine cycles (Haworth & Jansen 2000). Simulations were conducted for six consecutive engine cycles during LES calculations and the first three cycles
were discarded to minimise the effects of initial conditions. Results of the remaining three cycles were ensemble averaged to obtain mean quantities. However, for RANS simulations, only four consecutive cycles were computed and the first three cycles were discarded.

Figure 10.2: Computational mesh of the motored research engine. (a) Sectional view through the valve. (b) Full mesh (c) Sectional view across the cylinder region
Comparison of three engine cycles is not sufficient to obtain a statistically converged solution, as it requires a large number of independent data samples. However, the axisymmetric nature of this engine configuration can be used as an advantage to obtain an adequate number of data sets. Consequently, for a given crank angle, velocity data along the radial direction were extracted for every 20° azimuthal increments about the cylinder axis. This procedure yields 18 velocity data sets per each axial sampling station per engine cycle. Hence, a total of 72 data samples could be extracted during the four engine cycles, making it possible to obtain a sufficiently converged average value. This is somewhat similar to obtaining individual velocity profiles for 72 different engine cycles at a given location. A rough estimation could be made for the integral scale of turbulence, following standard scaling arguments. It should be equal to a fraction of the squish clearance height, when the piston is at TDC. In the annular jet during induction, the integral scale is proportional to the annulars width. These arguments, combined with experimental observations in similar sized engines, suggest an approximate upper bound of 4-5 mm for the integral scale of turbulence. The 20° increment corresponds to an approximate gap of 4.0 mm between two radial data extraction planes at a distance of 11 mm from the cylinder axis. Accordingly, the velocity data measured at larger radial distances than 11 mm from the cylinder axis could be considered as statistically independent, but for smaller radial distances, the 18 data samples may not be independent and the associated statistical uncertainty could be much higher.

Velocity and turbulent data were sampled at two crank angle positions (36° and 144°) measured after TDC of each cycle. For 36° case (early stage on intake), three axial locations were chosen and for 144° case (late stage on intake), 7 axial location were considered. The gap between two axial locations is about 10 mm and each location is designated by the z distance, measured from the cylinder head.

10.1.2 Results and Discussion

Predictions of three turbulence models: $k - \Delta$ and $k - kl$ in LES context and $k - \varepsilon$ in RANS context, are compared in these simulations. Due to the low Reynolds number (low engine speed) in this test case, the results may be relatively less sensitive to the SGS turbulence model. On the other hand, as coarser grids are used, it should make the results significantly model dependent. Plotted in Figure 10.3 are computed and measured ensemble averaged mean axial velocity profiles at 36° after TDC. Continuous solid lines and chained lines respectively show the results of $k - \Delta$ model and the $k - kl$ model. RANS predictions are indicated by the dashed lines. Symbols represent the corresponding measured values taken
from Morse et al. (1978, 1979). Note that, the velocity has been normalized by the mean piston speed. The value of resulting ratios at a given radial location should be read from the figure, with reference to the dashed vertical line, which indicates the corresponding $z$ location. Accordingly, the approximate maximum measured axial velocity at a distance of 20 $mm$ from the cylinder head is twice the mean piston speed as indicated in Figure 10.3.

Figure 10.3: Comparison of ensemble averaged mean axial velocity profile along the radial direction for three axial locations at 36° ATDC. Symbols show measured data

In general, very good agreement is seen between the measured and predicted LES results. RANS simulations have also predicted reasonable results, but a general tendency of under prediction at the peak velocity locations, particularly at $z = 20 \, mm$, can be noticed. Both LES models also under predict at this location, but the results are better than RANS. The peak velocity and its location close to the annular jet have been accurately predicted by all three turbulence models. During the initial trial simulations, it was noticed that, the mesh configuration plays an important role in determining the predicted peak pressure location. For example, if the mesh is coarser (even if the mesh in the annual passage and directly below the annulus is much finer) in the vicinity of the jet region, the flow was observed to deflect into the cylinder (not shown here), shifting the peak pressure location at $z = 10 \, mm$ towards the cylinder axis. As a result, in final simulations, the grid was made much finer in the squish area as already noted in Figure 10.2.
Comparison of measured and predicted root mean square (RMS) velocity fluctuations are shown in Figure 10.4. In general, none of the models shows a prefect agreement with measured values. However, $k - \Delta$ predictions were found to be the best and RANS results were the poorest among three models. Though, the high turbulence levels in the annular jet at $z = 10$ mm have been reasonably captured by both LES models, the overall results have been under-predicted. A similar trend has also shown at $z = 20$ mm, and a substantial difference in the measured and predicted peak values are observed. Note that, the computed RMS velocity $u'_{rms}$ contains the contributions from both resolved and sub-grid scales, as it was calculated using $u'_{rms} = u'_{resolved} + \sqrt{k_{sgs}/1.5}$ assuming isotropic turbulence (Sone & Menon 2003).

![Graph showing comparison of RMS velocity fluctuations](image)

**Figure 10.4:** Comparison of ensemble averaged RMS axial velocity profile along the radial direction for three axial locations at 36° ATDC. Symbols show measured data.

Predicted results of mean and RMS velocities corresponding to 144° ATDC crank location are shown in Figure 10.5 and Figure 10.6. Computed velocity magnitudes by $k - \Delta$ and $k - kl$ models are in very good agreement with the measured values and, are much accurate than RANS results at all locations up to $z = 20$ mm. None of the models have been able to capture the correct magnitude of axial velocity within a reasonable error margin at $z = 30$ mm location, but the general trends in magnitude variations have been grasped. In locations, where the distance from the cylinder head is higher and the magnitude of mean
velocity is significantly lower ($z > 40 \text{ mm}$), RANS has much accurately predicted the velocity profiles, whereas both LES models seem to overestimate. This could probably be a consequence of using a much coarser mesh in this region.

![Graph showing velocity profiles](image)

**Figure 10.5:** Comparison of ensemble averaged mean axial velocity profile along the radial direction for seven axial locations at 144° ATDC. Symbols show measured data.

Computed RMS velocity profiles at this crank position are also in reasonable agreement. $k - \varepsilon$ model has predicted comparatively a uniform turbulent intensity along the radial direction and, is highly insensitive to the apparent variations close to the jet region. Both LES models seem to grasp those variations, and their radial locations showing a reasonable agreement with the measured data. However, the actual magnitude is shown to be slightly different from the measured values, and this gap is much noticeable at a radius of 2.5 mm corresponding to $z = 10 \text{ mm}$ location, where the measured highest RMS velocity has been recorded. In general, neither of the LES model predictions are better than the other.
Figure 10.6: Comparison of ensemble averaged RMS axial velocity profile along the radial direction for seven axial locations at 144° ATDC. Symbols show measured data

The inherent unsteadiness of LES provides a prospect to look into the cycle-by-cycle variations in engines. Figure 10.7 and Figure 10.8 show the individual velocity profile along the radial direction for the 18 azimuthal planes corresponding to z = 10 mm and z = 20 mm locations at 36° ATDC in fourth, fifth and sixth engine cycles, as predicted by the two LES models. Symbols show the experimentally averaged values and dashed lines show averaged velocity profile of the particular cycle.

Generally, a substantial variation of the axial mean velocity profiles can be seen, between different engine cycles. Also, the variations of the velocity in different azimuthal planes, within the same cycle are also significant. However, at z = 10 mm location, where it is much closer to the high velocity intake jet stream, relatively a low level of variation is observed. At z = 20 mm, variations are maximum and instantaneous velocity profiles show a significant departure from axisymmetry.
Figure 10.7: Instantaneous axial velocity profile along the radial direction in azimuthal planes at $z = 10 \text{ mm}$ location at $36^0 \text{ ATDC}$
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Figure 10.8: Instantaneous axial velocity profile along the radial direction in azimuthal planes at \( z = 20 \text{ mm} \) location at 36° ATDC.
There is no any notable difference between the predictions made by each SGS turbulence model. Both models have shown a similar magnitude of variation of predicted axial velocity profiles.

Comparison of instantaneous RMS velocity profiles and the cycle averaged RMS values are shown in Figure 10.9 and Figure 10.10 corresponding to $z = 10 \text{ mm}$ and $z = 20 \text{ mm}$ axial locations respectively. The general trend of under prediction in both instantaneous and cycle averaged RMS values is apparent in these figures as previously noticed in ensemble averaged profiles. This is common in both $k – \Delta$ and $k – kl$ predictions. This could be a concern with the present configuration of the computational domain of the engine. As can be notice from the computational mesh in Figure 10.2, the inlet/outlet port is directly open to the atmosphere. As a result, there is only very little time/length is available for the development of turbulence, prior to the entrance into the engine cylinder. Whereas in the actual engine, there was a sufficiently long inlet passage available, for the development of turbulent fluctuations. No significant difference in performances between the two SGS models is noticed, with respect to the ability of predicting the instantaneous turbulence level. However, there is a noteworthy tendency of increasing the turbulence level in $k – kl$ model predictions. This might be an indication that, more number of simulation cycles would probably lead to improved results.

