Large Eddy Simulation of a High Aspect Ratio Combustor

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Dedicated to my family,

Babaannem, Annem, Babam, Selçuk, Ajda, Zeynep ve güzel eşim Betül,

for their support and love
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LIST OF SYMBOLS AND ABBREVIATIONS

Roman Symbols

\( c \) Speed of sound

\( c_p \) Specific heat at constant pressure per unit mass

\( c_v \) Specific heat at constant volume per unit mass

\( E \) Total energy per unit mass

\( H \) Total enthalpy per unit mass

\( k^{sgs} \) subgrid kinetic energy per unit mass

\( Le \) Lewis number

\( p \) Pressure

\( Pe \) Peclet number

\( Pr \) Prandtl number

\( R \) Gas constant

\( T \) Temperature

\( t \) Time

\( u_i \) Cartesian velocity vector component

\( W_k \) Molecular weight of species \( k \)

\( x, y, z \) Cartesian coordinate directions

\( x_i, \) Cartesian coordinate directions in indicial notation (\( i = 1 \ldots 3 \), for \( x, y \) and \( z \), respectively)

\( Y_k \) Mass fraction of species \( k \)
Greek Symbols

$\eta$  \hspace{1cm} Kolmogorov length scale

$\gamma$  \hspace{1cm} ratio of specific heats

$\kappa$  \hspace{1cm} thermal conductivity

$\mu$  \hspace{1cm} dynamic viscosity

$\nu$  \hspace{1cm} kinematic viscosity, $\mu/\rho$

$\Phi$  \hspace{1cm} equivalence ratio

$\rho$  \hspace{1cm} density

$\tau_{ij}$  \hspace{1cm} viscous stress tensor

$\varepsilon$  \hspace{1cm} turbulent kinetic energy dissipation rate

$\rho$  \hspace{1cm} Density

Superscripts

$n$  \hspace{1cm} Time step index of the numerical integration

$sgs$  \hspace{1cm} Subgrid scale

Subscripts

$0$  \hspace{1cm} Reference quantity

$sgs$  \hspace{1cm} Subgrid scale

$t$  \hspace{1cm} Turbulent quantity

Other Symbols

$f$  \hspace{1cm} Integral operator

$\nabla$  \hspace{1cm} Gradient operator
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\partial$</td>
<td>Partial derivation operator</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>Summation operator</td>
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**Acronyms**

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AR</td>
<td>Aspect Ratio</td>
</tr>
<tr>
<td>ATDC</td>
<td>After Top Dead Center</td>
</tr>
<tr>
<td>BDC</td>
<td>Bottom Dead Center</td>
</tr>
<tr>
<td>CFD</td>
<td>Computation Fluid Dynamics</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>EBU</td>
<td>Eddy Break-Up</td>
</tr>
<tr>
<td>HC</td>
<td>HydroCarbon</td>
</tr>
<tr>
<td>IC</td>
<td>Internal Combustion</td>
</tr>
<tr>
<td>ISAT</td>
<td>In Situ Adaptive Tabulation</td>
</tr>
<tr>
<td>LDKM</td>
<td>Localized Dynamic $k^{sgs}$ Model</td>
</tr>
<tr>
<td>LEM</td>
<td>Linear-Eddy Model</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>MPI</td>
<td>Message Passing Interface</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds-Averaged Navier-Stokes</td>
</tr>
<tr>
<td>SI</td>
<td>Spark Ignition</td>
</tr>
<tr>
<td>TDC</td>
<td>Top Dead Center</td>
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<tr>
<td>UHC</td>
<td>Unburned HydroCarbon</td>
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SUMMARY

The present research investigates the details of mixture preparation and combustion in a two-stroke, small-scale research engine with a numerical methodology based on large eddy simulation (LES) technique. A major motivation to study such small-scale engines is their potential use in applications requiring portable power sources with high power density.

The investigated research engine has a rectangular planform with a thickness very close to quenching limits of typical hydrocarbon fuels. As such, the combustor has a high aspect ratio (defined as the ratio of surface area to volume) that makes it different than the conventional engines which typically have small aspect ratios to avoid intense heat losses from the combustor in the bulk flame propagation period. In most other aspects, this engine involves all the main characteristics of traditional reciprocating engines. A previous experimental work has identified some major design problems and demonstrated the feasibility of cyclic combustion in the high aspect ratio combustor. Because of the difficulty of carrying out experimental studies in such small devices, resolving all flow structures and completely characterizing the flame propagation have been an enormously challenging task. The numerical methodology developed in this work attempts to complement these previous studies by providing a complete evolution of flow variables.

Results of the present study demonstrated strengths of the proposed methodology in revealing physical processes occurring in a typical operation of the high aspect ratio combustor. For example, in the scavenging phase, the dominant flow structure is a tumble vortex that forms due to the high velocity reactant jet (premixed) interacting with the walls of the combustor. Since the scavenging phase is a long process (about three quarters of the whole cycle), the impact of the vortex is substantial on mixture preparation for the next combustion phase. LES gives the complete evolution of this flow structure, from its beginning to its eventual decay after the scavenging period is over. In addition, LES is able to predict the interaction between the bulk flow at top dead center (TDC) and the turbulent
flame propagation. The success of this depends on the ability of the model in predicting turbulent flow structure including its length and velocity scales.

Another contribution of the LES analysis of this engine has been to determine the operating conditions (such as mass flow rate, trapping efficiency etc.) with as little uncertainty as possible. This aspect is perhaps one of the major strengths of the present methodology since determining these parameters in the experimental work proved to be a problem because of the limitations in accessing the flow.

Furthermore, LES findings were compared to $k - \varepsilon$ model predictions to assess the advantages of the proposed methodology in periodic flows. For example, in direct contrast to LES, $k - \varepsilon$ model predicted a highly smeared mean flow at all phases of the combustor, hence completely masking the unsteady character of the flow. It also proved to be more grid dependent than LES in predicting the combustion rate. In addition, the known deficiency of $k - \varepsilon$ model in predicting cycle-by-cycle variations has been shown for this particular engine. These observations regarding the quality and the nature of numerical predictions confirmed the expectations that LES may be the only option as a truly realistic tool for the analysis of this type of small-scale engine.
CHAPTER 1

INTRODUCTION

1.1 Background and Motivation

The internal combustion (IC) engine has contributed tremendously to the development of the civilization since its invention in the late 19th century. With little modification in working principles, it has become widespread in many aspects of the modern life as a dependable mechanical power generator. Equally important has been the rapid advances in the use of electrical power, with portable batteries as a prime example of its power in providing mobility to the end user.

Portable batteries, however, has the disadvantage of having a low power density. Power density is the ratio of the power available from a battery to its weight or volume. In certain applications or use of this technology, however, this feature is a liability and alternative portable energy producing technologies have been aggressively sought. In particular, small electrical power generators exploiting the repeatable and cyclic nature of IC engine have been recently suggested in many different forms [1, 29, 17].

In IC engines, the power is obtained as a result of a working fluid displacing the boundary (or chamber) that encloses the working fluid. More specifically, the engine chamber, with one side attached to a power transferring component (or piston), expands this boundary after the pressure in the chamber is higher than any opposing force (i.e., crankcase pressure, friction etc.). The pressure in the chamber increases mainly due to the combustion process. Combustion is an exothermic process in which fuel reacts with oxygen to release heat and is essential to engine operation. The IC engine combustion is initiated either by external heat addition (i.e., spark) or compression, whereby, the elevated temperature due to compression causes an explosion. Thus, there are two main types of IC engine: spark-ignition (SI) and compression ignition (diesel). In order for combustion to take place, the fuel and the oxidizer (oxygen) should be mixed at the molecular level. In SI engines, the fuel and air is
already mixed (hence the name premixed) prior to combustion. In the diesel engines, the fuel is introduced into the chamber in the form of liquid jet just before ignition. The fuel then should rapidly atomize to mix with the already present oxygen to form a combustible mixture.

Cyclic nature of IC engines is maintained by repeating 4 distinct phases that characterize their operation: (a) Charge preparation, (b) Compression, (c) Expansion, and (d) Exhaust. How this cycle of events is accomplished determines another classification type based on stroke. A stroke can be defined as the linear motion of the piston that is equivalent to 180 degrees revolution with respect to a reference point. In general, IC engine applications use either two-stroke or four-stroke cycle designs. The primary difference between the two is the way gas exchange process is accomplished. Each distinct phase has its own stroke in four-stroke engines. In contrast, some of the phases have significant overlaps with each other in two-stroke engines, for example, between (a)-(b) and (c)-(d)-(a).

One recent concept, shown schematically in Figure 1.1, that exploits the repeatability of IC engines was envisioned to provide a cheap and high power density alternative to traditional portable power generators. It consists of a free piston that is set into sustained oscillation by out-of-phase heat release in two opposed high aspect ratio (AR) combustors. Here, AR is defined as the area of the combustor to its volume. This device is placed inside a permanent magnetic coil where the motion of the piston leads to electric power generation [54].

With Micro-Electro-Mechanical Systems (MEMS) manufacturing techniques, the cost of such projects can be economical, provided simplified geometries are used in designing the engines. From manufacturing point of view, rectangular planforms are ideal candidates. Another desired requirement is to have less obtrusiveness [19]. This can be achieved by rectangular and flat (i.e., thin) chambers. Such a combustor would have a high AR. Hence, the combustion process in such chambers are expected to be different than the conventional engines which typically have small aspect ratios to avoid intense heat losses from the combustor in the bulk flame propagation period.
Figure 1.1: Schematic of a dual combustor power-generator. Also shown is the magnetic array.

How intense this adverse heat transfer effect would manifest itself depends on the selected spanwise dimension of the combustor. For example, the design dimensions comprising the planform area (i.e., the length and the width) can be expected to be influenced by thermodynamic cycle constraints or fluid mechanical considerations (i.e., methodology chosen to fill the chamber with fuel in intake stage and to purge the combustion products during exhaust stage). The final spanwise dimension is likely to be a function of the mass (or volume) of the combustible mixture at design conditions. The worst case scenario would occur when the thickness of the combustor is close to quenching limits of the fuel. In most other aspects, this conceptual engine involves all the main characteristics of traditional reciprocating engines. Given the complexity of internal combustion engine physics in general and the additional high AR effect for this engine in particular, it poses design challenges that need to be addressed by extensive studies.

The feasibility of this power generator concept depends on achieving repeatable combustion in small enclosures. A recent work by Faulkner [23] has investigated the combustion process in constant volume combustors that have rectangular planforms with spanwise dimensions of 12 mm, 6.35 mm and 3.125 mm. The emphasis in that study was on achieving flame propagation in the quenching limit. Heat transfer through and radical removal at the
walls were identified experimentally as major causes for the limited pressure rise following combustion in the chamber [23].

Subsequent work by Disseau [19] aimed at realizing cyclic combustion in a simpler configuration without coupling the two opposed high AR combustors. To this end, a research engine has been built to study the dynamics of cyclic combustion [19]. This device consists of a single combustor-spring configuration (Figure 1.2). A piston made of cast iron moves in a flat steel cylinder with optical access through Pyrex windows. The piston motion valves the inlet and exhaust ports and also triggers an ignition spark (approximately 200 mJ across 2 mm in less than 300 microseconds) generated by an automotive ignition circuit. To limit leaks, a dynamic wiper seal made of a double layer of Teflon-coated fiberglass is used along the longer sides. A split piston (whose two halves are pushed against the side walls by a spring) seals along the side walls while leaving a gap in its center, which is itself sealed by the dynamic frontal seal. Sealing is further improved using Diester synthetic oil.

The simplified design of Disseau [19] has demonstrated that cyclic and repeatable combustion is possible in very small and thin enclosures. This test engine is a two-stroke linear
generator and share many basic features of conventional larger scale engines. Several difficulties needed to be overcome in the design process, in particular with respect to scavenging and mass loss issues. In the working final version, the cyclic operation is started by pulling the piston back against the spring using a handle. This opens the inlet and exhaust ports and allows the combustion chamber to fill with fresh propane-air mixture, which is injected at an angle. When the handle is released, the spring propels the piston forward. Once the ports close, the mixture is compressed and then ignited by the spark. The subsequent pressure increase decelerates and eventually reverses the piston’s motion. Eventually, the ports re-open, the combustion products exhaust and fresh reactants enter the chamber. The spring is compressed until the piston motion is reversed and the cycle restarts.

These previous studies have concentrated on heat transfer effects in the quenching limit and its effect on cyclic combustion. Much has been learned about physical principles as well as manufacturing practices. For example, one striking difference between the constant volume combustor and the simplified engine studies is the combustion duration, being smaller by a factor of 3 in the latter. As pointed out by Disseau [19], the observed difference in combustion durations is due to the turbulence levels, wall heating and leakages. The impact of turbulence on the combustion duration has been realized since early times in combustion research. Similarly, the effect of wall temperature on heat transfer rates during combustion is well known. Therefore, from a combustion point of view, the levels of these quantities are of great importance at the time of ignition. While the turbulence levels and wall temperature is strongly modified in all phases of the cycle, their evolution during the scavenging phase is especially critical due to their impact on flame propagation characteristics.