It is expected from LES to resolve more flow structures than RANS in an unsteady flow field. Figure 10.11 shows the flow structures represented by vectors on an axial plane corresponding to $144^0 \text{ ATDC}$ crank position. The first two figures illustrate the instantaneous velocity vectors computed by $k – \Delta$ and $k – kl$ models. The third figure is the time averaged flow field computed using $k – \varepsilon$ model. As expected, RANS computation predicts a symmetric flow pattern, whilst the LES models have captured relatively a higher number of turbulent eddies with unsteady flow features. This can be further verified by the Figure 10.12, which shows contours of the axial velocity on the same plane as predicted by LES and RANS. One of the important observations in this type of engine configuration is the naturally induced weak swirl field about the cylinder axis. Figure 10.13 depicts the predicted flow contours and vector field across two axial locations at $144^0 \text{ ATDC}$ crank locations. It is interesting to see that, only the LES computations have been able to resolve this behaviour and RANS shows almost a zero swirl.
Figure 10.9: Instantaneous RMS velocity profile along the radial direction in azimuthal planes at $z = 10 \text{ mm}$ location at $36^\circ$ ATDC
Figure 10.10: Instantaneous RMS velocity profile along the radial direction in azimuthal planes at $z = 20\, mm$ location at $36^\circ ATDC$
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Figure 10.11: Comparison of predicted distribution of velocity vectors by RANS and LES turbulence models across an axial plane at 144° ATDC

Figure 10.12: Comparison of predicted axial velocity contours by RANS and LES turbulence models across an axial plane at 144° ATDC
Figure 10.13: Computed velocity magnitude and vectors on radial planes by RANS and LES turbulence models at 144° ATDC. Left column corresponds to $z = 15 \text{ mm}$ and the right column $z = 60 \text{ mm}$ axial locations.
10.1.3 Effect of Mesh Construction

Figure 10.14: Highly unstructured computational mesh of the motored research engine; i.e. mesh no. 2. (a) Full mesh (b) Sectional view across the cylinder region

The computational mesh (in Figure 10.2: mesh 1) used for previous simulations, is conceptually an unstructured hexahedral grid, but locally it exhibits largely a structured mesh distribution. As the computational mesh of the E6 engine used later in this work is highly unstructured, it has to be verified the performances of present LES implementation in such a configuration. Therefore, a second mesh (mesh 2) shown in Figure 10.14, was constructed with mostly an unstructured cell connectivity and the simulations were repeated using $k - \Delta$ and $k - kl$ SGS models. This mesh comprises nearly 260,000 hexahedral cell elements. The jet region and the annular passage have a similar mesh resolution as in mesh 1, but at the surrounding, the mesh gradually becomes much coarser towards the cylinder wall. Note that, only four engine cycles were simulated with this mesh for convenience and the first cycle was discarded. Comparison of the predictions in two mesh configurations and the measured values of the mean and RMS axial velocities corresponding to 360 ATDC crank position are plotted in Figure 10.15.
Figure 10.15: Comparison of ensemble averaged mean axial velocity profile along the radial direction for three axial locations at 36° ATDC in different mesh configurations.

Figure 10.16: Comparison of ensemble averaged RMS velocity profile along the radial direction for three axial locations at 144° ATDC in different mesh configurations.
It is encouraging to observe that, even with lesser number of cycles, both \( k - \Delta \) and \( k - kl \) models have been able to show similar performance as in the previous case. However, \( k - kl \) model seems to slightly under predict the level of turbulence, indicating that it needs more time for flow development. Remarkably, there is only very minute difference between the predictions of \( k - \Delta \) model. Results were also similar for 144\({}^0\) ATDC crank position. No notable difference was identified. Consequently, it can be concluded that, if the sufficient mesh resolution is provided in highly strained regions, the predictions of the present LES models are reasonably insensitive to the mesh configuration, at least for low Reynolds number flows.

The time spent on simulations is a crucial factor in LES simulations, as usually LES calculations are highly time demanding. Surprisingly, the time taken by the two SGS models in present calculations was very similar. For example, simulations using mesh 2 for 1270 crank degrees with the \( k - \Delta \) model consumed 226 CPU hours and during this time, \( k - kl \) mode was able to simulate approximately 1260 crank degrees. However, it should be noted here that, the automatic time step calculation technique of KIVA, which was originally developed for RANS calculations, was used here without any modification. Hence, there should be ample opportunities for optimisations of time step calculation to best suite each method.

Particularly, considering the facts that, \( k - \Delta \) model predicts better turbulent characteristic with relatively lesser number of engine cycles, \( k - \Delta \) SGS model was chosen to be used with the present LES combustion simulations. It is also worth mentioning that, this does not mean the \( k - kl \) model is poorer in predictions. It has a very good potential and should be thoroughly investigated to gain the confidence in a future study.

\subsection{10.2 Validation of Ignition and Flame Kernel Formation Model}

Having verified the accuracy of the present LES implementation for non-reacting flow problems in previous sections, now the attempts are made to validate the developed ignition and combustion models. Validation of the ignition and flame kernel model was performed by simulating the flame kernel growth in an engine swirl chamber. This is the same swirl chamber configuration of Herweg & Maly (1992), used in the validation process of extended DPIK model in RANS. A detailed description on the apparatus, measuring techniques and operating conditions can be found in Chapter 7.
The computational mesh of the swirl chamber used for LES is shown in Figure 10.17(a). The mesh has approximately 150,000 hexahedral cell elements. Only one half of the mesh was refined and it was ensured that, this region is large enough to enclose the whole flame kernel, during the entire period of simulation for all test cases. The nominal cell size in this region is about 0.5 mm. Initial swirl profile with superimposed random velocity fluctuations are shown in Figure 10.17(b). Location of the spark electrodes is also shown in the same figure. Note that, small length scale fluctuations shown in the contour plot correspond to the refined mesh region and the larger fluctuations are in coarser mesh region. This is only an artefact of plotting as a result of using two different mesh sizes. Fluctuating velocity scales have similar magnitudes in both mesh regions.

Figure 10.17: (a) Computational mesh of swirl chamber for LES of flame kernel growth
(b) Spark location and initial swirl velocity profile across spark plane
As in RANS simulations, a frozen turbulence field was assumed. Turbulent intensity at the integral length scale was estimated from experimental measurements (Herweg & Maly 1992). Required turbulent intensity at a given effective filter level was calculated assuming linear scaling of eddies according to Kolmogorov hypothesis. Swirl velocity, pressure and temperature were also initialized to match with the measurements. No slip and isothermal wall boundary conditions were used. A summary of the operating conditions corresponding to each of the simulated test cases, are provided in Table 10.1.

<table>
<thead>
<tr>
<th>Operating conditions and turbulence parameters in swirl chamber</th>
<th>Test case</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine RPM</td>
<td></td>
<td>300</td>
<td>500</td>
<td>750</td>
</tr>
<tr>
<td>Fuel-air equivalence ratios</td>
<td></td>
<td>1.0 &amp; 0.77</td>
<td>1.0 &amp; 0.77</td>
<td>1.0 &amp; 0.77</td>
</tr>
<tr>
<td>Pressure at ignition (bar)</td>
<td></td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Temperature at ignition</td>
<td></td>
<td>660</td>
<td>660</td>
<td>660</td>
</tr>
<tr>
<td>Turbulent intensity ((cms^{-1}))</td>
<td></td>
<td>44</td>
<td>73</td>
<td>109</td>
</tr>
<tr>
<td>Integral length scale ((cm))</td>
<td></td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>Mean flow velocity at peripheral spark location ((cm.s^{-1}))</td>
<td></td>
<td>750</td>
<td>1240</td>
<td>1870</td>
</tr>
<tr>
<td>Ignition energy supplied ((mJ))</td>
<td></td>
<td>60</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Ignition duration ((ms))</td>
<td></td>
<td>1.2</td>
<td>1.1</td>
<td>0.9</td>
</tr>
</tbody>
</table>

10.2.1 Simulation Results

Shown in the Figure 10.18 - Figure 10.20 are the measured and predicted flame area evolutions for the three simulated test cases in the swirl combustion chamber. The predicted area corresponds to the instantaneous surface area of the burned gas volume and the measured flame area has been calculated by averaging the flame area approximated using two dimensional schlieren photographs (Herweg & Maly 1992).

The predicted flame surface area is in close agreement with the measured flame area in all simulated test cases. A significant cyclic variation in flame area evolution has been observed in experiments (Herweg & Maly 1992). However, the variations in the present simulations are very limited, due to the employed modelling strategy. Basically, in simulations, the domain was taken as a closed chamber, whereas in experiments, it has been connected to the engine cylinder, so that the flow properties inside were changing dynamically. Simulation of both the engine cylinder and the swirl chamber requires a considerable computational time and therefore, only the swirl chamber volume was modelled. Initial swirl profile and the flow
velocity were artificially initialized to match with experimentally measured mean values. Gaussian random fluctuations were superimposed to mean velocity field based on measured mean turbulent intensity. However, as often observed (Lund et al. 1998), this turbulent field decays very fast, so that effect of turbulence reduces with time.

As a frozen turbulence field was assumed, where the turbulent intensity and the laminar flame speed were kept constant, estimation of wrinkling factors was based on the global values of these parameters. As a result, the predicted flame area remains very much closer to the cycle averaged mean flame area without a significant variation. Therefore, only the results of a single simulation are presented for each of the operating condition. However, the model has been able to successfully predict the changes in the flame growth rates under different turbulent levels and fuel properties. Accordingly, this model should also be able to grasp localized effects of turbulent, particularly in engine combustion. This will be demonstrated in the next section, where the modelling results of flame area growth in E6 engine is presented.

![Figure 10.18: Comparison of measured and predicted flame kernel surface area for case 1 in swirl chamber simulations](image-url)
Figure 10.19: Comparison of measured and predicted flame kernel surface area for case 2 in swirl chamber simulations

Figure 10.20: Comparison of measured and predicted flame kernel surface area for case 3 in swirl chamber simulations
10.3 Modelling Full Cycle Combustion in E6 Engine

The validation was extended by modelling the full cycle combustion process in a Ricardo E6 experimental engine at Loughborough University. Engine specifications, geometric parameters, testing procedure, data acquisition and analysing methods have already been presented in Chapter 6. Therefore, only the major operating conditions relevant to validation test cases are given in Table 10.2.

Table 10.2: Operating conditions of Ricardo E6 engine

<table>
<thead>
<tr>
<th>Case</th>
<th>φ</th>
<th>RPM</th>
<th>Spark advance (BTDC)</th>
<th>Comp. ratio</th>
<th>T_{in} (K)</th>
<th>T_{w} (K)</th>
<th>Injected fuel mass (mg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.967</td>
<td>1800</td>
<td>20</td>
<td>8.7</td>
<td>300</td>
<td>365</td>
<td>317</td>
</tr>
<tr>
<td>2</td>
<td>0.936</td>
<td>1500</td>
<td>16</td>
<td>8.7</td>
<td>298</td>
<td>360</td>
<td>368</td>
</tr>
<tr>
<td>3</td>
<td>0.953</td>
<td>1500</td>
<td>16</td>
<td>7.5</td>
<td>298</td>
<td>360</td>
<td>404</td>
</tr>
</tbody>
</table>

Case 1, running under part load conditions, was considered to be the reference test case; hence bulk of the results presented in this chapter corresponds to this test case. The other two test cases were set to investigate the predictability of present formulation in changing engine operating conditions. Both case 2 and 3 were running in full load conditions and spark advance was changed from case 1. In addition, the compression ratio has also been altered in case 3. Note that, the equivalence ratio is different in each case and corresponds to slightly lean conditions.

Continuous simulation of multiple LES engine cycles requires a large amount of computational time. Therefore, parallelized computer codes are often required (see Vermorel et al. 2009, Richard et al. 2007 & Ewald et al. 2007). As KIVA code used in this work is a serial code, simulations were limited to a number of separate individual cycles, and the effects of cycle-to-cycle variation were introduced by superimposing random fluctuations on the mean intake pressure. However, this approach does not exactly mimic the actual cycle-to-cycle variations of flow properties. Multi-cycle LES simulations of an SI engine have been reported in Goryntsev (2010), Vermorel et al. (2009), where the first engine cycle (at the start of the simulation) has been modelled by superimposing random fluctuations similar to the present approach. Comparison of the results obtained for this first engine cycle with rest of the results shows that, the current technique is capable of representing such cycle-to-cycle
variations to a reasonable degree. However, for more accurate results, continuous multi-cycle simulations are recommended.

Computational grids for all cases comprised of unstructured hexahedral cell elements. The engine mesh, in total contains 0.8 million cells and corresponds to a nominal cell dimension of 0.7 mm within the combustion chamber. Simulations were started at 20 BTDC in exhaust stroke. Initial properties and mass fractions were calculated using a thermodynamic analysis. Based on exhaust gas temperature measurements, in-cylinder and exhaust gas mixture temperatures were taken to be 750 K at the start of simulations. In-cylinder, fluid and turbulent properties were homogeneously initialized with superimposed random Gaussian fluctuations. Both intake and exhaust port openings were defined as pressure boundaries, with the allowance for possible back-flow phenomenon. Measured mean intake manifold pressure was set at the intake boundary with superimposed random fluctuations (maximum of 5% from the mean value) following Sone & Menon (2003). These fluctuations are the only source of external randomness introduced. No slip and isothermal wall conditions were assumed. Different wall temperature values were used in different surfaces as described in Chapter 7.

Figure 10.21: Computational mesh for the full cycle LES simulation of the Ricardo E6 engine
Flow in intake and exhaust ducts was solved even if the valve are closed as these conditions affects the flow during the valve overlap period and at the start of the next cycle. Ignition, flame kernel formation and the fully developed combustion were simulated using the new ignition model and the dynamic flame surface density model developed in Chapter 9. Single step fuel oxidisation is assumed and the laminar flame speed was calculated with the empirical relations proposed by Gülder (1984).

Ten engine cycles were simulated for the base case (i.e. case 1) and they are analysed in detail. Only five engine cycles were considered for other two test cases, as the purpose of those simulations is to verify whether the model reflects the correct behaviour in changing operating conditions. It should be noted that, this number of cycles may not be sufficient to make a firm judgment of the cyclic variability of an engine. Hence, the results shown here are primarily used to demonstrate the predictability of the present formulation.

10.3.1 Flow Evolution in Intake and Compression

In-cylinder bulk flow motion is predominantly important in determining the overall combustion duration and macro flame structure. The unsteady nature of LES can effectively be used to investigate in-cylinder flow development process on the cycle–by-cycle basis. Evolution of in-cylinder flow field during intake and compression strokes in cycle no. 1 is depicted from Figure 10.22 to Figure 10.31. Intake valve opens at the late stage of the exhaust stroke, when the piston is close to the TDC. At this time, in-cylinder pressure is greater than the intake port pressure and it forces burned gases to flow back into the intake port. When the piston passes TDC, the descent of the piston causes to drop the in-cylinder pressure below intake manifold pressure and this produces the required pressure gradient for the fuel-air mixture to flow into the cylinder. Smaller valve lift and the increasing speed of the piston descent generate a high speed jet though valves opening, which in the present case locally exceeds 150 m s\(^{-1}\) at the annular valve gap.

Variation of the velocity magnitude across the intake valve plane at 30\(^{0}\) after TDC is shown in Figure 10.22 (a). Shown in Figure 10.22 (b) is the velocity magnitude in a plane normal to the cylinder axis, located 1.5 cm below the cylinder head. Tangential velocity vectors on the same plane are also indicated with arrows. Mutual interaction of this jet stream and its impingement on the surrounding walls evolve very high turbulence levels and complex flow structures. These are clearly visible in the velocity contour plots in Figure 10.22 and Figure 10.23.
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Figure 10.22: Evolution of in-cylinder flow structure during intake at 30 ATDC.
(a) across the intake valve plane (b) 1.5 cm below the cylinder head

Figure 10.23: Evolution of in-cylinder flow structure during intake at 60 ATDC.
(a) across the intake valve plane (b) 1.5 cm below the cylinder head
Figure 10.24: Evolution of in-cylinder flow structure during intake at 90 ATDC. (a) across the intake valve plane (b) 1.5 cm below the cylinder head (c) 5.5 cm below the cylinder head
Figure 10.25: Evolution of in-cylinder flow structure during intake at 120 ATDC. (a) across the intake valve plane (b) 1.5 cm below the cylinder head (c) 5.5 cm below the cylinder head
Figure 10.26: Evolution of in-cylinder flow structure during intake at 150 ATDC. (a) across the intake valve plane (b) 1.5 cm below the cylinder head (c) 5.5 cm below the cylinder head
Figure 10.27: Evolution of in-cylinder flow structure during intake at BDC.
(a) across the intake valve plane (b) 1.5 cm below the cylinder head (c) 5.5 cm below the cylinder head (d) 9.5 cm below the cylinder head
Figure 10.28: Evolution of in-cylinder flow structure during compression at 210 ATDC.
(a) across the intake valve plane (b) 1.5 cm below the cylinder head
(c) 5.5 cm below the cylinder head
Figure 10.29: Evolution of in-cylinder flow structure during compression at 240 ATDC. 
(a) across the intake valve plane (b) 1.5 cm below the cylinder head 
(c) 5.5 cm below the cylinder head
Figure 10.30: Evolution of in-cylinder flow structure during compression at 270 ATDC. (a) across the intake valve plane (b) 1.5 cm below the cylinder head

Figure 10.31: Evolution of in-cylinder flow structure during compression at 300 ATDC. (a) across the intake valve plane (b) 1.5 cm below the cylinder head
Usually in engines, the configuration of valves and the motion of the piston results in large scale tumble motion perpendicular to the cylinder axis. In the present configuration in E6 engine, this motion is not that strong as in the case of a canted valve pent roof engine, but is considerable. This phenomenon can be clearly identified from Figure 10.25 and Figure 10.26 which correspond to the latter stage of the intake stroke. In addition, a significant development of flow structures in the axial plane is also apparent in these figures. Even though, no distinct swirling motion about the cylinder axis can be recognized, a number of local eddies has been formed generating a highly irregular flow pattern. Figure 10.27 shows a snapshot of the instantaneous in-cylinder flow at intake BDC, on the intake valve plane and three other axial planes, which are approximately located at 1.5, 5.5 cm and 9.5 cm from the cylinder head. It is worth noting that, the velocity magnitude has globally reduced to much lower values by this phase due to the dissipation of energy and the reduced pressure gradient across intake valve. Figure 10.28 and Figure 10.29 show the development of flow during the early stage of the compression stroke, after valves are fully closed and the in-cylinder and port regions are fully separated. It can be seen that, the upward piston motion has resulted in a much ordered flow motion with relatively less eddy structures. As shown in Figure 10.30 and Figure 10.31, which correspond to 270 ATDC and 300 ATDC respectively, the flow field becomes much weaker compared to the early stage of intake, but with localized large scale eddies with a moderate velocity.

Significant differences in the development of flow features in cycle-by-cycle basis can also be observed in SI engines. Velocity magnitude on the intake valve plane in three engine cycles at the bottom dead centre during the intake stroke are shown in Figure 10.32. Spatial variations of the in-cylinder flow structures among these three cycles are shown to be substantial. Global distribution of the magnitude of velocity seems to be common in all three cases, but local flow structures are entirely different from one another. These differences, particularly in direct injection engines, cause significant dissimilarities in air-fuel mixing between individual cycles. In addition, significant cyclic variations of the bulk convection flow pattern are also apparent in the present case, which must effectively result in subsequent variations in the flame propagation. In Figure 10.33, variation of the velocity field close to the spark plug plane, prior to the ignition is shown. In all cases, the variations are found to be substantial in magnitude and such variations are very much expected in these types of single cylinder engines. As a result, the variations of the flame propagation and the pressure rise should also be noticeable.
Figure 10.32: Variation of velocity magnitude across the intake valve plane at piston bottom dead centre during the intake stroke in three engine cycles of case 1

Figure 10.33: Variation of velocity magnitude across the spark plug plane just before ignition in three engine cycles of case 1
In addition to the investigation of engine flow features, these visualisations provide a qualitative assessment of the standard of the present LES model. It is clear that, even with relatively coarser meshes used in this work, present LES implementation has been able to resolve the evolution of a large number of in-cylinder flow structures. Particularly, flow features which are more influential for engine performance. This should be mainly due to the present SGS model, where a separate transport equation is solved for SGS kinetic energy as pointed out in Rutland (2011). A rudimentary SGS model requires finer meshes for good results whereas, a well-engineered model would provide better results with coarser meshes.

### 10.3.2 Ignition and Flame Kernel Formation in E6 Engine

Figure 10.34 shows the growth of mean flame kernel surface area during the ten engine cycles of case 1. Note that, the ignition is started at 40 BTDC in these simulations and the end of each curve is the transition point, after which the main combustion model is activated.

![Figure 10.34: Evolution of the computed flame surface area during the early stage of flame kernel development in E6 engine in case 1. The end of each curve is the transition point](image)

Accordingly, the predicted flame area and its growth rate have shown significant variations even at the early stage of the flame propagation. Variation of the transition point: i.e. the time taken to develop a resolvable flame front within the mesh, is also seen to be considerable. The shortest time elapsed until the transition is about 8 crank degrees and the longest is close to 14
crank degrees. Importantly, it seems that the transition point is determined not just by the flame area growth rate, as no distinct relation can be identified between rate of change of flame area and the time taken to form a fully developed flame profile. This can be clearly verified by Figure 10.35, in which the evolution of flame kernel surface is illustrated during the first three engine cycles.