However, this critical aspect of the cycle, mixture preparation, has been addressed only in limited extent. Mixture preparation, also called scavenging, involves all aspects of flow development from Exhaust Port Opening (EPO) to Exhaust Port Closure (EPC). In this phase, burned products from the previous cycle are purged and fresh reactants are filled. However, this process is imperfect, especially so in two-stroke engines, leading to dilution of the charge. Also, because of the short-circuiting seen in two-stroke engines employing port based scavenging strategies, the efficiency of the scavenging phase in terms of mass delivered
versus mass retained is not optimal. Furthermore, turbulence intensities in the combustor is strongly modified during scavenging phase, due to the injection of fresh reactants and their subsequent formation of large scale vortical structures. Depending on the design, these structures may persist up to the ignition timing [85].

From above observations, it is clear that further research is needed, both in terms of understanding the important parameters in the combustion process and applying this increased knowledge in realizing the power generator concept.

1.2 Issues Relevant for IC Engine Physics

1.2.1 Turbulence Generation Mechanisms

High turbulence intensities at the time of ignition promote fast burning [42, 34] and therefore are very desirable in IC engines, since the allowed time for combustion is very short (on the order of milliseconds). Generally speaking, the turbulence intensity is predominantly influenced by the injection strategy. For example, the turbulence structure created by a jet from a ported engine versus valved engine would be different, in terms of their impact on the large scale structures. Despite these differences, however, the increased shear generation during the intake phase between the reactant jet and in-cylinder mass is a common source of turbulence. This is basically called turbulence generation by shear production [57].

Another source of turbulence is the compression and the disintegration of large scale structures that forms in the intake phase. In the literature, two distant large scale structures that result in higher turbulence intensities are identified: swirl [46] and tumble [6, 84]. Swirl is characterized by a vortical structure whose rotation axis is in the direction of piston motion. The rotation axis of tumble (also called “barrel swirl” [85]) is, however, perpendicular to the direction of piston motion. In most engines, the global behavior and effect of these structures are similar. For example, in the intake, there is a progressive accumulation of kinetic energy. This kinetic energy decays during compression and just before the top dead center (TDC), these highly anisotropic structures persist on much smaller scales.

There are other strategies employed to increase TDC turbulence, mostly based on some
modification of piston-cylinder assembly. For example, bowl-in-piston geometries have been used in Gasoline Direct Injection (GDI) engines or Diesel engines. In engines with bowl-in-piston, the interaction of swirl structures with the bowl creates squish regions with high strain rates and consequent increase in turbulence levels.

Experimental observations indicate that the intensity of turbulence scales with engine speed [35]. The specifics of the scaling, however, depend on the engine geometry and intake methodology. For example, in valved engines, the flow rate is a function of the engine speed [42] and therefore some dependence on the engine speed is expected. A common finding for valved engines without swirl is that the turbulence intensity at TDC is about half the mean piston speed [42]. With additional turbulence generation mechanisms (i.e., swirl, tumble, squish etc.), this scaling is no longer correct [42]. In ported engines, turbulence intensities are usually larger, since the time for turbulence decay process (between the end of intake and TDC) is shorter [11]. However, in any case, there seems to be an upper limit due to increased damping effect of the walls with higher turbulence levels [11].

It must be noted that there is no consensus in the literature on how turbulence should be defined in periodic flows. The conventional understanding defines turbulence as the fluctuating component between the instantaneous velocity and its ensemble-averaged value [14]. An analysis based on determining turbulent fluctuations in this way is called “ensemble-averaged decomposition”, in which the the cycle-mean (as a function of crank angle window) is not recognized as a relevant quantity. However, it has been argued that the cycle-mean may exhibit large variations between cycles, and therefore turbulence from the ensemble-averaged decomposition may be unphysically large [11]. A more realistic description is to differentiate variations in the cycle-mean over many cycles and in the fluctuations about the cycle-mean. Hence, “Cycle-resolved decomposition” defines turbulence as the fluctuating component between the instantaneous velocity and the cycle-mean. As a result, cyclic changes can be defined based on the difference between the cycle-mean and the ensemble-averaged mean. A more comprehensive description and the related mathematical formulation on engine turbulence are given in Appendix B.
1.2.2 Cycle-by-Cycle Variations

All engines in practical applications exhibit cycle-by-cycle variations (CCV) in their power output. In broader terms, the concept of cyclic changes is related to how turbulence is defined in the context of periodic flows.

It is clear from above observations that cyclic changes occur only in the cycle-resolved decomposition paradigm. Heywood [44] lists several causes of cyclic variations, as given in Table 1.1. This is a comprehensive list in the sense that some of the factors influencing CCV are interrelated. For example, items c, d, e and g are all turbulence related. Similarly, items b and h are related to bulk flow motion. Hence, bulk flow structure and turbulence characteristics near the ignition location are mainly responsible for CCV [44, 47, 48]. Therefore, engines can not be made free from cyclic changes and it is important that any particular design accounts for its effect on the performance.

Early stages of ignition and the subsequent delay period are occurring in laminar conditions until the flame reaches sizes comparable to integral scales of the bulk flow. Here, the process is strongly non-adiabatic and heat losses determine spark energy deposition rate, which becomes cycle dependent because of the local turbulence characteristics near the plug. However, the variability caused exclusively by spark energy deposition rate is negligible with modern ignition systems [47]. Also, in the early stages with ignition kernel less than about 10 mm [44], the bulk flow is able to convect the flame kernel away from the ignition zone, distorting the spherical like structure of the flame [48]. This indicates that turbulence is influencing the flame surface, changing its shape to become more convoluted and wrinkled. Flame convection in the early stages is a major cause of CCV, changing the dynamics of the subsequent bulk flame propagation period [48, 64].

This early phase in the flame development is clearly affected markedly by the bulk flow and shows dependence on cyclic changes in the structure of the bulk flow near TDC and around the spark plug. After this initial phase, the flame becomes increasingly larger and turbulence is less able to convect the flame. However, the influence of turbulence characteristics of the flow now determines if the combustion burn rate is fast or slow in the main burn period. It is obvious that a fast combustion will decrease the cyclic changes [12]
Table 1.1: Causes of SI engine cycle-by-cycle variations, reproduced from Heywood [44]. Each of these, primarily, affects (1) the early stages of flame development, (2) the main flame propagation process, or (3) the later stages of combustion.

| (a) Spark energy deposition gas (1) |
| (b) Flame kernel motion (1,3) |
| (c) Heat losses from kernel to spark plug (1) |
| (d) Local turbulence characteristics near plug (1) |
| (e) Local mixture composition near plug (1) |
| (f) Overall charge composition—air, fuel, residual (2,3) |
| (g) Average turbulence in the combustion chamber (2, 3) |
| (h) Large-scale features of the in-cylinder flow (3) |
| (i) Flame geometry interaction with the combustion chamber (3) |

since this will prevent the flow structure to have time to affect the combustion period. This in turn requires that the flow (i.e., the turbulence structure) is nearly homogeneous with high turbulence intensity. However, the turbulence intensity should not be too high to cause quenching due to stretch [56] since quenching may lead to misfire (a cycle with no apparent heat release).

1.3 Numerical Methods in IC Engine Applications

Requirements of predicting engine output necessitated mathematical analysis even in the early period of IC engines. Review by Heywood [41] provides with the early efforts (late 19th century to mid 20th century) in IC engine modeling, which typically involve simple cycle analysis to estimate operating conditions and efficiency parameters. Modern understanding of engine analysis, however, has dramatically changed with the advent of computers. A contemporary classification of numerical methods in IC engines is given by Heywood [41] based on the suggestions by Bracco [10]. According to this, there are three basic groupings in IC engine modeling (with Heywood’s nomenclature):

(i) zero-dimensional models where thermodynamic relations and approximations (heat
transfer, burn rate etc.) are applied to the entire cycle or parts of the cycle to obtain order of magnitude analysis for parameters of interest. These group of techniques typically return fast results, and are still used in initial design work of IC engines.

(ii) quasi-dimensional models where physical arguments relating turbulence to combustion are used to have a more realistic account of combustion period

(iii) multidimensional models where governing equations of fluid motion are solved (with models and approximations) for the engine geometry of interest. These efforts can be one, two or three dimensional, depending on the accuracy needed from the analysis. Obviously, even the three dimensional simulation may not be correct, if correct simplifications are not used and if the geometric fidelity of the engine is not observed in the numerical simulations.

1.3.1 Multidimensional Methods

In principle, Navier-Stokes (NS) equations that represent the conservation principles as applied to flow variables can be used to solve combustion problems since they are general and applicable to both reacting and non-reacting flows. There are two main aspects to typical combustion processes that need to be addressed: the turbulent nature of the bulk flow and the heat release due to the combustion process. Analysis of either one of these phenomena is complex by itself. Moreover, the fact that they are strongly coupled to each other is an additional complexity. This coupling is strongly nonlinear and mathematically expressed as a chemical source term in the conservation equations.

In theory, both turbulence and chemical kinetics (as a basic science related to combustion) should not pose any challenge. This is because both of their respective theoretical principles have long been known. For example, turbulence is fully incorporated in Navier-Stokes equations and chemical kinetics (of species) have been available for mechanisms of interest to combustion with sufficient accuracy for a long time. In order to address both turbulence and heat release without any model, smallest hydrodynamic and chemical scales need to be resolved on the numerical grid. Since this is not possible due to computational resources, models are developed to simulate the effect of turbulence and chemistry on the combustion process. This development activity is still an ongoing process.
A flow simulation that employs NS equations discretized on a computational mesh (grid) without any “model” is called Direct Numerical Simulation (DNS). A DNS attempts to resolve all scales of the flow, both time and spatial, from energetic largest scales (identified here as $L_t$) to the smallest Kolmogorov scales ($\eta$). Small scales are affected most by viscous dissipation (i.e., viscous forces) while large scales (and their characteristics) are determined by bulk flow (inertial forces) and boundary conditions. The Reynolds number, defined as $Re = \rho UL_t/\mu$, determines the relative importance of these two competing forces. Turbulent flow, characterized by random eddies and fluctuations, occurs when the Reynolds number is high. The critical $Re$ number at which transition to turbulence happens depends on both geometry and bulk (or mean) flow. At high Reynolds numbers (i.e., turbulent flow), the separation between these scales are wide apart, and the ratio $L_t/\eta$ is large. This ratio is a function of Reynolds Number, and scales as $Re^{3/4}$. Most industrial applications require that all three dimensions of the flow be resolved. In that case, the required number of grid points (an indication of how finely the domain is divided into smaller volumes) scales as $Re^{9/4}$. At present, computational resources allow simulation of modest $Re$ numbers (about 10000). However, a typical combustor (for instance, an IC engine) has a $Re$ number on the order of 100000 or above. Hence, a DNS of such high $Re$ number flows is computationally very demanding.

It must be noted that the level of accuracy (and detail) obtained by DNS is usually not necessary for industrial applications. Rather, predicting the mean flow and its lower order statistics is of prime importance since these usually suffice for successful prediction of complex 3D flows. There are two approaches that attempt to provide the optimal detail (not in the strictest sense since what is optimal is problem specific) using a modified (averaged) form of NS equations. When the averaging is done over time or an ensemble of equivalent flows, the resulting equations are called Reynolds Averaged Navier-Stokes (RANS) equations. This type of simulation is also called Reynolds Averaged Simulation (RAS). If, on the other hand, one uses a spatial filter to average the NS equations, Large Eddy Simulation (LES) equations are obtained. Averaging (in both RAS and LES sense) results in correlations of variables (i.e., velocity, pressure etc.) that require closure. The closure is
obtained by devising approximations (e.g., gradient diffusion hypothesis) to these correlations and introduces errors. This is one of the factors that will determine if the averaged equations are a good working replacement for DNS. Another obvious factor is relaxing the requirement that all scales must be resolved.

At present, RANS is the model of choice for practical applications due its robustness and less stringent numerical grid requirements. However, the level of detail (including emission characteristics and unsteady features) demanded by recent regulations for more efficient combustion devices can not be met by statistical RANS methods. Furthermore, when resolving the wall is absolutely required, the advantages of RANS are less clear. Therefore, with its inherent potential in addressing these outstanding issues, LES has been increasingly favored by practitioners, in parallel with the advances in computational resources.

1.3.2 Literature Review

Because of the limited scope of zero-dimensional and quasi-dimensional models, the present review of numerical IC engine applications is limited to multidimensional models. However, introductory texts [94, 43] may serve as a good starting point for zero-dimensional design methodologies. Because of the large volume of work in the IC engine literature, only representative work will be cited, without being too specific.

1.3.2.1 Pre-1980

Heywood [41] summarizes developments prior to 1980. This period is dominated by applications of simple turbulence models in predicting motored or firing engine cycles, mostly in one-dimensional or two-dimensional (axisymmetric) configurations. Turbulence models are generally algebraic eddy viscosity models, with time dependent diffusivities [83, 91]. Engine geometries are usually simplified, both in the main body as well as around intake or exhaust valves. The first three dimensional engine study with all four strokes using Computational Fluid Dynamics (CFD) is reported by Griffin et al. in 1978 [32]. Combustion is modeled by constant-volume heat addition. Major finding of that study is the strong coupling between localized combustion and the recirculating flow structures in the piston [32]. This study, however, did not simulate turbulence effects, limiting the applicability of the simulation to
1.3.2.2 1980-1990

The next decade, 80’s, witnessed major developments in IC engine CFD work as evidenced in the scope of the work done [22]. Advanced algorithms to accurately simulate three-dimensional geometries as well as rapid advances in computational resources have enabled researchers to use larger grid densities (although still far from resolving wall regions and high gradient regions) in their simulations, typically on the order of 20000-200000 finite volume cells [22]. In parallel to these developments, advanced turbulence models are increasingly used. $k-\varepsilon$ model, originally developed for incompressible flows, were extended to compressible IC engine flows [71, 86, 21]. Numerous other studies employing $k-\varepsilon$ model have been reported, for example [83, 21, 20]. CFD was applied to prediction of heat transfer, spray modeling, intake flow physics and mixture preparation, among others. In general, CFD findings increasingly contributed to a better understanding of in-cylinder structures near TDC, especially in the late compression stroke. For example, work by Gosman et al. [31, 22] highlighted the importance of intake generated tumble vortex in increasing the turbulence levels near TDC. All sorts of geometrical improvements to the piston shape (i.e., variety of bowl configurations) were investigated by numerical simulations with emphasis on combustion characteristics due to these modifications. In some designs (particularly in diesel and stratified-charge SI engines), the piston has the important function of enhancing turbulence levels at the time of ignition [94, 22].

Differential second-moment (DSM) closures, however, have been less popular because of their increased cost due to additional transport equations in the turbulent closure. In one of the early works in IC engines, El Tahry [20] compared a DSM model with $k-\varepsilon$ model in an axisymmetric chamber with annular intake valve open. The comparison did not yield any major discrepancy between DSM and $k-\varepsilon$ predictions in the mean flow and both simulations fairly agreed with the experimental data of the engine simulated. DSM, however, was found to be better at predicting turbulence intensities. The findings of the study by El Tahry were later disputed by Lea et al. [58] on the grounds that compression
effects were not simulated in El Tahry’s work. Hence, it was argued that one of the major motivations for using DSM (i.e., predicting complex flows with straining and streamline curvature) was not realized [58]. Their work included compression effects by simulating both intake and compression strokes. The results confirmed the earlier finding of El Tahry [20] that both models generally agree with each other when there is no compression (i.e., in the intake stroke). However, DSM performed much better during the compression stroke both in the mean flow and turbulence intensities. This observation is attributed to anisotropic stress generation by DSM in the early stages of the compression stroke that suppressed the main vortical structure [58]. This feature is absent in $k − \varepsilon$ modeling paradigm. Despite its potential theoretical advantages, however, DSM closures have not found widespread use in IC engines [30].

Since the IC engine geometries are complex and involve moving parts (i.e., valves), numerical stability is given higher priority in most of the earlier studies, typically employing first order accurate spatial schemes with upwinding methods. KIVA code [3] developed at Sandia National Laboratories have found increasing use in this period.

1.3.2.3 1990-Present

Contemporary trends in IC engine modeling are given in several recent reviews [15, 40, 39, 30]. As a result of advancements in computing power, the complex in-cylinder processes have increasingly been simulated with more refined grids. $k − \varepsilon$ model remains to date the popular choice due to its simplicity and robustness. Efforts generally concentrated on the ability of turbulence models to predict scales of turbulence in the compression stroke (due to its relevance in TDC turbulence levels). Han et al. [36] compared $k − \varepsilon$ predicted turbulence parameters with Laser Doppler Velocimetry (LDV) measurements in a motored diesel engine. The computations were three-dimensional. Standard interpretation of the integral length scale (obtained from the model, $L_e \approx k^{3/2}/\varepsilon$) failed to reproduce measured trends. This result is attributed to the incapability of the equilibrium turbulence model in rapidly strained non-equilibrium flows. In equilibrium flows, the model predicted length scale $L_e$ is proportional to the integral length scale $L_I$ (as can be obtained from spatial auto-correlation
curve). An alternate formulation, based on scaling arguments, revealed a Reynolds number dependence ($L_e \approx L_T Re$) in non-equilibrium flows. With this modification, the numerical results were in fair agreement with the measured data [36].

The limitations of RANS methods, including DSM, have sparked an interest in LES recently, although the published LES literature in IC engine applications is limited [15, 38, 39]. The work of Naitoh et al. [72] seems to be the first LES of a premixed spark-ignition engine. In that work, LES is applied to a 4-valve engine using the full three-dimensional geometry, with a flamelet subgrid combustion model. The grid resolution is very coarse, about 122500 cells in the intake stroke, 101728 cells in the compression stroke and 47488 cells in the expansion stroke. The proposed scheme in [72] is used only in the compression and expansion strokes. The simulation of the intake and the compression strokes were carried out by a different scheme [72]. Despite the coarse resolution, flame propagation characteristics were in fair agreement with the experimental data. Moreover, as part of the investigation, 2 full cycles were simulated to assess the ability of LES in reproducing cyclic changes. It was suggested that variations in turbulence levels was the cause of cyclic variations. The lack of similarity in the streamline pattern at 330 degrees ATDC (late compression) was given in support of their argument. In addition, the numerical pressure history of 2 cycles was compared to ensemble-averaged (of 100 cycles) pressure signal. Their conclusion that LES was able to predict cyclic variation, while theoretically expected, is inconclusive since individual cycle LES results were compared to ensemble-averaged measured pressure.

In another study, Celik et al. [16] applied LES to investigate the evolution of turbulence in a bowl-in-piston geometry using the popular KIVA software [3, 2] under motored conditions. The engine is a 4-stroke, 2 valve diesel engine [13], with a compression ratio of 18, stroke of 86 mm and bore of 79.5 mm. Two mechanisms of turbulence generation (intake generated and bowl induced) were studied. In the first part, the energy spectra of velocity fluctuations were compared to measurements in selected locations near TDC during the intake phase. The motored engine speed was 1600 revolutions per minute (rpm). The computational grid in this case did not include the bowl, which was the case in experimental
study. Two computational grids of 220000 and 440000 nodes, including the intake and exhaust ducts, were used. Typical grid size was about 1-2 mm. In the second part, the effect of the bowl on the instabilities and turbulence generation during the compression stroke were investigated at 1500 rpm, with 20000 computational cells. The numerical simulation was not continuous in the sense that the turbulence generated at the intake phase was not used. Rather, the turbulence level was initialized to zero. The occurrence of instabilities during the computations was attributed to the flow separation triggered at the corner (between the flat part of the piston and the bowl).

The examples provided by these representative studies indicate that the numerical solutions of IC engine physics are still limited in several ways. For example, in the majority of the reviewed literature, emphasis has been on modeling the intake and compression phases only. This usually stems from the fact that simulations of dynamic systems, which require meticulously resolving the time accurate nature of the flow with refined grids, are difficult. This is in contrast to statistically stationary flows where the main aim is to simulate just long enough to obtain averaged information. Furthermore, the cost of IC engine simulations also limits their applicability in predicting variations over multiple cycles. The cyclic variations of IC engines can not be addressed in RANS methods because of their accepted feature of providing only an ensemble-averaged realization of the periodic flow [38]. It can only be addressed with LES, provided that efficient algorithms and refined grids are used in the simulation.

1.4 Objectives Of This Thesis

In this work, the study of mixture preparation and combustion characteristics of a two-stroke, high AR combustor is carried out with a multidimensional numerical methodology over multiple cycles. This would complement, to a certain degree, previous works [19, 23] that have emphasized manufacturing issues and quenching effects due to heat losses in high AR combustors. In particular, the following steps are considered major objectives of the present study:
(1) To develop an accurate large-eddy simulation (LES) methodology to simulate complex flow dynamics in a realistic combustor.

An algorithm based on a second-order accurate (in time and space) predictor-corrector time stepping scheme will be extended to efficiently simulate periodic, in-cylinder flows. The numerical complexity of such problems is inherently more difficult due to the unsteady, periodic nature of the flow. Physical phenomena such as turbulence generation, heat transfer and bulk flow structures interact with each other continuously and in constantly changing conditions as the piston is moving. To accomplish this, an algorithm for piston motion needs to be developed that will handle strong shear and compression dominated flows. The developed algorithm should be robust and accurate. Formal accuracy (of the numerical scheme) is especially important to reduce or prevent the numerical noise from contaminating the computed turbulence quantities. This condition is usually not met in standard predictive tools currently used in the literature. For example, KIVA usually employs first-order upwind schemes and therefore a definitive assessment on the ability of turbulence models in IC engine flows is not possible [40]. Therefore, a second-order central scheme is employed to reduce the effect of uncertainties originating from the numerical discretization. The numerical scheme will be implemented employing Message Passing Interface (MPI) paradigm in domain decomposition mode to reduce the computational burden typical of engine flows.

(2) Analysis of mixture preparation and turbulence characteristics in the high aspect ratio combustor.

Since the mixture composition and turbulence intensities at the time of ignition is a direct consequence of the scavenging period, the study of mixture preparation has a significant effect on the combustion period. Issues that need to be addressed are the mixture composition, turbulence intensities and the dominant structures that promote turbulence. Experimentally, a quantitative study regarding these aspects of the two-stroke engine has not been done. Optical access and manufacturing difficulties are some of the issues that have hindered full characterization of IC engine flows in the past for similar configurations. Therefore, the present numerical work, with its potential to provide full field information
of flow variables in a continuous and cycle-resolved manner, might lead to a more advanced interpretation of the physical processes occurring in the high AR combustor. Moreover, the findings are likely to be relevant for other similar practical systems as well.

(3) Comparison of LES and RANS in predicting in-cylinder flows.

Periodic flows pose tremendous challenges to turbulence models. The LES methodology has the potential to resolve many deficiencies of traditional RANS based methods. The most important strength of LES is the explicit account of large scale structures of the mean flow. As a result, the unresolved effects of turbulence are limited to relatively isotropic small scales, which can be modeled even by traditional closures without substantial effect on predictions. RANS methods, on the other hand, model the entire spectrum. This distinction between LES and RANS has serious repercussions in providing an assessment on the nature of turbulence in engine flows since an accurate prediction of turbulent structures is a significant requirement for correctly modeling the combustion period. Furthermore, the performances of the investigated methodologies in revealing the nature of cyclic variations need to be understood. This is because a capability in predicting cyclic variations is crucial if full advantage of design limitations is to be realized.

(4) To provide directions for future studies of the power generator concept.

The present methodology has the potential to simulate highly coupled physical processes in a consistent manner. As a result, a better understanding of important parameters in the engine workings may emerge. This is likely to improve future studies of more specialized basis. For example, if some relation between the accuracy of predictions and the employed numerical grid can be established in the intake phase, this information may be used to seek strategies in which optimum use of resources is targeted. This is based on the observation that the intake and the early compression stages constitute a relatively long period in the entire engine cycle, yet compared to the flame propagation period may require less grid density. On the other hand, the combustion period, while much shorter (several milliseconds), will be likely to require more grid density due to the additional need of resolving
the flame structure. Therefore, a quantified understanding in obtaining the mixture conditions prior to combustion period in a more economical manner will improve the chances of multidimensional methods to become truly involved in the design process. As a result, the predictions of the combustion phase may be simulated using more refined grids and more advanced combustion mechanisms to extract more specialized information such as dynamic flame-wall interaction parameters. Furthermore, averaged quantities such as mixture composition and mixture temperature as a function of piston position will be known for the simulated (based on an experimentally available pressure data) engine conditions. This level of detail is likely to be not possible for some time to come, given the limitations of experimental measurement techniques in the context of providing full 3D field information in a time accurate manner. As such, the findings of the present study may be used in developing lower order prediction tools that incorporate integrated effects of mixture and turbulence in a more physical basis.
CHAPTER 2

GOVERNING EQUATIONS

The concept of “conservation” for any fluid mechanics variable is the starting point of any derived methodology (i.e., LES and RANS) and are fully expressed by Navier-Stokes equations as the general form of the governing equations. In this chapter, a fully compressible version of the governing equations is presented first for completeness. Although incompressible formulations are usually better in terms of computational turnaround time, the compressible formulations allow a complete framework to couple all relevant physical processes (i.e., acoustics, fluid mechanics and combustion). Following the presentation of this general framework, the set of conservation equations used in LES and RANS methodologies are described. A brief introduction of heat release modeling concludes the discussion of the numerical tools used in the present work.