![Flame kernel evolution during three engine cycles in case1. The final figure in the sequence shows the flame surface at transition. Flame surface is represented by ĉ = 0.5 iso surface. Ignition at 340 CAD](image)

It is interesting to see significant differences in the evolution of flame kernel shape in these three cycles. The flame kernel has been deformed, wrinkled and slightly convected away from spark centre (especially in cycle no 1) by the local bulk flow motion, even early as 10 degrees after ignition.
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Figure 10.36: Evolution of the computed flame surface area during the early stage of flame kernel development in Ricardo E6 engine in case 2. The end of each curve is the transition point.

Figure 10.37: Evolution of the computed flame surface area during the early stage of flame kernel development in Ricardo E6 engine in case 3. The end of each curve is the transition point.
Further, it can be noticed in all three cycles that, the flame kernel is much smaller in size up to 10 degrees after ignition and the iso-\( \tilde{c} \) surface remains roughly spherical. This has been often observed in experiments and a crank interval of 10 degrees after ignition has been defined as an upper limit, in which this spherical behaviour prevails (Heywood 1994). After this period, the flame starts to show fully developed characteristics. Promisingly, the present simulations further verify this fact, as turbulent characteristics are apparent only after 10 crank degrees from ignition. Usually in RANS modelling, transition to the main combustion model takes place before 10 crank degrees. However in LES, the transition criterion is different and it needs to from a resolvable flame profile in the computational mesh. This makes the transition point a function of the grid and combustion filter widths.

Figure 10.36 and Figure 10.37 also show the variations in growth rate of mean flame kernel surface area in case 2 and case 3 respectively. As illustrated, the variations in these cases are also substantial. Note that, no fine tuning of any of the model constant was made in these simulations for all three test cases. Standard values obtained during model derivation in Chapter 9 were used unchanged.

### 10.3.3 Predicted Flame Propagation Characteristics

In this section, the result of the present dynamic flame surface density model for the fully developed stage of combustion is presented. As in the ignition model, standard values of model constants were used with the combustion model for all three test cases without any adjustment. Mean cell size in the combustion chamber used for these simulations is about 0.7 mm and the combustion filter width is about 3.5 mm. These parameters indicates an approximate simulated flame brush thickness of 7.0 mm. Accordingly, the present LES simulations found to capture the flame wrinkling larger than this limit, generated by the resolved scale eddies. Shown in Figure 10.38 are some of the most important combustion model parameters at two different crank angles in case 1. Shown in the first row is the variation of filtered progress variable across the flame front while, second row shows the variation of test filtered progress variable. As expected, at test filter level wrinkling of the flame is reduced but the thickness is increased. A smooth gradient has been maintained, near walls indicating that the current test filtering approach is capable of producing acceptable results. The local values of the wrinkling exponent \( \xi \) are shown in the third row. It was found to be close to zero at the leading edge of the flame front while, a value close to 1.0 in the fully burned region within the flame.
Figure 10.38: Distribution of the progress variable, test filtered progress variable and the exponent of the wrinkling term for two crank positions during the combustion phase in case 1.
The reason for $\xi$ to become unity is the presence of a near zero gradient of $\tilde{c}$, behind the reaction zone. Also, it has an average value of 0.5 inside the reaction zone. This is completely in agreement with the currently published literatures for these types of dynamic combustion models (Wang et al. 2012, Yoshikawa et al. 2012). This indicates a fractal dimension close to a value of 2.5. In general this value for engine applications is found to be quite high, compared to the typical range of 2.2 – 2.4, often found in experimental literature (North & Santavicca 1990).

Substantial variation in the instantaneous flame propagation is also observed for all the simulated engine cycles as presented in Figure 10.39. The flame front is represented by the iso-progress variable surface equal to 0.7. Even though the instantaneous flame surfaces demonstrate significantly different localized geometric profiles, the global trend in the propagation direction and enflamed volume is shown to be similar. Wrinkling of the flame surface caused by a wide spectrum of turbulent eddies is clearly evidenced throughout the flame propagation, more importantly the variations are apparent even from the very early stage of combustion. Interaction of flame front with combustion chamber walls results in flame quenching. The importance of making proper allowance to incorporate quenching effects in engine calculations have been discussed in detail in Chapter 5 and 8 of this thesis. However, no allowance was made in this LES work to model the flame quenching phenomenon as the primary aim was to investigate the combustion model performance. Thus, implementation of a suitable flame quenching model is highly recommended. For this purpose, the newly developed flame quenching model in chapter 5 of this work, can be easily adapted.
Figure 10.39: Flame surface propagation during three combustion cycles in case 1. Flame surface is represented by the iso-progress variable surface of $\bar{c} = 0.5$. Ignition at $340^\circ$
The main objective of an engine combustion model is to predict the in-cylinder pressure rise and the heat release rate during combustion. Present predictions of these parameters corresponding to the conditions in case 1, are shown in Figure 10.40 and Figure 10.41 respectively. The predicted pressure is well within the experimentally measured range and varies close to the cycle averaged pressure trace. The maximum variation of the experimental peak pressure from the cycle averaged value is slightly above ± 6 bar and the simulated value is about ± 3 bar. The difference, in the two quantities could mainly be a consequence of the present approach (imposing random fluctuations) used to specify the intake pressure boundary conditions for different engine cycles. Hence, it is clear that, initial assumption of the amplitude of pressure fluctuations (i.e. 5% maximum) has caused a considerable under estimation of cycle-by-cycle variations in this case.

Note that, the magnitude of peak in-cylinder pressure during the cycle (Figure 10.40) and the flame area growth rate during the early stage of the flame kernel formation (Figure 10.34) are not directly interrelated for the present cases. This is mainly caused by the differences in trapped fuel mass and the variations in the in-cylinder turbulence in different cycles.
Figure 10.41: Comparison of predicted heat release rate and computed heat release rate from measured pressure data in case 1

Computed heat release rate curves for case 1, during the combustion process are shown in Figure 10.41. Note that, these results have been processed by applying a low pass filter for clarity of representation. Shown by the chained line is the cycle averaged heat release rate, computed using experimentally measured pressure data. As in the case of in-cylinder pressure, substantial variation of heat release rates can be seen. A general trend of over prediction during the early and latter stages of combustion is apparent, but in the middle phase, the measured and predicted values are comparable. A significant irregularity of heat release is seen in this phase, indicating rigorous flame turbulent interactions.

Variation of pressure and heat release rate corresponding to case 2 is shown in Figure 10.42 and Figure 10.43. Those parameters relevant to case 3 are plotted in Figure 10.44 and Figure 10.45 respectively. In case 2, the predicted pressure curves are within the experimental limits, but in case 3, the peak pressure of the cycle no 1 and 5 exceed the experimental maximum. In both cases, the predicted mean peak pressure seems to be larger than the mean experimental peak. These effects can also be seen in the heat release curves as well, where a distinct early start is shown compared to the mean experimental heat release rate. However, in general, the model has been able to successfully grasp the global changes in engine parameters, particularly the peak cylinder pressure and its location, caused by the changes in operating conditions.
Chapter 10: Results & Discussion: LES Applications

Figure 10.42: Comparison of computed and measured in-cylinder pressure variations for the Ricardo E6 engine in case 2

Figure 10.43: Comparison of predicted heat release rate and computed heat release rate from measured pressure data in case 2
Figure 10.44: Comparison of computed and measured in-cylinder pressure variations for the Ricardo E6 engine in case 3

Figure 10.45: Comparison of predicted heat release rate and computed heat release rate from measured pressure data in case 3
Finally, considering the level agreement between experimentally measured and predicted flow and combustion parameters, it can be concluded that, present LES formulation has been considerably successful in prediction premixed combustion characteristic in SI engines. However, despite the successfulness, several key points have still to be verified. Mainly, the grid dependency of the models should be evaluated in detail, probably in much simpler configuration. Assessments of the sensitivity of the test filter width and the combustion filter has also to be accomplished. On the other hand, more importantly, the model behaviour in a range of different engine operating conditions has also to be thoroughly investigated. Then only the capability of the dynamic methods can be properly understood.

10.4 Concluding Remarks

- Flow in an axisymmetric research engine was modelled using the newly developed LES code and the predictions were compared with experimental data.
- This LES formulation has been able to successfully predict overall flow features and to sufficiently resolve instantaneous large flow structures,
- Application of present LES model in Ricardo E6 engine has been able to resolve the evolution of a large number of in-cylinder flow structures, which are more influential for engine performance.
- This is believed to be a result of the higher accuracy of the present SGS turbulence models, where a transport equation is solved for SGS kinetic energy.
- Application of ignition and flame kernel model together with the dynamic flame surface density formulation, has also accurately predicted the global features of flame propagation, reaction rate and in-cylinder pressure rise.
- It has also been able to demonstrate the limits of cyclic fluctuations to a reasonable degree even with a fewer number of simulation cycles.
- A significant variation of flame propagation has also been predicted by the simulations indicating that LES is a much better tool for simulating engine combustion with an acceptable level of computing cost.
CONCLUSIONS AND RECOMMENDATIONS

The main objective of the present study was to develop CFD based turbulent combustion models for premixed spark ignition engine applications. The first phase of this study considered the development of RANS techniques for combustion modelling. In the second stage, the potential of LES techniques were investigated for reacting and non-reacting engine flow modelling. Both RANS and LES tasks undertaken were completed successfully and good comparisons with experimental data have been achieved. Having completed the study, followings have been identified as the most important achievements of this research.

- The potential of the BML model for combustion modelling in wall bounded systems has been successfully demonstrated. This has been achieved by making sufficient allowances to account for wall-flame interaction effects and spatial inhomogeneity in turbulence.

- The capability of LES techniques for capturing unsteady behaviour in SI engines, even with low order numeric in predominantly unstructured hexahedral deforming coarse meshes has been successfully manifested.

- The first ever application of dynamic flame surface modelling techniques in premixed SI engine combustion simulations has been successfully demonstrated.

During these accomplishments, a number of challenges had to be overcome, which ultimately resulted in several novel contributions to the knowledge. Important outcomes are summarised in the section 11.1. Main conclusions drawn from this work are outlined in section 11.2. Recommendations to be considered in a future study, in the course of implementation or enhancement of present modelling strategies are given in section 11.3.
Chapter 11: Conclusions and Recommendations

11.1 Present Contribution

The present work can be broadly specified as the development of premixed combustion models for RANS and LES applications in SI engines. In RANS work, special emphasis was given to develop techniques for modelling ignition, flame kernel formation, fully developed combustion and wall flame quenching effects. Accordingly, a complete set of models addressing each of the above aspects was developed and comprehensively validated with experimentally measured engine combustion data, obtained during the present research. Whereas in LES, the primary attention was to adapt dynamic combustion modelling techniques to suite wall bounded combustion in SI engines. However, in order to achieve this goal, a number of other requirements had to be fulfilled. In the context of LES, special methods are needed to model the ignition and early stage of flame kernel formation. Consequently, a separate sub-grid formulation was developed to address this issue. The present work was based on the open source engine code KIVA-4, which solves the governing equations using RANS methods. Therefore, the modification of this code to make it capable of performing LES calculations and implementation of suitable SGS turbulence models and their validation were also parts of this work. This code is capable of using unstructured grids, but it does not have any facility to generate unstructured grids. Hence, the development of a suitable unstructured mesh generation tool was undertaken as an objective of the present study.

At the completion of this research and having accomplished its objectives, following achievements comprises the major contributions and, are presented in the order of appearance in this thesis.

- A complete computer programme: N2K, was developed and tested, which is capable of converting GAMBIT generated mesh data into KIVA-4 format. This enabled the easy meshing of complex CAD geometries and their importation into KIVA-4 code. A descriptive user guide has also been prepared to be used with the code.

- A comprehensive experimental data set was obtained for a range of operating conditions of the Ricardo E6 engine, as a part of the present work. This data set may be effectively used in the validation of premixed combustion models.

- The DPIK ignition model was improved to account for the local bulk flow convection effects on early flame growth. The model was successfully validated against experimental data in both engine and non-engine applications.
Chapter 11: Conclusions and Recommendations

- A new combustion model based on the BML flame surface density formulation was developed and comprehensively validated. This model uses a new procedure for the dynamic determination of flame wrinkling scale.

- A novel correlation to account for the reduction in flame surface density near solid walls, due to wall-flame quenching, was developed and validated in the context of premixed SI engine combustion. This effectively solved the wall flame acceleration problem associated with the standard BML model.

- KIVA-4 RANS code was successfully modified to perform LES calculations. Two sub-grid scale turbulence models ($k - \Delta$ and $k - kl$) were implemented. The code was validated against experimental data in engine and non-engine applications.

- A new spark ignition and flame kernel formation model was developed in the LES context, for the simulation of early stage of flame propagation in SI engines and validated with experimental data.

- A new dynamic flame surface density model combined with a SGS flame wrinkling model was implemented and investigated its performance was investigated in SI engine configurations.

- A test filtering procedure, particularly suitable for dynamic LES combustion modelling in wall bounded systems was developed and implemented. The performance of this model was assessed by modelling the premixed combustion in SI engines, combined with the dynamic flame surface density model.

11.2 Conclusions

11.2.1 Mesh Generation

- Meshing with conventional block structured grid generation approach of KIVA is a tedious task and it suffers from some inherent drawbacks. Lack of facilities for localized mesh refinements, difficulty of meshing non-conventional engine geometries, unavoidable skewed and concave cells are some of the major deficiencies.

- More importantly, KIVA-4 is capable of handling unstructured grids, but it has no facility for unstructured grid generation. This deficit largely hindered the extraction of its full potential.
• Use of N2K: the developed mesh conversion tool in this study, is quite attractive for high quality unstructured grid generation of complex shaped geometries, as it is a low cost solution, but with greatest flexibility and user-friendliness.

• This provides a seamless approach to use CAD geometries for meshing and importing mesh data in to KIVA-4, whereas it was not at all possible with the inbuilt grid generator.

• In contrast to the conventional block structured meshing approach, the use of the present approach has made a large reduction in the time spent in mesh generation.

• The N2K code may be easily customized for any shape of geometry or its mathematical concepts and logic formulations may be easily adapted to be used with other freely available meshing tools.

11.2.2 RANS Modelling of SI Engines

Ignition and Flame Kernel Formation

• DPIK is a sufficiently accurate model for spark ignition and early stage flame kernel formation modelling, but it assumes the flame kernel to be perfectly spherical, and it lacks the provisions for bulk flow convection effects on the early stage flame propagation.

• In engine like conditions, flame kernel is convected away from the electrodes by the local bulk flow, and the flame surface wrinkling and deformations become apparent after few cranks degrees form the spark onset, making the flame kernel irregularly shaped.

• A realistic flame kernel model should provide adequate allowances for bulk flow convection effects and non-spherical nature of the incipient flame kernel.

• Present improved implementation of the DPIK model has such properties and it accounts for the bulk flow convection effects and non-spherical nature of the flame kernel.

• This formulation has been able to predict the mean flame area growth rate with a very high accuracy for a range of turbulence levels in SI engines.

• Present results further confirms that, making sufficient allowances for the bulk flow convection effects and non-spherical nature of the flame kernel is very important in engine combustion modelling, particularly if the spark electrodes are located close to walls, where a strong swirling field is usually present.
Fully Developed Phase of Combustion

- Combustion in SI engines is essentially influenced by turbulence. Flame is wrinkled by a range of eddies having different length scales and the rate of flame wrinkling is spatially non-uniform due to the inhomogeneity of turbulence.

- Interaction of flame fronts with combustion chamber walls results in quenching owing to heat losses and this phenomenon results in partial burning of fuels.

- BML model produces good results in open stagnation flame modelling, but it fails in engine like wall bounded configurations due to wall flame acceleration problem.

- BML model often involves several modelling constants, which need fine tuning on case by case basis, within a considerable range.

- Present fractal based improvement has successfully eliminated many of these constants from the BML model, leaving only one model constant to be specified. Rest of the constants are dynamically calculated using the information from local flow data.

- The novel dynamic procedure for the flame wrinkling scale calculation has been able to successfully incorporate the effects of inhomogeneity of turbulence in flame surface wrinkling.

- Significant differences of the values of dynamically calculated model parameters were noticed across the flame front and highly strained areas like walls. It verifies the necessity of making sufficient provisions to account for spatial inhomogeneity of turbulence in combustion modelling studies.

- The new wall flame quenching correlation has also been able to successfully capture the reduction of flame area and the reaction rate, so that eliminating the wall flame acceleration problem of the BML model. More importantly, this model can be used with any of the available FSD modelling approaches and no further modification is required.

- Application of the present FBML model (the improved version of the BML model with allowance for spatial inhomogeneity in turbulence and wall flame quenching effects with dynamically calculated model coefficients) in SI engine simulations have produced very good results demonstrating its potential for accurate predictions in engine like dynamic configurations.
Chapter 11: Conclusions and Recommendations

11.2.3 LES Modelling of SI Engines

Turbulence Modelling

- Large eddy simulation is an attractive tool for engine flow modelling as it provides the opportunity to investigate the unsteady dynamic nature of flow and combustion.

- Often, the use of LES in engine simulations is hindered due to the requirement of excessively refined meshes.

- However, present LES simulations demonstrate that, by using a well-engineered SGS model, a sufficiently accurate LES solution with adequate details can be obtained even with a moderately refined mesh than a typical RANS grid.

- Both $k - kl$ and $k - \Delta$ models are found to produce much better results than the conventional RANS $k - \varepsilon$ model in engine applications, even with low order numeric in predominantly unstructured deforming coarse grids.

- Application of the $k - \Delta$ model in engine simulations has been able to resolve the evolution of a large number of in-cylinder flow structures, which are more influential for engine performance.

Ignition and Flame Kernel Formation

- During the early stage of flame kernel formation, its size remain much smaller than the combustion filter width, so that special techniques are required in modelling.

- The newly developed spark ignition flame kernel model considers this aspect in addition to the flame straining effects due to curvature and sub-grid scale turbulence.

- Predictions of this model in the swirl combustion chamber have shown that, it is very much capable of computing the flame kernel surface area growth under non-equilibrium conditions.

- Application in multi-cycle engine simulations have successfully shown its capability of capturing unsteady cycle-to-cycle variations of flame surface growth and winkling effects even after few crank degrees from ignition.

Fully Developed Phase of Combustion

- Dynamic combustion modelling techniques in LES provide the opportunity to formulate problem independent combustion models, but has never been investigated their applicability to SI engines.
Present, dynamic flame surface density model reports the first ever application of such techniques in premixed combustion modelling in SI engines.

Agreement between model predictions and experimental pressure and mass burn data is reasonably good.

It has been able to demonstrate the potential of LES combustion modelling techniques to capture cycle-to-cycle variations and unsteady effects of engine combustion.

The adapted test filtering procedure near solid boundaries has proven to be efficient and successful for dynamic combustion modelling.

Present model is attractive, due its simplicity and is low computation cost compared to a FSD transport equation, hence very much suitable for multi cycle combustion modelling.

11.3 Recommendations for Future Work

11.3.1 Mesh Generation

At present, the $N2K$ code is best suited for the conversion of vertical valve engine geometries with hexahedral unstructured grids. Development of a universal procedure, which may be used with pent-roof engines with canted valves, has been initialized and this work should be continued as explained in Chapter 2. However, this improvement also considers only on unstructured hexahedral grids.

KIVA-4 allows using non-hexahedral mesh elements in any of the regions, except squish and valves. Use of such elements makes meshing much easier. However, procedures for the conversion of non-hexahedral elements in $N2K$ code are still have not yet been adequately tested and they may be considered as unstable. Thus, further testing and optimisations are highly recommended.

In addition, it would be much handy to use full tetrahedral grids for the entire engine geometry. However, implantation of such a procedure would be much challenging as it requires on the fly mesh generation techniques for maintaining the grid quality in the squish and valve regions.

Currently, a single mesh for the entire engine cycle. However, the resolution requirements in the various stages of engine cycle are different from each other. For example, a higher mesh resolution is required in the combustion phase, whereas a coarse mesh would be sufficient during the exhaust. Accordingly, implementation of an accurate data interpolation procedure between different meshes of the same engine would be quite
advantageous as it provides a way to maintain a sufficient mesh resolution, but with less overall computational cost. Alternatively, implementation of an adaptive mesh refinement scheme also remains as an option.