2.1 Navier-Stokes Equations

In the continuum limit, Navier-Stokes equations completely determine the description of a flow with given initial conditions. The form adapted here is the compressible and multi-species form and basically describe the conservation of mass, momentum, total energy and chemical species[53]:

Conservation of mass:

\[
\frac{\partial p}{\partial t} + \frac{\partial p u_i}{\partial x_i} = 0 \tag{2.1}
\]

Conservation of Momentum:

\[
\frac{\partial p u_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ p u_i u_j + p \delta_{ij} - \tau_{ij} \right] = 0 \tag{2.2}
\]

Conservation of Total Energy:

\[
\frac{\partial p E}{\partial t} + \frac{\partial}{\partial x_i} \left[ (p E + p) u_i + q_i - u_j \tau_{ij} \right] = 0 \tag{2.3}
\]
Species:
\[
\frac{\partial \rho Y_m}{\partial t} + \frac{\partial}{\partial x_i} [\rho Y_m (u_i + V_{i,m})] = \dot{w}_m, \; m = 1, \ldots, N_s
\] (2.4)

where \(\rho\) is the density, \(u_i\) is the velocity, \(Y_m\) is the mass fraction of species "m", \(E\) is the total internal energy per unit mass and \(p\) is the pressure. \(N_s\) is the number of species. The pressure, \(p\), is obtained from the equation of state, \(p = \rho RT\). The mixture gas constant is given by \(R = \sum_{m=1}^{N_s} Y_m R_m\). Similar expressions can be used for the mixture specific heats. For example, \(c_p = \sum_{m=1}^{N_s} Y_m c_{p,m}\) and \(c_v = \sum_{m=1}^{N_s} Y_m c_{v,m}\). The total energy per unit volume is determined from

\[
\rho E = \rho (e + \frac{u_i u_i}{2})
\] (2.5)

where the repeated indices imply summation and the internal energy per unit mass is defined as

\[
e = \sum_{m=1}^{N_s} Y_m h_m - p/\rho
\] (2.6)

The viscous stress tensor is given by

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial}{\partial x_k} \delta_{ij}
\] (2.7)

where \(\mu\) is the molecular viscosity computed from Sutherland’s Law. Also, \(\dot{w}_m\) is the mass destruction (production) of the species in the domain of interest per unit volume per unit time. Heat flux vector have contributions from thermal conduction and enthalpy flux. For the heat conduction, Fourier’s Law can be used to compute the heat flux. Dufour effect and radiation losses are neglected in the present study. Hence

\[
q_i = -\kappa \frac{\partial T}{\partial x_i} + \rho \sum_{m=1}^{N_s} h_m Y_m V_{i,m}
\] (2.8)

where \(\kappa\) is the mixture averaged thermal conductivity coefficient. The general expression for species diffusion velocities in a multi-component system are very complex and includes Soret effect, Dufour effect and cross-diffusion effects [45]. However, incorporating these effects in the computations is costly. A simplified approach based on Fick’s law are used here instead, with

\[
V_{i,m} = -\frac{D_m \partial Y_m}{Y_m \partial x_i}
\] (2.9)
where $D_m$ is the diffusion coefficient of the species. For a thermally perfect gas, enthalpy per unit mass for species $m$ is obtained from

$$h_m = \Delta h_{f,m} + \int_{t_0}^{T} c_{p,m} T' dT'$$

where $\Delta h_{f,m}$ is the standard heat of formation at temperature $T_0$.

### 2.2 Large Eddy Simulation Formulation

The LES equations of motion are obtained by spatially filtering the governing equations. The filtering operation essentially removes high wave number contributions by acting as a low-pass filter. In the physical space, the following expression defines [95] this operation for any flow variable $f$

$$\bar{f}(x_1,x_2,x_3) = \int \int \int f(x,y,z) \left( \prod_{j=1}^{3} G_j(x_j',x_j) \right) dx_1' dx_2' dx_3'$$

where the filtering operation is symbolically represented by an “over-bar” and $G$ is the kernel function satisfying the normalization condition

$$\int \int \int \left( \prod_{j=1}^{3} G_j(x_j',x_j) \right) dx_1' dx_2' dx_3' = 1$$

There are several filter kernels used in physical space, the most popular being the box filter [18] and the Gaussian filter [24]. In the present work, the box filter defined as

$$G_j(x_j - x_j') = \begin{cases} 1/\Delta_j & |x_j - x_j'| \leq \Delta_j/2 \\ 0 & \text{otherwise} \end{cases}$$

is used. The result of this filtering operation has an easy interpretation as the volume-averaged value of $f$. One drawback of the box filter is that it does not preserve the signal below the cut-off scale but rather attenuates it, as opposed to spectral cut-off filter [75] which does. Nevertheless, it provides ease of implementation in implicit filtering of LES equations since the numerical grid acts as the filter and does not require any explicit filtering. The spatial filtering as defined above commutes with temporal derivatives in the governing equations when the grid is not changing in time. Hence,

$$\frac{\partial \bar{f}(x_i,t)}{\partial t} = \frac{\partial \overline{f(x_i,t)}}{\partial t}$$

(2.14)
However, it does not commute with spatial derivatives in the general case where the kernel function \( G \) is changing in space [79]. Only when the grid is uniform (i.e., \( G \) is constant) that it does commute with spatial derivatives. For simple flows, it is usually possible (and affordable) to have a uniform grid. But in applications with complex geometries (for instance high-Re wall bounded flows or gas turbine combustors), this is usually difficult and grid stretching is used inevitably. In this case, special attention must be paid to make sure that grid spacing does not change too much (usual practice is on the order of \( \%5 \) or less) so that commutation error can be kept to a small level\(^1\). In the present study, the commutation in spatial derivatives is assumed to hold, hence

\[
\frac{\partial f(x_i, t)}{\partial x_i} \approx \frac{\partial \tilde{f}(x_i, t)}{\partial x_i}
\]

(2.15)

In compressible flows, spatial filtering results in correlations involving density fluctuations that need to be closed. This can be avoided by applying Favre filtering defined by the following expression

\[ \tilde{f} = \frac{\overline{pf}}{\overline{p}} \]

(2.16)

where \( f \) is any flow variable and “tilde” represents this operation. As a result of Favre filtering, a density weighted spatial filtering of \( f \) is obtained, denoted by \( \tilde{f} \). Defining a residual component by \( f'' \) completes the relation between \( f \) and its two components such that \( f = \tilde{f} + f'' \). In the context of LES, the residual component is called subgrid scale or unresolved scale. Similarly, \( \tilde{f} \) is called supergrid or resolved scale.

The LES equations for a reacting, compressible flow can be obtained by applying filtering rules described above to Navier-Stokes Equations. The final set of LES equations become

Continuity:

\[ \frac{\partial \overline{p}}{\partial t} + \frac{\partial \overline{p} \overline{u}_j}{\partial x_j} = S_1 \]

(2.17)

Momentum:

\[ \frac{\partial \overline{p} \overline{u}_i}{\partial t} + \frac{\partial \overline{p} \overline{u}_i \overline{u}_j}{\partial x_j} = - \frac{\partial \overline{p} \delta_{ij}}{\partial x_j} + \frac{\overline{\tau}_{ij}}{\partial x_j} - \frac{\overline{\tau}^{\text{ss}}_{ij}}{\partial x_j} + S_i \]

(2.18)

\(^1\)the limitation to maximum grid stretching is important even without filtering operation since with stretching the original accuracy of a discretization scheme is reduced.
Total Energy:

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho \bar{E}_j}{\partial x_j} = \frac{\partial \rho \bar{u}_j}{\partial x_j} + \frac{\partial \bar{q}_j}{\partial x_j} - \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial \bar{H}_{ij}^{gs}}{\partial x_j} + S_j + \dot{E}_i \tag{2.19}
\]

Species:

\[
\frac{\partial \rho \bar{Y}_m}{\partial t} + \frac{\partial \rho \bar{u}_m}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \bar{p} D_m \frac{\partial \bar{Y}_m}{\partial x_j} \right) - \frac{\partial \Phi_{j,m}^{gs}}{\partial x_j} - \frac{\partial \Theta_{j,m}^{gs}}{\partial x_j} + \bar{w}_m \tag{2.20}
\]

where \( S_1 \) through \( S_5 \) are mass loss source terms as explained in chapter 3. \( \dot{E}_i \) is the ignition source term (see chapter 3). As a result of filtering, several terms (denoted by superscript “gs”) that represent subgrid scale correlations of certain flow variables are produced in the governing equations. These terms are unknown and their closure strategies constitute the main theme of subgrid modeling in the literature.

The total internal energy per unit mass, \( \bar{E} \), is the sum of the internal energy (\( \bar{e} \)), resolved kinetic energy and the unresolved part of the kinetic energy

\[
\bar{E} = \bar{e} + \frac{\bar{u}_l \bar{u}_l}{2} + \frac{\bar{u}_l \bar{u}_l - \bar{u}_l \bar{u}_l}{2} \tag{2.21}
\]

where the filtered internal energy is given by

\[
\bar{e} = \sum_{k=1}^{N_s} \left[ \bar{Y}_k \bar{h}_k + (\bar{Y}_k (\bar{h}_k - \bar{h}_k)) - \bar{p}/\bar{\rho} \right] \tag{2.22}
\]

In the present formulation, unresolved kinetic energy term, \( \frac{\bar{u}_l \bar{u}_l - \bar{u}_l \bar{u}_l}{2} \), plays an important role by providing an estimate for velocity scales of subgrid turbulent fluctuations, and in what follows it will be referred to as the subgrid kinetic energy, \( k^{gs} \). The magnitude of this term depends on the state of the flow (turbulent versus laminar) and can not be computed a priori. A transport equation (defined later) is solved to determine its evolution along with the filtered governing equations described above.

Filtering the equation of state produces an additional term

\[
\bar{p} = \bar{p}_R \sum_{k=1}^{n} \frac{\bar{Y}_k \bar{T}}{W_k} + \frac{\bar{Y}_k \bar{T} - \bar{Y}_k \bar{T}}{W_k} \tag{2.23}
\]

that represents temperature-species correlation, \( T^{gs} = [\bar{Y}_k \bar{T} - \bar{Y}_k \bar{T}] \). It is neglected in this study due to uncertainties and difficulties in modeling. It was shown, however, that modeling the correlation might be necessary at high heat release rates [25].
The heat flux vector after filtering becomes

\[ \tilde{q}_i = -\kappa \frac{\partial \tilde{T}}{\partial x_i} + \bar{\rho} \sum_{k=1}^{N_s} \tilde{h}_k \tilde{Y}_{i,k} \tilde{V}_{i,k} + \sum_{k=1}^{N_s} q_{i,k}^{sgs}. \]

where \( q_{i,k}^{sgs} = \tilde{h}_k D_k \partial Y_k / \partial x_i - h_k D_k \partial Y_k / \partial x_i \) is the unresolved heat transfer due to turbulent convection of species and is neglected here. Filtered diffusion velocities of species are expressed by Fick’s law, following the discussion in the first part of this chapter, but this time in terms of resolved quantities

\[ \tilde{V}_{i,k} = (-\bar{D}_k / \bar{Y}_k)(\partial \tilde{Y}_k / \partial x_i) \quad (2.23) \]

The subgrid terms \( \tau_{i,j}^{sgs}, H_j^{sgs} \) and \( \Theta_{k,j}^{sgs} \) result from filtering of the convective terms in the governing equations. \( H_j^{sgs} \) and \( \Theta_{k,j}^{sgs} \) represent total enthalpy and mass fluxes due to subgrid fluctuations. \( \sigma_j^{sgs} \) and \( \Theta_{k,j}^{sgs} \) result from correlations of the velocity field with the viscous stress tensor, and the species mass fractions with the diffusion velocities respectively. These terms can be closed by defining a turbulent viscosity (\( \nu_T \)). The method to compute the turbulent viscosity will be described later in this chapter, but for purposes of developing closure strategies for the unclosed terms of LES equations, it is sufficient to assume that it can be defined.