11.3.2 RANS Combustion Modelling

Ignition and Flame Kernel Formation

- One of the major drawbacks of the present DPIK ignition model is that, it does not account for the influence of ignition circuit design on the flame kernel onset. They may be easily incorporated as already explained in Chapter 4. However, re-striking and multiple ignition kernel formation are also some important phenomena, which may be considered in a future implementation.

- Lagrangian particle tracking technique is somewhat unattractive when the mesh is excessively fine or the number of ignition particles is high. The only use of Lagrangian particles in this work is to distribute the total flame area among individual cells. Thus, the possibility of developing an Eulerian based method for this purpose could be considered.

Fully Developed Phase of Combustion

- Smaller eddies have reduced effect on flame surface wrinkling. In the present FBML formulation, these effects are accounted for in the form of fractal dimension to a certain extent. However, it is seen that, even with the present improvements, the flame wrinkling scale has a direct dependency with the turbulent intensity. Consequently, at walls, or at very low turbulent intensities, the estimated flame surface density is still higher than the actual value. Therefore, this issue has to be addressed in a future study. The ITNFS function which defines the overall efficiency of flame wrinkling by eddies of different sizes would provide a background for such an implementation.

- Present wall flame quenching model could be improved by accurately taking into account the effects of equivalence ratio; particularly at rich conditions, fuel type, temperature and pressure. A proper expression has also to be correlated for the minimum and maximum values of the Peclet number for varying mixture conditions. However, these investigations need fair amount of experimental data, which is unavailable at present.

- In general, further, validation of the present formulation in range of engine operation conditions and in different geometrical configurations is highly recommended.
11.3.3 LES Modelling of SI Engines

Turbulence Modelling

- One of the main concerns of KIVA-4 is its serial nature. It is now extremely essential to be parallelized for multi-core processing, using a message passing interface (MPI) approach. OpenMP would be an alternative option but the achievements would be limited. Use of a parallel version would be much useful in multi-cycle simulations of LES studies. In addition, it provides an opportunity to investigate the accuracy of RANS RSM like complex modelling approaches in practical engineering configurations.

- Presently, in the $k - \Delta$ model, two SGS turbulent model constants need case by case calibration, even though the standard values were used in this work. In order to get rid of this deficiency, a dynamic calculation procedure may be implemented following the explanation given in Chapter 8.

- Only the SGS turbulence models for momentum transport was validated in this work. Thus, SGS scalar transport models should also be comprehensively validated.

- No any boundary layer model was used in this work other than the no-slip conditions. Consequently, a suitable wall layer model; preferably a log-law wall function, for turbulent and thermal boundary layers should be implemented.

- In order to assess the performance, present SGS model should be compared with the widely used Smagorinsky model in detail. In this way, it would be possible to identify the relative advantages/disadvantages in the current approach.

- Present investigation revealed that, the $k - kl$ model is also equally suitable for LES modelling. It would be interesting to examine it’s potential in combustion modelling.

Ignition and Flame Kernel Formation

- Similar to the RANS DPIK model, present LES ignition model has also to be improved by making allowances to incorporate re-striking, multiple ignition kernel formation and the effect of the ignition circuit.

- Estimation of the FSD and flame wrinkling factor during the kernel formation period, is currently based on global mean values of those parameters. Investigations should be made to identify a more accurate locally based method to evaluate those quantities.

- In the current model, the magnitude of turbulent intensities at different scales is estimated using simple scaling laws, which is just a simple approximation. Therefore, a more accurate advanced method could be considered in a future study.
**Fully Developed Phase of Combustion**

- An alternative method to compute progress variable gradients, required in dynamic calculation of wrinkling factor, is to directly compute their gradients without using any model form. It should be interesting to investigate the effect of this approach and necessary information is provided in Chapter 7.

- The inner cut off scale plays a vital role in the present combustion model. Current method for approximation of this parameter is solely based on the conclusions made via experimental observations. There are several model forms available in the literature to compute the inner cut off scale and investigation of the applicability of such expressions is encouraged.

- Incorporation of the effects of dissociation and equilibrium reactions in engine combustion is important and still remains to be achieved in the context of present LES model. As the rates of these reactions are often computed with Arrhenius type expressions, coupling with the FSD approach and combustion filtering concept would be a challenging task.

- Wall flame quenching effects are yet to be accounted for in the present fully developed phased LES combustion model. The wall flame quenching model developed in RANS work of this research may be used without significant modifications in LES as well.

- Finally, most of the today’s gasoline engines are of direct injection type. Therefore, present fully premixed combustion models have to be adapted to suite such engines, where the fuel-air mixture may be significantly inhomogeneous at the time of combustion.
This section provides a brief introduction to the GAMBIT neutral file format and the kiva4grid file format based on the following simple mesh shown in Figures A.1 and A.2.

![Figure A.1](image)

(a) Node addresses of the GAMBIT generated mesh as indicated in the neutral file

(b) Corresponding cell addresses shown in an exploded view

This figure shows a computational mesh of a rectangular engine cylinder comprising of 8 cell elements. The entire mesh has been grouped into the squish_lower region. The face boundary conditions were assigned as shown in the Figure A.2. The mesh file has been named as Box_engine_8elements. It should be noted that, the information provided here is only a guideline to understand the mapping concept presented in Chapter 2. GAMBIT and KIVA-4 user manuals should be referred for more information where necessary.
Figure A.2  Face labels of the rectangular engine mesh. Some of the hidden mesh lines are not shown for clarity.

A.1 neutral File Format

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Box_engine_8elements
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Oct 2010
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27         8         1         3         3         3
ENDOFSECTION
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  27
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ELEMENT GROUP 2.4.6
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squish_lower

ENDOFSECTION

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6 4 6
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7 4 3
4 4 3
8 4 3
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3 4 5
2 4 5
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5 4 1
1 4 1
6 4 1
2 4 1

ENDOFSECTION

BOUNDARY CONDITIONS 2.4.6
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5 4 4

ENDOFSECTION

BOUNDARY CONDITIONS 2.4.6
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2 4 2
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### A.2 kiva4grid File Format

**Box_engine_8elements**

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A.3 neutral File Definitions

CONTROL INFO: HEADER SECTION

Header section contains the information on programme version, date and the file name of the GAMBIT file. In this example, Box_engine_8elements is the name of the file. In addition, it contains the following information. Only the first four variables are required for the conversion process.

- **NUMNP** - Total Number of nodes
- **NELEM** - Total Number of cell elements
- **NGRPS** - Total Number of cell groups
- **NBSETS** - Total number of boundaries

NODAL COORDINATES

This section contains the information about node numbers and their coordinates. The first index is the node number and it is followed the *x*, *y* and *z* coordinates of the node respectively.

ELEMENTS/CHECKS

Information about cell elements and their connectivity is included here. The first index in a row is the cell address. The second is the element type. GAMBIT uses the number 4 as the label to represent hexahedral cells as indicted. The third index indicates the number of nodal points of the given cell. It is 8 here in this example, as the cell is a regular hexahedron. Note that, there are special hexahedral cell types in GAMBIT, which is made of different number of nodes. Rest of the indices in the row show the node addresses according to the GAMBIT node numbering convention.

ELEMENT GROUP

Each of the regions defined in the mesh file is assigned a group number and written in this section under the assigned label. First record defines the assigned number of the group. In this example, the entire mesh has been grouped to a single region during meshing. The second record shows the number of cell elements containing in this group and the third is the region type; i.e. solid or fluid. The next is a solver dependent flag and not required for the present purpose. The label assigned for the region in the mesh file: squish_lower in this case, is written as the next record. The index followed by the region label is also an unused solver
dependent flag. The rest of the indices show the cell addresses of all the elements belong to this group.

**BOUNDARY CONDITIONS**

Boundary face labels assigned during meshing and faces of cell elements, which recline on the particular boundary face, are given in this section. Each of the boundary face with a label is written in a separate section. In this example, there are three of these sections for the three boundaries defined: *cyl_wall*, *cyl_head* and *piston_top*. The first record is the boundary face name and the second indicates the type of the boundary i.e. (nodes or cell faces). The third index is the total number of cell faces contained in this boundary. The next two flags are solver dependent flags and are not used in the conversion programme. The first index of the next line is the cell address and the second is the type of that cell. This record shows the index of the face, which lies on the boundary. Note that, the faces of a cell are indexed according the conversions highlighted in the chapter 2.

**A.4 kiva4grid File Definitions**

The first record is the name of the mesh file. Second and third are respectively the total number of elements and nodes. Next section is the corresponding $x$, $y$ and $z$ coordinates of each of the nodes starting form node 1 and ordered in the ascending order. The next section includes the cell connectivity information. Note that, the node addresses are not explicitly written in these records, as data is written in the ascending order of node addresses. Each row contains the 8 node addresses of the cell, written according to the KIVA-4 indexing convention. As in the previous section, the cell information is presented in ascending order omitting the cell address. Face boundary data is presented in the next section. As usual, the cell number has been omitted from these records. The first record of a row in this section indicates the region index of the cell. KIVA-4 uses a unique index flag for each of the regions. The other records in the row show the face type of the each face of that cell element, according to the KIVA-4 boundary flags.

The last record shows the number of periodic boundaries and if there are such boundaries, corresponding periodic vertices are to be followed.
The concept behind the dynamic approach is to use the information from the smallest resolved scale to model the sub-grid scale effects. If the scale similarity of SGS scale eddies is assumed, the variation of the wave number in SGS range may also be assumed to be linear as depicted by Figure B.1.

Figure B.1: The concept of test filtering. $T_{xy}$ – SGS stresses in test filter scale. $\tau_{sgs_{xy}}$ – SGS stresses in grid filter scale. The difference results in Leonard stresses $L_{xy}$, at test scale (adapted from Poinsot & Veynante 2005)
The wave number and the corresponding turbulent kinetic energy are represented by $W$ and $E$ respectively. The stress contribution from the shaded area can be calculated by double filtering the grid-filtered results with a larger filter width than the grid filter size. This filtering operation is normally called test filtering and the test filter width is denoted by $\Delta$. The same contribution can also be calculated from the Smagorinsky model and by equating the two components the SGS model constant can be evaluated.