### 2.2.1 Subgrid Stress Closure

The most important unclosed term is the subgrid stress tensor, \( \tau_{i,j}^{sgs} = \bar{\rho} (\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) \). Because of the formal similarity of this term with the Reynolds stress tensor from conventional statistical averaging, it is also called unresolved Reynolds stress tensor [98]. In compressible flows, it can be decomposed into anisotropic and isotropic components [87]

\[ \bar{\rho} \tau_{ij}^{sgs} = \bar{\rho} \tau_{ij}^{sgs} - \frac{1}{3} \bar{\rho} \tau_{ii}^{sgs} \quad (2.24) \]

The anisotropic part is modeled in terms of resolved strain rate, \( \tilde{S}_{ij} = (1/2)(\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) \), and the turbulent eddy viscosity as

\[ \tau_{ij}^{sgs,a} = -2\nu_T \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) \quad (2.25) \]
The isotropic part of the stress tensor, $\tau_{ii}^{\text{gs}}/3$, is usually not modeled in incompressible flows, but rather added to the filtered pressure [87]. This approach, however, causes the filtered pressure to be unknown (since the modified pressure is solved) and therefore not desirable for compressible flows where unambiguous determination of the filtered pressure term is required, for example, in the equation of state. Also, it is a fundamental quantity in the enthalpy balance (i.e., energy equation) [99]. Models are proposed to determine the isotropic part of the stress tensor. It was pointed out by Schumann [90] that unresolved part of the stress tensor should be positive semidefinite (realizable). A set of conditions that satisfy this requirement are

$$\tau_{ii}^{\text{gs}} \geq 0 \quad i=j \quad (2.26)$$

$$|\tau_{ij}^{\text{gs}}| \leq \left( \tau_{ii}^{\text{gs}} \tau_{jj}^{\text{gs}} \right)^{1/2} \quad i \neq j \quad (2.27)$$

$$\det(\tau_{ij}^{\text{gs}}) \geq 0 \quad (2.28)$$

According to Germano [26], a generalized turbulent kinetic energy can be defined such that $\tau_{ii}^{\text{gs}} = 2k$. It follows from the realizability conditions that $k$ is positive. Conversely, this definition introduces a requirement that if the isotropic part is to be modeled, it should be positive. Several approaches are available to model the isotropic part of the subgrid stress tensor (or $k$). For example, Moin et al. [70] used $k = C_l \Delta^2 (2\tilde{S}_{kl}\tilde{S}_{kl})$, with dynamic determination of the coefficient $C_l$. Alternatively, a transport equation for $k$ has been solved in several studies [89, 53, 28]. In the present study, the transport equation approach of Kim et al. [53] is adapted where subgrid kinetic energy ($k^{\text{gs}}$) is solved with the governing equations in a coupled manner (cf. 2.2). With the adaption of the subgrid kinetic energy approach, the final expression for the subgrid stress tensor becomes

$$\overline{p} \tau_{ij}^{\text{gs}} = \overline{p}(\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) = -2\overline{p} v_t \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \overline{p} k^{\text{gs}} \delta_{ij} \quad (2.29)$$

### 2.2.2 Scalar Transport Closure

Unresolved Enthalpy flux, $H_j^{\text{gs}}$, and unresolved species flux, $\Phi_{k,j}^{\text{gs}}$, are modeled through a gradient transport hypothesis:

$$H_j^{\text{gs}} = \overline{p} \left( \tilde{H}_j u_j - \tilde{H} \tilde{u}_j \right) = -\overline{p} v_t \frac{\partial h}{\partial x_i} \quad (2.30)$$
\[ \Phi_{k,j}^{\text{sgs}} = \bar{p} \left( \bar{Y}_k u_j - \bar{V}_k \bar{U}_j \right) = -\bar{p} \frac{V_i}{S_{CT}} \frac{\partial \bar{Y}_m}{\partial x_i} \]  

(2.31)

Under certain conditions, however, it was shown experimentally [60] that scalar turbulent fluxes might occur in the opposite direction to that of Equation 2.30 or 2.31. This phenomenon is called counter-gradient transport (CGT) and usually considered to be caused by differential buoyancy effects. DNS studies by Veynante et al. [97] recovered theoretical conclusions that counter-gradient transport is promoted by low turbulence intensities (\(u'/S_L\)) and high heat release rates. Note that counter-gradient is captured at the resolved scales in LES [8] and uncertainties due to gradient transport hypothesis is limited to the unresolved scales only. In the RANS context, CGT is neglected unless BML (Bray-Moss-Libby) model is used.

Unresolved Diffusive mass flux, \(\Theta_{k,j}^{\text{sgs}} = \bar{p} \left( \bar{Y}_k V_{k,j} - \bar{V}_k \bar{V}_{k,j} \right)\), and subgrid viscous work, \(\sigma_{k}^{\text{sgs}} = \bar{p} \left( \bar{u}_i \bar{\tau}_{ij} - \bar{u}_i \bar{\tau}_{ji} \right)\), are neglected in the present study. Unresolved diffusive mass flux is neglected since it is shown to be relatively small compared to the subgrid species mass flux [53]. Subgrid viscous work is small compared to other terms in the energy equation for high Reynolds number flows [55].

### 2.2.3 Subgrid Kinetic Energy Transport Equation

It was shown in the previous two sections that several unresolved correlation terms due to the LES filtering operation can be closed by defining a turbulent eddy viscosity. In the first subgrid closure by Smagorinsky [92], the eddy viscosity is defined as

\[ \nu_T = C_S^2 \Delta^2 |\bar{S}| \]  

(2.32)

where \(|\bar{S}| = \left( 2 \bar{S}_{ij} \bar{S}_{ij} \right)^{1/2}\) and \(C_S\) is the Smagorinsky constant. The subgrid stress term is still defined by Equations 2.24 and 2.25. Using the definition of subgrid stress tensor (Equation 2.24) in the realizability condition implies that the subgrid energy \((k)\) defined by the isotropic part of the stress tensor should satisfy [99]

\[ k^{\text{sgs}} \geq \frac{1}{2} \sqrt{3} C_S^2 \Delta^2 |\bar{S}|^2 \]  

(2.33)
which can be expressed in a slightly different form by defining a second coefficient, $C_k$, to obtain the subgrid kinetic energy $k^{sgs}$

$$k^{sgs} = C_k \Delta^2 |\bar{S}|^2$$

(2.34)

where the second constant $C_k$ now is given by the inequality $C_k \geq \frac{1}{2} \sqrt{3} C_S^2$. Suggested values [103] for the model coefficients are $C_S = 0.16$ and $C_k = 0.0886$. According to Kolmogorov hypothesis, small scales are isotropic in the limit of high Reynolds numbers. In this view, also called the cascade hypothesis, energy is created in the large scales and dissipated at small scales by viscous dissipation, with a wide range of scales separating the largest and smallest scales. This intermediate region is called the inertial subrange and primarily serves as transferring the energy from large scales to small scales. In the LES context, subgrid models are designed to mimic this global energy transfer which, on average, is from large to small scales and therefore dissipative.

In the formal derivation of Smagorinsky model, the dissipation and production of kinetic energy are assumed to be equal, implying equilibrium between small scales and large scales. In that case, small scales adjust to any deformation in the mean flow instantaneously. But in reality, this is exactly true only when the entire inertial range is numerically resolved, which leaves only the real dissipation scales to be modeled. In typical applications, however, the grid cut-off wavenumber is in the inertial range, usually $k_I > k_c > k_\eta$, and therefore what the model sees as small scale and actual small scales are different. As a consequence, a substantial fraction of kinetic energy might be unresolved. This has the important implication that the adjustment rate to equilibrium is now dictated by a different time scale [62, 76]. Smagorinsky model, however, compute the time scale of subgrid from resolved large scales, which is usually the inverse of the mean strain rate magnitude, $|\bar{S}|^{-1}$. Therefore, the time rate of change of this time scale is infinite, necessarily implying that small scales adjust to the new equilibrium level instantaneously. Hence, relaxation to equilibrium is not accounted for because separate determination of time scale is not built into the model. Recognizing this, a transport equation that models the time rate of change of the unresolved kinetic energy ($k^{sgs}$) has been proposed by several researchers [89, 53, 28]. In the present study, the
transport equation of Kim [53] is used:

\[
\frac{\partial \bar{\rho} k^\text{gs}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i k^\text{gs})}{\partial x_i} = P^\text{gs} - D^\text{gs} + \frac{\partial}{\partial x_i} \left( \bar{\rho} \frac{v_i}{Pr_i} \frac{\partial k^\text{gs}}{\partial x_i} \right)
\]  

(2.35)

Here, \(P^\text{gs} = -\tau^\text{gs}_{ij} \frac{\partial \bar{u}_i}{\partial x_j}\) and \(D^\text{gs} = C_e\bar{\rho} (k^\text{gs})^{3/2}/\bar{\Lambda}\) are the production and dissipation of subgrid kinetic energy. In the closure approach used in the previous sections, it was assumed that a turbulent viscosity can be defined. For this task, appropriate length and velocity scales need to be determined to compute turbulent eddy viscosity, \(\nu_T \approx (\text{LengthScale}) \times (\text{VelocityScale})\). In LES, the natural choice for length scale is the filter width, \(\bar{\Lambda}\). The velocity scale is computed from \(\sqrt{k^\text{gs}}\). Hence, the turbulent viscosity can be determined from

\[
\nu_T = C_v (k^\text{gs})^{1/2} \bar{\Lambda}
\]

(2.36)

where \(C_v\) is a model coefficient. The two coefficients of the model, \(C_v\) and \(C_\varepsilon\), need to be determined. In high Reynolds number applications, \(C_v\) and \(C_\varepsilon\) are taken as 0.067 and 0.916, respectively [53]. However, this approach would be purely dissipative (similar to Smagorinsky model), and will not be able to predict any reverse energy transfer (from small to large scales). Also, the assumption that a single set of model coefficients will provide accurate results are dubious, since there can be substantial differences in different flow configurations as well as in different locations of the same flow geometry. Hence, calibration of the coefficients may be difficult in complex flows. However, there is an approach that can be used to compute these coefficients as the flow evolves [67]. This is the method employed in the present study. A brief summary of dynamic determination of model coefficients is given in Appendix A.

### 2.3 Reynolds-Averaged Navier-Stokes Formulation

The equations employed for the RANS simulation of the flow is the Favre-ensemble averaged Navier-Stokes equations with a \(k - \varepsilon\) turbulence closure extended for near wall flows, as detailed by Gerolymos et al. [27]. The equations read as follows:

**Continuity:**

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = S_1
\]

(2.37)
Momentum:

\[
\frac{\partial \bar{\rho} \bar{u}_j}{\partial t} + \frac{\partial}{\partial x_j} \left[ \bar{\rho} \bar{u}_i \bar{u}_j + p \delta_{ij} \right] = \frac{\partial}{\partial x_j} \left[ \bar{\tau} - \bar{\rho} \bar{u}_i' \bar{u}_j'' \right] = S_{j+1} \tag{2.38}
\]

Energy:

\[
\frac{\partial (\bar{\rho} \bar{E})}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{h}_i}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \bar{u}_i (\tau_{ij} - \bar{\rho} \bar{u}_i' \bar{u}_j'') \right] + (\bar{q}_j + \bar{\rho} e' \bar{u}_j'') + P_k - \bar{\rho} e^* = -2\mu \left( \frac{\partial \sqrt{k}}{\partial x_j} \right)^2 = S_\delta + \bar{E}_i \tag{2.39}
\]

\[k\] equation:

\[
\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j k}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] - P_k + \bar{\rho} e^* + 2\mu \left( \frac{\partial \sqrt{k}}{\partial x_j} \right)^2 = 0 \tag{2.40}
\]

\[\varepsilon\] equation:

\[
\frac{\partial \bar{\rho} \varepsilon^*}{\partial t} + \frac{\partial \bar{\rho} \varepsilon^* \bar{u}_j}{\partial x_j} - \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \varepsilon^*}{\partial x_j} \right] - C_{e1} P_k \frac{\varepsilon^*}{k} + C_{e2} \bar{f}_2 \frac{\varepsilon^*}{k} = \frac{\lambda}{k} \left( \frac{\partial^2 \bar{u}_i}{\partial x_i \partial x_j} \right) \left( \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_l} \right) = 0 \tag{2.41}
\]

Species:

\[
\frac{\partial \bar{\rho} Y_m}{\partial t} + \frac{\partial \bar{\rho} Y_m \bar{u}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \bar{\rho} D_m \frac{\partial Y_m}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu_T}{P_{RT}} \frac{\partial Y_m}{\partial x_j} \right) + \bar{w}_m \tag{2.42}
\]

Here, \(S_1\) through \(S_5\) are mass loss source terms and \(E_i\) is the ignition source term (see chapter 3). The viscous stress tensor and the Reynolds stress tensor are given by \(\tau_{ij} = \mu \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] - \frac{2}{3} \mu \frac{\partial \bar{u}_i}{\partial x_i} \delta_{ij}\) and \(-\bar{\rho} \bar{u}_i' \bar{u}_j'' = \mu_T \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] - \frac{2}{3} \mu \frac{\partial \bar{u}_i}{\partial x_i} \delta_{ij} - \frac{2}{3} \bar{\rho} k \delta_{ij}\), respectively. The production term is \(P_k = \frac{1}{2} \bar{\rho} \bar{u}_i' \bar{u}_j'' \left[ \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right] \). The viscous heat flux and the turbulent heat flux are \(\bar{q}_i = -\kappa_T \frac{\partial \bar{T}}{\partial x_i}\) and \(-\bar{\rho} e' \bar{u}_j'' = -\kappa_T \frac{\partial \varepsilon^*}{\partial x_i}\), respectively. \(\bar{\rho}\) is the pressure, \(\bar{T}\) is the temperature and \(\bar{h}_i = \bar{h} + \frac{1}{2} \bar{u}_i \bar{u}_i\) is the total enthalpy of the flow not including the kinetic energy term. \(e^*\) is the isotropic part of the turbulence kinetic energy dissipation term \((e^* = e - 2\nu \left[ \text{grad} \sqrt{k} \right]^2)\) where \(e\) is the dissipation rate and \(k\) is the turbulence kinetic energy per unit mass. The model constants and various near-wall terms are \(C_{e1} = 1.44\), \(C_{e2} = 1.92\), \(\sigma_k = 1\), \(\sigma_\varepsilon = 1.3\), \(f_{e2}(Re_T) = 1 - 0.3 \exp^{-Re_T^2}\), \(Re_T = k^2/e^*\), and \(f_{\mu}(Re_T) = \exp \left[ \frac{-3.4}{1+0.02(Re_T)^2} \right]\). Then, the expression for turbulent viscosity is \(\mu_T = C_{\mu} f_{\mu}(Re_T) \mu Re_T\) where \(\mu\) is the molecular viscosity.

This formulation is adapted into the numerical solver originally developed for LES. Only minor modifications were necessary in the overall structure since the governing equations
in both cases are very similar, with the exception of the additional transport equation for the dissipation ($\varepsilon$) of the turbulent kinetic energy ($k$) in RANS.

The traditional approach in high-Reynolds number statistical models is to use wall functions, but uncertainty of such practices is simply too high in engine flows because of the highly unsteady and periodic nature of the flow as a result of which the conditions dictating the placement of the first grid off the wall can not be determined with any confidence. The present low-Reynolds number variant of the $k - \varepsilon$ model attempts to remove this ambiguity by modifying the dissipation equation to account for wall effects. However, one important requirement is the need to use refined grids near the walls to resolve the length scale decrease. A consequence is that this resolution requirement may reduce the motivation of using RANS based closures in engine flows if the combustion chamber is strongly influenced by walls. In such cases, the advantages of using RANS over LES may be less obvious.

### 2.4 Combustion Modeling

The following 5 species, single-step reaction mechanism is used for fuel (propane) oxidation following Westbrook [101]:

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2 \quad (2.43)$$

The reaction rate of the fuel is

$$d[C_3H_8]/dt = -8.6 \times 10^{11} \exp(-15100/T)[C_3H_8]^{0.1}[O_2]^{1.65} \quad (2.44)$$

where units are [mol, cm, sec, and K]. This expression is strictly valid in DNS (Direct Numerical Simulation). However, when an averaging procedure is used (as in RANS or LES), the nonlinear reaction rate term would produce high-order correlations of temperature that are difficult to model. Various approaches are available in the literature to model the effect of chemistry on the flow field, from simpler models such as G-equation [74] to more complicated models like the Linear Eddy Model (LEM) [67]. In the G-equation, chemistry may be decoupled from the computation by tracking the G surface that represent the flame. This model is limited to flamelet regime of turbulent combustion, but a recent extension of the model to thin-reaction zones regime is available [74]. LEM is a more refined model and the
crucial scalar mixing process is accounted for much better due to the increased resolution at the subgrid level and a more realistic representation of the turbulent stirring by a stochastic model. LEM has the potential in simulating any combustion regime [67]. Nevertheless, because of its cost, the potential benefits of LEM can not be realized in the present study.

An alternative is to use a much simpler approach to globally model the heat release. This can be justified by the observation that the present work attempts to model the physical processes occurring in the scavenging phase over multiple cycles, and in that point of view, globally predicting the heat release may be enough to consume the combustible mixture so that the next cycle’s scavenging phase may be started in the computations. Hence, the combustion model here may be thought simply as a link between multiple scavenging phases, whose purpose is to provide realistic initial conditions (i.e., temperature, pressure etc.) just before exhaust port opening for the scavenging phase.

In the present study, the eddy-breakup type closure described by Said et al. [88] is used. EBU model assumes that turbulent eddies bring cold reactants and hot products into contact before subsequent reaction period which is controlled by the frequency of the mixing process. This mixing controlled reaction rate can be expressed as

\[ w_{\text{mix}} = -\frac{C_{EBU}}{\tau_{\text{mix}}} \left( 1 + \frac{4.4}{1 + 3.2 \left( \frac{u_{L}}{S_L} \right)^{1/2}} \right) \tilde{Y}_{FUEL} \left( 1 - \frac{\tilde{Y}_{\text{FUEL}}}{\tilde{Y}_{\text{FUEL}}^{0}} \right) \]  

where \( C_{EBU} \) is a coefficient of order one and \( \tau_{\text{mix}} \) is the integral time scale of turbulent eddies.

The time scale for computations involving RANS is \( \tau_{\text{mix}} = k/\epsilon^{*} \). Similarly, for LES, the time scale is computed from \( \tau_{\text{mix}} = \overline{k^{gs}}/\epsilon^{gs} \). Consequently, in EBU, the mean reaction rate of fuel is modeled as the minimum of Equation 2.44 and Equation 2.45. The laminar flame speed, \( S_L \), in the reaction rate expression can be computed using the correlation below [96],

\[ S_L(T_u, P) = 33.34 \left( \frac{T_u}{T_{u, \text{ref}}} \right)^{2.18} \left( \frac{p}{P_{\text{ref}}} \right)^{-0.16} \]  

where \( T_u \) is the unburned mixture temperature, \( T_{u, \text{ref}} \) is 300 K, \( p \) is the pressure and \( P_{\text{ref}} \) is 1 atm.

A thermally perfect gas assumption is used for the species to more realistically represent the heat release period in the combustor. For this, a linear fit is devised to species data of CHEMKIN [49] to obtain the data used in the present study, as given in Table 2.1.
Table 2.1: Curve-fit coefficients for linear variation of specific heat at constant pressure, $C_{p,k} = a_k T + b_k$.

<table>
<thead>
<tr>
<th>Species, k</th>
<th>$C_3H_8$</th>
<th>$O_2$</th>
<th>$CO_2$</th>
<th>$H_2O$</th>
<th>$N_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_k$</td>
<td>0.8877</td>
<td>0.0487</td>
<td>0.1012</td>
<td>0.3491</td>
<td>0.0770</td>
</tr>
<tr>
<td>$b_k$</td>
<td>2924.3</td>
<td>1022.2</td>
<td>1114.1</td>
<td>1970.2</td>
<td>1087.2</td>
</tr>
</tbody>
</table>
CHAPTER 3

NUMERICAL IMPLEMENTATION DETAILS

3.1 Integration of Governing Equations

In the present study, the LES and RANS forms of the governing equations are integrated in time using a finite-volume approach that employs the MacCormack predictor-corrector time-stepping scheme [65]. The integration is explicit and second-order accurate both in time and space. The generic integration formula of the finite volume scheme can be obtained after noting that the governing equations of LES and RANS can be written in the strong conservation form

\[
\frac{\partial Q}{\partial t} + \nabla \cdot f = \Phi \quad (3.1)
\]

where \( Q \) is the vector of conserved variables, \( \Phi \) is the source vector and \( f \) is the flux vector, with \( f = f_x \hat{i} + f_y \hat{j} + f_z \hat{k} \). Equation 3.1 is integrated over a finite volume to obtain

\[
\int_V \frac{\partial Q}{\partial t} dV + \int_S f \cdot \hat{n} dS = \int_V \Phi dV \quad (3.2)
\]

where \( dV \) is the differential volume. Applying Green’s theorem to Equation 3.2, we obtain the final version of that expression to be used in the finite volume formulation

\[
\int_V \frac{\partial Q}{\partial t} dV + \int_S f \cdot \hat{n} dS = \int_V \Phi dV \quad (3.3)
\]

with \( \hat{n} \) being the surface normal unit vector. This expression is valid for any subdivision of the problem domain. In the present study, the problem domain is divided into small volumes called cells that have 6 faces. This is a natural and easy way of creating structured meshes consisting of hexahedrons. The number and distribution of these cells depend on the required accuracy requirements from the solution. In addition, it is assumed that the conserved variables are uniform over the cells and their values are stored at the cell centers. Figure 3.1 describes a typical finite volume cell, shown here in 2D for clarity. Both physical and computational coordinate systems are shown. The cell face area vectors, \( S_\xi, S_\eta \), and
$S_z$, are computed at the cell interfaces, halfway between cell centers for their respective coordinate (computational) directions. Using these conventions, Equation 3.3 can be further simplified as

$$\frac{\partial Q}{\partial t} \Delta V + \sum_{l=1}^{6} f_l \cdot S_l = \Phi \Delta V$$  \hspace{1cm} (3.4)

where $f_l$ is the flux vector and $S_l$ is the area vector, both defined at face $l$. Here, $l$ can be any one of the 6 faces enclosing the discrete (finite) volume, and its identification with computational coordinates is described later in this part.

In the MacCormack scheme, the integration (i.e., finding the value of the conserved variable at time level $n+1$ from the known value at level $n$) is carried out in two steps:

$$Q^* = Q^n + dQ^n$$  \hspace{1cm} (3.5)

$$Q^{n+1} = \frac{1}{2} (Q^n + Q^* + dQ^*)$$  \hspace{1cm} (3.6)

where $n$ denotes the discrete time level before the integration, $*$ denotes the predicted value and $n+1$ denotes the corrected value. The variations of the conserved variable over the predictor and corrector steps, $dQ^n$ and $dQ^*$ respectively, are given by

$$dQ^n = - \frac{\Delta t}{\Delta V} \left( \sum_{l=1}^{6} f_l^{(n)} \cdot S_l - \Phi^n \Delta V \right)$$  \hspace{1cm} (3.7)

$$dQ^* = - \frac{\Delta t}{\Delta V} \left( \sum_{l=1}^{6} f_l^{(*)} \cdot S_l - \Phi^* \Delta V \right)$$  \hspace{1cm} (3.8)

Note that the fluxes need to be computed at the cell faces based on how the fluxes are defined for predictor and corrector stages in the MacCormack scheme. Since the numerical mesh is structured, the flux summation over six faces can be carried out in 3 sweeps, represented by $\xi$, $\eta$ and $\zeta$, as follows

$$\sum_{l=1}^{6} f_l \cdot dS_l = \left( f_{(i+1/2,j,k)} \cdot S_\xi(i+1/2,j,k) + f_{(i-1/2,j,k)} \cdot S_\xi(i-1/2,j,k) \right) \xi \text{ sweep}$$

$$+ \left( f_{(i,j+1/2,k)} \cdot S_\eta(i,j+1/2,k) + f_{(i,j-1/2,k)} \cdot S_\eta(i,j-1/2,k) \right) \eta \text{ sweep}$$

$$+ \left( f_{(i,j,k+1/2)} \cdot S_\zeta(i,j,k+1/2) + f_{(i,j,k-1/2)} \cdot S_\zeta(i,j,k-1/2) \right) \zeta \text{ sweep}$$  \hspace{1cm} (3.9)

These sweep directions correspond to numerical storage indexes of conserved variables. During each sweep, only the index of that particular sweep is changing. The computation
Figure 3.1: Schematic showing the finite volume convention used in the present study. Variables are stored at cell centers, for example, at \((i,j,k)\), \((i+1,j,k)\) etc. Fluxes are computed at cell faces, corresponding to half the distance between two consecutive cell centers. For clarity, only 2D view is shown.

of fluxes at cell faces is based on forward (+) and backward (-) differencing, defined in the following relations for each sweep direction:

\[
\begin{align*}
    f_{i+1/2,j,k} &= f_{i+1,j,k} & \text{(forward differencing, } \xi \text{ sweep)} & (3.10) \\
    f_{i+1/2,j,k} &= f_{i,j,k} & \text{(backward differencing, } \xi \text{ sweep)} & (3.11) \\
    f_{i,j+1/2,k} &= f_{i,j+1,k} & \text{(forward differencing, } \eta \text{ sweep)} & (3.12) \\
    f_{i,j+1/2,k} &= f_{i,j,k} & \text{(backward differencing, } \eta \text{ sweep)} & (3.13) \\
    f_{i,j,k+1/2} &= f_{i,j,k+1} & \text{(forward differencing, } \zeta \text{ sweep)} & (3.14) \\
    f_{i,j,k+1/2} &= f_{i,j,k} & \text{(backward differencing, } \zeta \text{ sweep)} & (3.15)
\end{align*}
\]

At any time step, both of these differencing schemes are used. For example, if (+) differencing is used in the predictor step (n), that means (-) differencing should be used in the corrector step (*). To reduce the bias in the solution, however, the sequence of differencing is alternated between the sweep directions. A possible combination in this operation is given in Table 3.1.