Favre filtering is always preferred in variable density flows. Test filtering of a grid filtered variable $\tilde{\phi}$ is defined in the following way.

$$\tilde{\phi} = \frac{\phi_{\tilde{\phi}}}{\tilde{\rho}}$$  \hspace{1cm} (B.1)

The hat symbol represents the test filtering operation.

### B.1.1 Germano Dynamic Model

Germano et al. (1991) model for dynamic evaluation of SGS model constants is based on the double filtering concept of Bardina et al. (1980) and the redefinition of turbulent stresses of Germano (1986). The following equation is derived by applying the test filtering operation on the grid filtered (LES filtered) momentum equation.

$$\frac{\partial (\tilde{\rho} \tilde{U})}{\partial t} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U}) = - \frac{\partial \tilde{\rho}}{\partial x} + \frac{\partial \tilde{T}_{xx}}{\partial x} + \frac{\partial \tilde{T}_{yx}}{\partial y} + \frac{\partial \tilde{T}_{zx}}{\partial z} + F_x$$  \hspace{1cm} (B.2)

To proceed with the derivation, conventionally, the term $\nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U})$ is introduced as already shown in Eq. (8.16). However, if this procedure is followed it is needed to evaluate $\nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U})$ term, but no simple mathematical model is available for this purpose. Therefore, in order to avoid this difficulty, a new term $\nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U})$, was introduced and its use in practical calculations has been justified by Germano (1986).

$$\nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U}) = \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U}) + \left[ \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U}) - \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{U}) \right]$$  \hspace{1cm} (B.3)

The new definition for the test level SGS stresses is then given by:

$$T_{xy} = \tilde{\rho} (\tilde{u} \tilde{v} - \tilde{u} \tilde{v})$$  \hspace{1cm} (B.4)

where, $T_{xy}$ is a general component of the test level stress tensor. If the resolved stress tensor is test filtered, the following is obtained.
\[ \hat{\tau}_{sgs_{xy}} = \hat{\rho}(\bar{u}\ddot{v} - \ddot{u}\bar{v}) \] (B.5)

\[ L_{xy} \text{ at test level is obtained by subtracting Eq. (B.4) from Eq. (B.5). It is worth to note here that } L_{xy} \text{ is equivalent to the Leonardo stress tensor at test level and the relation given in Eq. (B.6) and Eq. (B.7) is called the Germano Identity.} \]

\[ L_{xy} = T_{xy} - \hat{\tau}_{sgs_{xy}} \] (B.6)

\[ L_{xy} = \hat{\rho}(\bar{u}\ddot{v} - \ddot{u}\bar{v}) \] (B.7)

If the test level stresses are computed using the Smagorinsky model, the following set of equations from Eq. (B.8) to Eq. (B.11) is obtained.

\[ T_{xy} - \frac{1}{3}(T_{kk})\delta_{xy} = -2\mu^{s}_{sgs}\hat{S}_{xy} \] (B.8)

\[ \hat{S}_{xy} = \left[ \hat{S}_{xy} - \frac{1}{3}(\nabla \cdot \vec{U})\delta_{xy} \right] \] (B.9)

\[ \mu^{s}_{sgs} = (c_{sgs}\Delta)^2 \hat{\rho} |\hat{S}| \] (B.10)

\[ |S_{xy}| = \sqrt{2\hat{S}_{xy}\hat{S}_{xy}} \] (B.11)

A similar set of equation can be obtained by test filtering grid level relations of Smagorinsky model as given in Eq. (B.12) – Eq. (B.15).

\[ \hat{\tau}_{sgs_{xy}} - \frac{1}{3}\hat{\tau}_{sgs_{kk}}\delta_{xy} = -2\mu^{g}_{sgs}\hat{S}_{xy} \] (B.12)

\[ \hat{S}_{xy} = \left[ \hat{S}_{xy} - \frac{1}{3}(\nabla \cdot \vec{U})\delta_{xy} \right] \] (B.13)

\[ \mu^{g}_{sgs} = (c_{sgs}\Delta)^2 \hat{\rho} |\hat{S}| \] (B.14)

\[ |S_{xy}| = \sqrt{2\hat{S}_{xy}\hat{S}_{xy}} \] (B.15)

Subtraction of Eq. (B.8) from Eq. (B.12) yields:

\[ L_{xy} - \frac{1}{3}L_{kk}\delta_{xy} = -2c_{sgs}^2 \hat{\rho} \left( \Delta^2 \hat{S}_{xy} |\hat{S}_{xy}| - \Delta^2 \hat{S}_{xy} |\hat{S}_{xy}| \right) \] (B.16)
This equation provides a way to calculate $C_{sgs}$ as a function of local flow properties in both the space and time. However, the computed viscosity field from this model was found to be highly fluctuating, sometimes resulting negative viscosities as well.

To avoid this problem, Lilly (1992) suggested an averaging procedure using the least square method.

$$M_{xy} = \hat{\rho} \left( \hat{\Delta}^2 \hat{S}_{xy} \left| \hat{\Delta} \hat{S}_{xy} \right| \right)$$  \hspace{1cm} (B.18)

$$C_{sgs}^2 = \frac{\langle L_{xy} M_{xy} \rangle}{\langle M_{xy} M_{xy} \rangle} \hspace{1cm} (B.19)$$

Angle brackets indicate some form of averaging, usually in the homogeneous direction of the flow. In complex flows, where no homogeneous direction exists, time averaging for a small time interval is performed. The test filter width can be of any size larger than the grid filter width. Germano et al. (1991), after a comprehensive study found out $\hat{\Delta}/\Delta = 2$ produces optimum results. However in general, the results are quite insensitive to the test filter width.

**B.1.2 Dynamic $k_{sgs} - \Delta$ Model**

The concept of test filtering and the Germano identity can be easily extended for dynamic determination of model constants in other models as well. Kim et al. (1999) suggested a formulation, in which the two model constants in $k_{sgs} - \Delta$ model are calculated dynamically. This formulation was tested by modelling a gas turbine combustor and reasonably better results were obtained compared to the static version of the $k_{sgs} - \Delta$ model. It should be noted that, this approach does not follow the exact derivation of Germano et al. (1991), instead some of the conclusions are based on experimental evidence.

The test scale kinetic energy $k_{test}$, can be expressed using the Germno et al.’s (1986) redefinition of SGS stress as:

$$k_{test} = \frac{1}{2} \left[ \left( \hat{u} \hat{u} - \hat{u} \hat{u} \right) + \left( \hat{v} \hat{v} - \hat{v} \hat{v} \right) + \left( \hat{w} \hat{w} - \hat{w} \hat{w} \right) \right]$$  \hspace{1cm} (B.20)

Based on the experimental data of Liu et al. (1994), it was shown that $L_{xy}$ can also be modelled in the form of sub-grid stress tensor $\tau_{sgs,xy}$. 

$$L_{kk} = L_{xx} + L_{yy} + L_{zz}$$  \hspace{1cm} (B.17)
Using the least square minimisation technique, the model coefficient $C_v$ can be given by:

$$C_v = \frac{L_{xy}^\prime M_{xy}}{M_{xy} M_{xy}}$$  \hspace{1cm} (B.22)

$$L_{xy}^\prime = L_{xy} - \frac{2}{3} \hat{\beta} k_{test} \delta_{xy}$$  \hspace{1cm} (B.23)

$$M_{xy} = -\hat{\beta} \sqrt{k_{test} \Delta} \left[ \hat{\delta}_{xy} - \frac{1}{3} (\nabla, \vec{U}) \delta_{xy} \right]$$  \hspace{1cm} (B.24)

$C_e$ is also obtained in a similar way.

$$C_e = \frac{\hat{\Delta} \left( \mu + \mu_{sgs} \right) / \mu}{\hat{\beta} (k_{test})^{3/2}} (\alpha \hat{\beta} - \alpha \beta)$$  \hspace{1cm} (B.25)

$\alpha = \sum \tau_{sgs_{xy}}$ and $= \sum \frac{\partial u}{\partial x}$ : where the summation is over all the possible derivatives of velocity components in three dimension. Compared to other methods, several advantages are identified in this formulation. In Eq. (B.22), $C_v$ is calculated without any form of averaging. This is not possible with the dynamic Smagorinsky model, because $M_{xy}$ in Eq. (B.18) can locally be zero or negative arising an ill-posed condition. As a result, some form of averaging with algorithmic adjustments is essential. Conversely, with the present form of $M_{xy}$ in dynamic $k_{sgs} - \Delta$ model, such mathematical inconsistency is avoided ensuring $C_v$ is always positive.

### B.1.3 Discretised Form of Filtering

It should be noted here that LES governing equations are derived by filtering the unsteady Navier-Stokes equations. Therefore, no specific filtering operation is required within the computation code. However, if dynamic LES models are used, test filtering is required where grids filtered terms are explicitly filtered by a secondary filter. Traditionally, Gaussian and Box filter kernels are mainly used for this purpose.

Filtering is mathematically equivalent to spatial averaging. In numerical computations, filtering is performed by weighted averaging the flow properties within the filter domain. For
a symmetric filter kernel with \( 2m + 1 \) point stencils, the discrete finite deference filtering operation can be defined as:

\[
\hat{\phi}_i = \sum_{n=-m}^{m} a_n \hat{\phi}_{i+n}
\]  

(B.26)

\[
\sum_{n=-m}^{m} a_n = 1
\]  

(B.27)

Weighting coefficients are calculated by converting the filter kernel in to discrete form by expanding in a Taylor series. Discretised form of a 4\(^{th}\) order Gaussian filter can be written as (Garnier et al. 2009):

\[
\hat{\phi}_i = \frac{\epsilon^4 - 4\epsilon^2}{1152} (\hat{\phi}_{i+2} + \hat{\phi}_{i-2}) + \frac{16\epsilon^2 - \epsilon^4}{288} (\hat{\phi}_{i+1} + \hat{\phi}_{i-1}) + \frac{\epsilon^4 - 20\epsilon^2 + 192}{192} \hat{\phi}_i
\]  

(B.28)

where, \( \epsilon \) is the ratio between the filter cut-off scale and the mesh size. Second order Gaussian filter for \( \epsilon = 2 \) may be reduced to

\[
\hat{\phi}_i = \frac{1}{6} (\hat{\phi}_{i-1} + 4\hat{\phi}_i + \hat{\phi}_{i+1})
\]  

(B.29)

with box filtering, the tradition is to use three point symmetric filter given by:

\[
\hat{\phi}_i = \frac{1}{4} (\hat{\phi}_{i-1} + 2\hat{\phi}_i + \hat{\phi}_{i+1})
\]  

(B.30)

Hence, if these formulae are adopted for test filtering, \( \hat{\phi} \) represent a conventional LES filtered quantity and \( \hat{\phi}_i \) denotes a test filtered quantity. \( \epsilon \) is equivalent to the filter width ratio given by \( \hat{\Delta}/\Delta \).