The fluxes, described by \(f\), contain both inviscid and viscous terms. The (+) and (-) differencing schemes for MacCormack schemes are directly applicable for inviscid components of the flux term. However, the flux components with derivative expressions need to
be treated somehow differently. For example, during the $\xi$ sweep, a representative viscous term would be in the form of $A\frac{\partial Y}{\partial t}$, where $A$ and $Y$ are two variables. The discretization of this expression would involve two steps. First, the variable $A$ would be projected onto the surface $(i+1/2, j, k)$ by
\[
A(i+1/2, j, k) = \frac{A(i, j, k) + A(i+1, j, k)}{2}
\] (3.16)
regardless of if it is the predictor step or the corrector step. Second, the derivative expression will be written in the physical space by the chain rule
\[
\frac{\partial Y}{\partial x}
\bigg|_{(i+1/2, j, k)} = \left( \frac{\partial Y}{\partial \zeta} \right)_{(i+1/2, j, k)} \left( \frac{\partial \zeta}{\partial x} \right)_{(i+1/2, j, k)} + \left( \frac{\partial Y}{\partial \eta} \right)_{(i+1/2, j, k)} \left( \frac{\partial \eta}{\partial x} \right)_{(i+1/2, j, k)} + \left( \frac{\partial Y}{\partial \zeta} \right)_{(i+1/2, j, k)} \left( \frac{\partial \zeta}{\partial x} \right)_{(i+1/2, j, k)}
\] (3.17)
where the underbrackets show the evaluation location for each expression. It is clear that all metrics are directly evaluated at the cell face. However, this is only true for some of the derivative expressions. For example, the normal derivative (i.e., in the direction of sweep) term will be computed directly at the surface from the following expression:
\[
\frac{\partial Y}{\partial \zeta}
\bigg|_{(i+1/2, j, k)} = \frac{Y(i+1, j, k) - Y(i-1, j, k)}{2}
\] (3.18)
Remaining cross-derivative terms (with respect to the sweep direction) will be direction biased, i.e., they will be computed based on the direction of differencing summarized in Equation 3.11. For example, the cross-derivative in the $\eta$ direction will be given by
\[
\frac{\partial Y}{\partial \eta}
\bigg|_{(i+1/2, j, k)} = \frac{Y(i+1, j+1, k) - Y(i+1, j-1, k)}{2} \quad \text{(forward)}
\] (3.19)
\[
\frac{\partial Y}{\partial \eta}
\bigg|_{(i+1/2, j, k)} = \frac{Y(i, j+1, k) - Y(i, j-1, k)}{2} \quad \text{(backward)}
\] (3.20)
The integration scheme described above is stable only if the time step, $\Delta t$, is selected to be smaller than the time step of any cell in the entire computational domain. The time step of a computational cell is determined from [50]
\[
\Delta t = CFL \times \frac{V}{\upsilon}
\] (3.21)
Here, $\upsilon$ is defined as $\upsilon = \upsilon_c + \upsilon_u + \upsilon_d$, with individual components given by
\[
\upsilon_c = |uS_\xi| + |uS_\eta| + |uS_\zeta|
\] (3.22)
Table 3.1: An example of possible sequencing in the differencing scheme chosen as a function of MacCormack predictor/corrector stages (P/C) and the sweep direction.

<table>
<thead>
<tr>
<th>Time Step</th>
<th>$\xi$ Sweep, P/C</th>
<th>$\eta$ Sweep, P/C</th>
<th>$\zeta$ Sweep, P/C</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>(+)/(-)</td>
<td>(+)/(-)</td>
<td>(-)/(+)</td>
</tr>
<tr>
<td>n+1</td>
<td>(+)/(-)</td>
<td>(+)/(-)</td>
<td>(+)/(-)</td>
</tr>
<tr>
<td>n+2</td>
<td>(+)/(-)</td>
<td>(-)/(+)</td>
<td>(-)/(+)</td>
</tr>
<tr>
<td>n+3</td>
<td>(+)/(-)</td>
<td>(-)/(+)</td>
<td>(+)/(-)</td>
</tr>
<tr>
<td>n+4</td>
<td>(-)/(+)</td>
<td>(+)/(-)</td>
<td>(-)/(+)</td>
</tr>
<tr>
<td>n+5</td>
<td>(-)/(+)</td>
<td>(+)/(-)</td>
<td>(+)/(-)</td>
</tr>
<tr>
<td>n+6</td>
<td>(-)/(+)</td>
<td>(-)/(+)</td>
<td>(-)/(+)</td>
</tr>
<tr>
<td>n+7</td>
<td>(-)/(+)</td>
<td>(-)/(+)</td>
<td>(+)/(-)</td>
</tr>
</tbody>
</table>

$u_a = c|S|$  \hspace{2cm} (3.23)  

$u_d = \frac{2\mu |S|}{\bar{p}Pr V}$ \hspace{2cm} (3.24)  

where $c$ is the speed of sound, $V$ is the volume of the cell, $u$ is the velocity vector and $|S|$ is the magnitude of cell face area vectors. CFL number is taken as 0.5 for a second-order scheme.

3.2 The Computational Grid

The computational grid used in the present study follows closely the details of the real engine. However, certain simplifications are inevitable. For instance, inlet ports are modeled as if there are physical ports connected to the engine body to simplify boundary conditions. Also, since charging of the engine is done by a pipe not connected to the body, one of the ports is used as exhaust at the initial stages of the scavenging process, but at later phases when the pressure in the chamber is low enough a portion of that port is dedicated to inflow charge. The extent of this partition is based on the estimated experimental mass flow rate into the engine (see the next chapter).

The computational grid (Grid-1) is shown in Figure 3.2 and the details are given in
Figure 3.2: Typical grid geometry in $x-y$ plane and $y-z$ plane. Here, every other grid point is shown for Grid-1. All dimensions in mm. A second grid (Grid-2) is also used, having similar structure except near the walls and the port region where a more refined grid distribution is employed (see Figure 3.3).

Figure 3.3: The distribution of grid spacing in the main combustor, shown for all three directions and for both grids (Grid-1 and Grid-2).
Table 3.2: Numerical details of Grid-1. Also shown are the minimum and maximum grid spacing in each direction.

<table>
<thead>
<tr>
<th>Domain</th>
<th>Dimensions</th>
<th>Min. $\Delta x$, $\Delta y$, $\Delta z$ (mm)</th>
<th>Max. $\Delta x$, $\Delta y$, $\Delta z$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$47 \times 109 \times 13$</td>
<td>0.264, 0.264, 0.264</td>
<td>0.264, 0.264, 0.264</td>
</tr>
<tr>
<td>2</td>
<td>$269 \times 192 \times 25$</td>
<td>0.264, 0.264, 0.264</td>
<td>0.264, 0.264, 0.264</td>
</tr>
<tr>
<td>3</td>
<td>$47 \times 109 \times 13$</td>
<td>0.264, 0.264, 0.264</td>
<td>0.264, 0.264, 0.264</td>
</tr>
</tbody>
</table>

Table 3.3: Numerical details of Grid-2. Also shown are the minimum and maximum grid spacing in each direction.

<table>
<thead>
<tr>
<th>Domain</th>
<th>Dimensions</th>
<th>Min. $\Delta x$, $\Delta y$, $\Delta z$ (mm)</th>
<th>Max. $\Delta x$, $\Delta y$, $\Delta z$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$62 \times 109 \times 17$</td>
<td>0.057, 0.057, 0.057</td>
<td>0.264, 0.264, 0.264</td>
</tr>
<tr>
<td>2</td>
<td>$322 \times 233 \times 46$</td>
<td>0.057, 0.057, 0.057</td>
<td>0.264, 0.264, 0.264</td>
</tr>
<tr>
<td>3</td>
<td>$62 \times 109 \times 17$</td>
<td>0.057, 0.057, 0.057</td>
<td>0.264, 0.264, 0.264</td>
</tr>
</tbody>
</table>

Table 3.2. Domain-1 and Domain-3 are the port regions while Domain-2 is the main combustor. For the main combustor, grid point distribution in “x”, “y” and “z” directions are shown in Figure 3.3. TDC region in this figure is where the flame propagates after ignition and has constant spacing. Similarly, the grid is uniform in “y” and “z” directions, matching the spacing in “x” direction in the TDC region. Ports have geometrically clustered grids in y direction, with minimum spacing at the domain interfaces matching the spacing in the main combustor. Grid-1 is used as the main investigation grid in this study. However, a second grid (Grid-2, Table 3.3) is also used for a complete cycle to investigate the effect of grid resolution on the solution and heat transfer. Grid-2 is the finer grid with regions close to walls and the port region are clustered to have a grid spacing of 57 $\mu$m. A comparison of Grid-2 and Grid-1 can be seen in Figure 3.3.

For cycle-resolved analysis of turbulence, a set of probe positions is chosen in the combustor for continuous signal sampling, as given in Figure 3.4. Table 3.4 details the coordinates of the probe points.
**Figure 3.4:** Schematic showing the location of probe points used for acquiring instantaneous time trace of flow variables (center plane, z=3.175 mm).

**Table 3.4:** Probe coordinates (cf. Figure 3.4) at center plane, z=3.175 mm

<table>
<thead>
<tr>
<th>Probe</th>
<th>2</th>
<th>5</th>
<th>8</th>
<th>11</th>
<th>14</th>
<th>17</th>
<th>20</th>
<th>23</th>
<th>26</th>
<th>29</th>
<th>32</th>
<th>35</th>
</tr>
</thead>
<tbody>
<tr>
<td>x(mm)</td>
<td>35</td>
<td>35</td>
<td>35</td>
<td>35</td>
<td>45</td>
<td>45</td>
<td>45</td>
<td>45</td>
<td>45</td>
<td>55</td>
<td>55</td>
<td>55</td>
</tr>
<tr>
<td>y(mm)</td>
<td>6</td>
<td>19</td>
<td>32</td>
<td>45</td>
<td>6</td>
<td>19</td>
<td>32</td>
<td>45</td>
<td>6</td>
<td>19</td>
<td>32</td>
<td>45</td>
</tr>
</tbody>
</table>
3.3 Boundary Conditions

3.3.1 Wall Conditions

At the wall, no-slip condition is applied for velocity components. In addition, the subgrid kinetic energy (in LES), the turbulent kinetic energy (RANS) and the dissipation of the turbulent kinetic energy (RANS) are also zero at the wall. Since wall reaction mechanisms are not used, the wall-normal gradient of any species is assumed to be zero. All walls are assumed to be iso-thermal at $T_w = 500$ K. The density at the wall is assumed to be simply its value at the first flow cell. These conditions are enforced for each respective flow variable by the help of a ghost cell, added to each sweep direction at the end of physical boundaries. Consistent with the convention used before (Figure 3.1), the wall is at the interface of the first flow cell and the ghost cell, as shown in Figure 3.5. Consequently, the wall boundary condition is automatically enforced for any variable $Q$ when the relation

$$Q(i, j, k) = 2Q_{wall} - Q(i, j + 1, k)$$

is applied at the ghost cell. In this expression, $Q_{wall}$ is the value of the flow variable at the wall. This type of boundary condition implementation at the wall greatly facilitates computation of viscous derivatives of various quantities needed in the viscous fluxes. The boundary conditions for euler fluxes at the wall are applied directly due to simplicity provided with the zero mass-flux condition.

3.3.2 Characteristic Boundary Conditions

The treatment of the boundary conditions is very critical to the success of the simulation. This is especially important in the present simulation model because there are both inflow boundaries and outflow boundaries and at times they may operate at the same time. Characteristic boundary conditions developed for multicomponent mixtures by Baum et al. [7] is used for the present simulation for both inflow and outflow boundary conditions.