Usually in LES, test filtering only up to second order is used. Hence for example, a total of 27 adjacent cells, including the centre cell, are considered, when test filtering in a structured three dimensional hexahedral mesh, where a maximum of 8 cells are attached to a given node. A two dimensional view of the test filter domain with a filter width ratio of 2 in a structured hexahedral mesh is shown in Figure B.2.
Filtering in three-dimension is mathematically equivalent to the consecutive application of the corresponding one-dimensional filter in the three directions. Hence, in computer codes, this procedure is often adopted. Figure B.2 corresponds to the test filtering of cell centred flow variables. Whereas, for vertex associated variables, such as the velocity field, interpolation of nodal values into the cell centres is required prior to test filtering is performed. Subsequently, the resultant cell centred values maybe re-interpolated, back onto the cell vertices. Further, in variable density flows, test filtering should also be appropriately density weighted.

**B.1.4 Test Filtering in Unstructured Hexahedral Grids**

The above procedures cannot be directly applied in an unstructured grid, due to a couple of reasons. Mainly the number of cell elements attached to a node is not definite and may be higher or lower than 8. In addition, there may not be such elements located in due East \((i+1)\) or West \((i-1)\) directions. Hence, a slightly different procedure is adopted. Often, in LES calculations, linear filtering is used. Gaussian filters are used only in test filtering of combustion related quantities. In fact, test filtering in combustion modelling requires somewhat advanced methods due to conceptual reasons. Thus, test filtering procedures in this section apply only for linear test filtering in LES flow calculations. Techniques of test filtering in combustion modelling are described in the next chapter.

Shown in Figure B.3 is a two dimensional view of a typical cell configuration in an unstructured hexahedron grid. In the present procedure, cell centred variables are initially
averaged (interpolated) on to the nodes as give in Eq. (B.31) using equal weights. Represented by \( n \) is the number of cell elements attached to the node \( \varphi_j \). This number may vary from node to node depending on the local mesh distribution. In a similar way, all 8 (for a hexahedron cell) \( \varphi \) values can be calculated. Subsequently, the \( \varphi \) values are averaged with equal weights, in to the cell centres, in order to obtain the test-filtered value following the relation given in Eq. (B.32). The summation is over the all 8 eight nodes of the cell.

\[
\varphi_j = \frac{1}{n} (\hat{\varphi}_1 + \hat{\varphi}_2 + \cdots + \hat{\varphi}_i + \cdots + \hat{\varphi}_n)
\]

(B.31)

\[
\hat{\varphi}_i = \frac{1}{8} \sum_{j=1}^{8} \varphi_j
\]

(B.32)

In the case of test filtering node-associated quantities, such as velocity components, the node values are interpolated into the cell centres prior to test filtering. Subsequently, those intermediate test filtered values located in cell-centred are interpolated back on to cell nodes. This interpolation procedure has been successfully applied in IC engine non-reacting flow modelling with the dynamic Smagorinsky model by Haworth & Jansen (2000). Several other alternative methods, especially for unstructured tetrahedron grids, have also been suggested by Jansen (1994). Many of these methods are only suggestions and not adequately validated.
NOMENCLATURE

Alphanumeric Symbols

\( \mathcal{A} \) - Surface area vector
\( A \) - Total flame area
\( \bar{c} \) - Mean progress variable
\( c_p \) - Constant pressure specific heat capacity
\( c_v \) - Constant volume specific heat capacity
\( C \) - Isentropic speed of sound
\( C_D \) - Diffusion Courant number
\( C_{kk} \) - Cross stress term
\( COV \) - Coefficient of Variation
\( d \) - Distance
\( d_e \) - Inter electrode distance
\( \mathcal{D} \) - Diffusivity
\( D \) - Fractal dimension
\( D_l \) - Fractal dimension for a smooth flame surface
\( D_t \) - Maximum fractal dimension for a turbulent flame surface
\( D_Q \) - Non-dimensional normalized quenching distance
\( Da \) - Damköhler number
\( E \) - Total internal energy, Activation energy, Turbulence kinetic energy corresponding to a given wave number
\( f_{wall} \) - Heating rate per unit area of wall
\( f_x \) - Flamelet crossing frequency
\( F \) - Force
\( g \) - Gravitational acceleration
\( h \) - Enthalpy
\( h_c \) - Convective heat transfer
\( i \) - Unit vector in \( x \)-direction
\( I \) - Specific internal energy
\( \mathbb{I} \) - Unit tensor
\( I_0 \) - Stretch factor
\( I_{QR} \) - Quenching rate parameter
\( j \) - Unit vector in \( y \)-direction
\( k \) - Unit vector in \( z \)-direction, Turbulence kinetic energy, Coefficients of Arrhenius reaction rate
\( \mathcal{K} \) - Thermal conductivity
\( K \) - Effective strain rate
\( K_a \) - Karlovitz number
Nomenclature

\( K_C \) - Curvature stretch rate
\( K_C^r \) - Concentration equilibrium constant
\( K_T \) - Turbulent strain rate (Karlovitz stretch factor)
\( l \) - Characteristic length
\( L \) - Length
\( L_e \) - Lewis number
\( L_G \) - Gibson scale
\( L_f \) - Active length of the flame front
\( L_i \) - Integral length scale of turbulence
\( L_{Ma} \) - Markstine length scale
\( L_q \) - Quenched length of the flame front
\( L_{xy} \) - Leonard stress term
\( L_y \) - Integral scale of flame wrinkling
\( L_x \) - Dissipation length scale
\( L_\lambda \) - Taylor micro scale
\( m_k \) - Flame kernel mass
\( \dot{m}_k \) - Rate of change of flame kernel mass
\( M \) - Mass of a control volume
\( n \) - Unit wall normal vector
\( n \) - Polytropic index
\( n_y \) - Number of flamelet crossings per unit length
\( N \) - Number of particles, Total number of species
\( N \) - Unit normal vector
\( p \) - Pressure
\( Pe \) - Peclet number
\( Pr \) - Prandtl number
\( q \) - Heat flux vector
\( Q \) - Energy/Heat source
\( r \) - Radius of the spherical flame
\( r_k \) - Equivalent flame kernel radius
\( R_{kk} \) - SGS Reynolds stresses
\( Re \) - Reynolds number
\( R_f \) - Residual gas mass fraction
\( R_{th} \) - Theoretical flame radius
\( R_u \) - Universal gas constant
\( S \) - Closed surface area, Flame speed
\( S_C \) - Consumption speed
\( S_D \) - Displacement speed
\( S_C \) - Schmidt number
\( S_l^0 \) - Unstrained laminar burning velocity
\( t \) - Time
\( t_\eta \) - Kolmogorov time scale
\( T_{0G} \) - Characteristic time
\( T \) - Temperature
\( T \) - Transpose
\( T_{xy} \) - SGS stresses
\( u \) - Velocity component in \( x \)-direction
\( u_\eta \) - Kolmogorov velocity
\( \nu \) - Relative flow field velocity
**Nomenclature**

- $U$ - Velocity, Internal energy
- $v$ - Velocity component in $y$-direction
- $V$ - Diffusion velocity, Volume
- $V_d$ - Displacement volume
- $V_m$ - Diffusion velocity
- $w$ - Velocity component in $z$-direction
- $W$ - Molecular weight, Wave number
- $y$ - Distance from the solid wall
- $Y_m$ - Mass fraction of species $m$

**Greek Letters**

- $\gamma$ - Heat capacity ratio
- $\delta_c$ - Inner cut off scale
- $\delta_l$ - Laminar flame thickness
- $\delta_{xy}$ - Kronecker delta
- $\varepsilon$ - Rate of dissipation of turbulent kinetic energy
- $\zeta$ - Local wall Reynolds number, Temperature exponents
- $\zeta'$ - Characteristic temperature Reynolds number
- $\eta$ - Unit normal vector, Efficiency, Kolmogorov scale
- $\theta$ - Angle
- $\lambda$ - Second viscosity
- $\mu$ - Dynamic molecular viscosity
- $\mu'$ - Bulk viscosity
- $\mu_t$ - Eddy viscosity or turbulent viscosity
- $\rho$ - Density
- $\sigma''$ - Fluctuating component of the viscous stress tensor
- $\tau$ - Viscous stress tensor, Heat release factor
- $\tau_c$ - Chemical time scale
- $\tau_t$ - Representative time scale
- $\varphi$ - Weighting power of the inverse distance interpolation
- $\phi$ - Equivalence ratio, A general flow property
- $\phi_D$ - Variable implicitness parameter for scalars
- $\phi_p$ - Variable implicitness parameter for pressure
- $\psi$ - A general flow property
- $\bar{\omega}_{m,s}$ - Consumption rate of species $m$
- $\bar{\omega}$ - Unburned mass consumption rate per unit volume
- $\dot{\omega}_r$ - Reaction rate
- $\omega_x$ - Reaction rate per unit flamelet crossing
- $\hat{\Delta}$ - Filter width
- $\hat{\Delta}$ - Test filter width
- $\Delta_c$ - Combustion filter width
- $\bar{\Delta}_e$ - Effective filter width
- $\Theta_{sgs}$ - SGS scale molecular diffusion fluxes
- $\Xi$ - Flame wrinkling factor
- $\Sigma$ - Flame surface density
- $\Phi$ - SGS convective mass fluxes
- $\Omega$ - Global filter domain
Subscripts

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Superscripts

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Abbreviations

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References


References


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*Loughborough University*


Xu J., Behrendt F. and Warnatz J. (1994) 2D-LIF Investigation of Flame Kernel Development during Spark Ignition, COMODIA.