3.3.2.1 Outflow Boundary Conditions

At the outflow, numerical disturbances from the computational boundary may propagate back into the problem domain, and hence, may cause deterioration in the solution. Hence,
the condition that waves do not reflect back into the domain should be imposed by the boundary conditions. The characteristic boundaries are in “y” direction. The convective terms can be expressed in the following form

\[
\frac{\partial p}{\partial t} + \rho \frac{c_p}{c^2} (\ell_1 + \ell_{N_i+7}) + \tilde{C}_1 = 0 \tag{3.26}
\]

\[
\frac{\partial \rho v}{\partial t} + \nu \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) + \frac{\rho c_p}{c} (\ell_{N_i+7} - \ell_1) + \tilde{C}_3 \right) = 0 \tag{3.27}
\]

\[
\frac{\partial \rho u}{\partial t} + u \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) + \rho \ell_2 + \tilde{C}_2 \right) = 0 \tag{3.28}
\]

\[
\frac{\partial \rho w}{\partial t} + u \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) + \rho \ell_3 + \tilde{C}_4 \right) = 0 \tag{3.29}
\]

\[
\frac{\partial \rho k^{gs}}{\partial t} + k^{gs} \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) + \rho \ell_4 + \tilde{C}_7 \right) = 0 \tag{3.30}
\]

\[
\frac{\partial p E}{\partial t} + \left( \frac{1}{2} u_i^2 + k^{gs} + \sum_{i=1}^{N_i} h_i Y_i \right) \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) \right) + \rho u \ell_2 + v \frac{\rho c_p}{c} (\ell_{N_i+7} - \ell_1) + \rho w \ell_3 + \rho \ell_4 + \rho \sum_{i=1}^{N_i} (c_p - h_i R) \ell_{i+5} = 0 \tag{3.31}
\]

\[
\frac{\rho Y_1}{\partial t} + Y_1 \left( \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_i+7} + \ell_{N_i+6}) \right) + \frac{R}{R_1} (- \frac{\rho}{T} \ell_6 - \ell_{N_i+6} + \tilde{C}_8) = 0 \tag{3.32}
\]
\[
\frac{\partial \rho Y_j}{\partial t} + Y_j \left( \frac{\rho c_p}{c} (\ell_1 + \ell_{N_s+7}) + \ell_{N_s+6} \right) - \frac{R \rho}{R_j T} \ell_{j+5} + \tilde{C}_{j+7} = 0
\] (3.33)

where terms of the form \(C_1, C_2\) etc. are the viscous terms (not shown for simplicity) and \(\ell_j\) terms are the the amplitudes of the characteristic waves given by

\[
\ell_1 = (v - c) \left( \frac{\gamma - 1}{2} \frac{T \partial \rho}{\rho \partial y} + \frac{\gamma - 1}{2} \frac{T \partial T}{T \partial y} - \frac{c}{2c_p} \frac{\partial v}{\partial y} + \sum_{i=1}^{N_s} \frac{\gamma - 1}{2} \frac{R_i T \partial Y_i}{R \partial y} \right)
\] (3.34)

\[
\ell_2 = \frac{\partial u}{\partial y}
\] (3.35)

\[
\ell_3 = \frac{\partial w}{\partial y}
\] (3.36)

\[
\ell_4 = \frac{\partial k_{gs}}{\partial y}
\] (3.37)

\[
\ell_5 = v \left( \frac{1 - \gamma T \partial \rho}{\gamma \rho \partial y} + \frac{1}{\gamma} \frac{T \partial Y_i}{T \partial y} - \frac{R_i T}{R} \frac{\partial Y_i}{\partial y} + \sum_{i=1}^{N_s} \frac{R_i T}{\gamma R} \frac{\partial Y_i}{\partial y} \right)
\] (3.38)

\[
\ell_{5+j} = v \left( - \frac{R_i T}{R} \frac{\partial Y_i}{\partial y} \right) \quad j = 2, \ldots, N_s
\] (3.39)

\[
\ell_{N_s+6} = v \left( \frac{\gamma - 1}{\gamma} \frac{\partial \rho}{\partial y} - \frac{\rho}{\gamma T} \frac{\partial T}{\partial y} - \sum_{i=1}^{N_s} \frac{R_i \rho}{\gamma R} \frac{\partial Y_i}{\partial y} \right)
\] (3.40)

\[
\ell_{N_s+7} = (v + c) \left( \frac{\gamma - 1}{2} \frac{T \partial \rho}{\rho \partial y} + \frac{\gamma - 1}{2} \frac{T \partial T}{T \partial y} + \frac{c}{2c_p} \frac{\partial v}{\partial y} + \sum_{i=1}^{N_s} \frac{\gamma - 1}{2} \frac{R_i T \partial Y_i}{R \partial y} \right)
\] (3.41)

The characteristic form of the governing equations are solved on the boundary and does not contain any approximation in this form. If the outflow is supersonic, then all the waves leave the domain and imposing boundary conditions is trivial because all characteristics can be computed from the solution inside the domain. However, when the outflow is subsonic, one characteristic wave \((v - c)\) enters the domain. Hence, one condition should be imposed from the outside. Imposing perfectly non-reflecting condition by setting \(\ell_1\) equal to zero is ill-posed [78]. Instead, a fraction of the difference of the pressure between the domain and environment is used as a relaxation parameter to allow smooth behavior on the boundary. Poinos [78] suggests the approximation

\[
\ell_1 = K (p - p_\infty)
\] (3.42)

where \(K\) is a constant that determines the rate of relaxation toward the imposed ambient pressure. A typical value of \(K\) is on the order of \((1 - M^2)c/(2pc_pL)\) where \(M\) is the maximum
Mach number in the domain and $L$ is a characteristic size of the domain. Thus, only $\ell_1$ is imposed while other $\ell_i$'s are computed from the information already known in the domain. This formulation is for an outflow boundary in positive “y” direction. When there is an outflow boundary in the negative “y” direction, the information from outside into the domain is carried by $\ell_{N_s+7}$ and hence the relaxation parameter is applied to this characteristic wave amplitude.

3.3.2.2 Inflow Boundary Conditions

Inflow boundary conditions follow a similar procedure. For a boundary in positive “y” direction, all characteristics except one enter the domain. The characteristic with wave speed $v - c$ is leaving the domain. Hence, either pressure or density should be determined by the flow. In non-conservative form, the governing equations can be written as:

\[
\frac{\partial \rho}{\partial t} + \frac{\rho c_p}{c^2} (\ell_1 + \ell_{N_s+7}) + \ell_{N_s+6} = 0 \tag{3.43}
\]

\[
\frac{\partial T}{\partial t} + (\ell_1 + \ell_{N_s+7}) + \sum_{i=6}^{N_s+5} \ell_i = 0 \tag{3.44}
\]

\[
\frac{\partial u}{\partial t} + \ell_2 = 0 \tag{3.45}
\]

\[
\frac{\partial v}{\partial t} + \frac{c_p}{c} (\ell_{N_s+7} - \ell_1) = 0 \tag{3.46}
\]

\[
\frac{\partial v}{\partial t} + \ell_3 = 0 \tag{3.47}
\]

\[
\frac{\partial k^{gs}}{\partial t} + \ell_4 = 0 \tag{3.48}
\]

\[
\frac{\partial Y_1}{\partial t} - \frac{W_1}{WT} \ell_6 - \frac{W_1}{W \rho} \ell_{N_s+6} = 0 \tag{3.49}
\]

\[
\frac{\partial Y_j}{\partial t} - \frac{W_j}{WT} \ell_{j+5} = 0 \quad j=2, \ldots, N_s \tag{3.50}
\]

In the present formulation, temperature and chemistry is imposed and constant. Thus $\ell_{j+5}$ for $j=2, \ldots, 5$ is zero. From the first species characteristic equation $\ell_{N_s+6} = -(\rho/T)\ell_6$ and from the temperature equation $\ell_6 = -(\ell_1 + \ell_{N_s+7})$. Also velocities are imposed but may be time dependent. From the “y” direction velocity component characteristic equation $\ell_{N_s+7} = -(c/c_p) \frac{\partial v}{\partial t} + \ell_1$. Hence, all characteristics in density equation can be expressed in terms of the outgoing characteristic wave at the inflow. With density known through the
integration of its respective equation, pressure can be computed by the equation of state. Time dependent nature of the velocity imposed is important because it allows specification of random turbulence levels.

The effect of inflow turbulence is simulated by introducing isotropic turbulence data (obtained from a database). The basic features of the data set is reflected in the turbulence parameters, with turbulence intensity level of $u' = 25$ m/sec [86] and the integral length scale of about $l_t = 5$ mm. The data set is interpolated in time (using assumption of frozen turbulence) before applying to the inflow plane.

### 3.4 Piston Motion Algorithm

The combustor of current focus has a piston to convert the thermal energy to mechanical energy. As described earlier, the retarding force to the piston has been provided by a spring mechanism. The trajectory of the piston motion, $x(t)$, is available experimentally. The algorithm described in this section has the ability to follow this trajectory with accuracy over multiple cycles.

For piston kinematics, position $x(t)$ is measured from the ignition wall. In the present study, piston motion is handled by a cartesian cut-cell approach [102]. This method is particularly helpful for moving boundary problems on fixed cartesian grid systems. The method, adapted for the present model, works as follows: at each time step, the displacement of the piston is determined from the known expression $x(t + \Delta t) - x(t)$. Since the time steps of the integration is very small (on the order of $10^{-7}$ sec), usually an interpolation procedure is required to exactly determine the displacement. In this work, a cubic spline interpolation procedure is used.

Based on the computed displacement for the time step, the first layer of cells next to the piston are moved to their new positions. Consider Figure 3.6 where a cut cell (the first cell adjacent to the piston), piston surface and a ghost cell is shown. Subscript “s” is for surface values of the flow variables, while subscript “f” is the flow variables at the first cell (i+1). Depending on the actual piston (moving surface) velocity $u_s$, there can be two situations:
If $u_s > u_f$, the pressure on the wall can be determined from the relation:

$$\frac{p_s}{p_f} = \left(1 - \frac{\gamma - 1}{2} \frac{u_s - u_f}{c_f}\right)^\frac{2\gamma}{\gamma - 1} \tag{3.51}$$

In this case, both waves (left and right) from the surface are rarefaction waves. However, if $u_s < u_f$, the waves moving right and left are both shock waves. Thus, normal shock relations are used to obtain the pressure on the surface

$$\frac{p_s}{p_f} = 1 + \frac{(u_f - u_s)^2}{2C^2_f} + \frac{(u_f - u_s)^2}{2C^2_f} \sqrt{\frac{8\gamma}{\gamma + 1} C^2_f + (u_f - u_s)^2} \tag{3.52}$$

where $C_f = 2p_f/(\gamma + 1)\rho_f$ and $\rho_f$ is the flow density at the first cell. With the surface value of pressure known, all other variables at the ghost cell can be computed by a procedure similar to wall boundary conditions described before.

During piston motion, the cell adjacent to the moving surface will change in volume\(^1\). Hence, to maintain accuracy and stability, maximum and minimum cell volumes are specified as $V_{\text{min}} = 0.55V_{\text{ref}}$ and $V_{\text{max}} = 1.55V_{\text{ref}}$ where $V_{\text{ref}}$ is the volume of the original cell in the fixed grid (i.e., no piston motion). As the volume increases (or decreases) with respect to the reference value, volume limitations are enforced through cell merging and cell creation, as depicted in Figure 3.7.

For example, “cell creation” is applied during the expansion stroke when the volume of cell $(i+1)$, $V(i+1)$, becomes larger than $1.55V(i+1)_{\text{ref}}$, where $V(i+1)_{\text{ref}}$ is the reference value. When this condition is detected, cell $(i+1)$ is split into cells $(i)$ and $(i+1)$. As a result

---

\(^1\)Others do not change because they are treated on a fixed grid.
of this operation, the volume of the new cell (i+1) is equal to its reference value \( V(i)_{ref} \). The volume of cell (i) is determined from the condition that \( V(i) + V(i+1) \) after the operation is equal to \( V(i+1) \) before the operation.

On the other hand, “cell merging” is applied during the compression stroke when the volume of cell (i), \( V(i) \), first becomes smaller than 0.55\( V(i)_{ref} \). When this condition is detected, cells (i) and (i+1) are merged to create the cell (i+1). Hence, the first flow cell becomes (i+1), with the ghost cell now being represented by index (i). The volume of cell (i+1), \( V(i+1) \), after the operation is equal to the sum of volumes \( V(i) \) and \( V(i+1) \) before the operation.

During this process, the conservation principle is used for flow variables in their new state with respect to their previous state. For example, in the cell creation process, the volume weighted sums of any variable in cells (i) and (i+1) after the operation is equal to volume weighted sum of cell (i+1) before the operation. Similarly, in the cell merging process, the volume weighted sum of any variable in cell (i+1) after the operation is equal to the volume weighted sums of cells (i) and (i+1) before the operation.

### 3.5 Modeling the Mass Loss from Engine

Leakage due to poor sealing have a penalizing impact on any engine work output. This has been reported to be the case for the present engine [19] as well, and shown to cause
variations in peak pressures obtained from the cycle. The effect of mass losses between the piston and engine body is modeled in a simplified manner. The main assumptions are that of quasi-one dimensional isentropic flow and constant leakage area. Hence, the total mass flow rate out of the combustion chamber, \( \dot{m} \), for a subsonic flow is given by

\[
\dot{m} = C_d A_t \frac{p_0}{RT_0} (\gamma RT_0)^{1/2} \left( \frac{2}{\gamma - 1} \left[ \left( \frac{p_s}{p_0} \right)^{2/\gamma} - \left( \frac{p_s}{p_0} \right)^{(\gamma+1)/\gamma} \right] \right)^{1/2} \tag{3.53}
\]

where \( A_t \) is the area gas escapes, \( C_d \) is a coefficient of discharge, \( \gamma \) is the ratio of specific heats, \( p_0 \) and \( T_0 \) are the stagnation pressure and temperature and \( p_s \) is the pressure near the sealing [82]. If the flow is sonic [82], \( p_s/p_0 < (2/(\gamma + 1))^{\gamma/(\gamma - 1)} \), \( \dot{m} \) is expressed as

\[
\dot{m} = C_d A_t \frac{p_0}{RT_0} (\gamma RT_0)^{1/2} \left( \frac{2}{\gamma + 1} \right)^{(\gamma+1)/(2(\gamma-1))} \tag{3.54}
\]

In these equations, \( C_d \) is a tunable coefficient and its value is determined by matching the experimental pressure data. Determining the coefficient is further explored in the next chapter. In actual implementation of the mass loss algorithm, this total mass loss rate \( \dot{m} \) is distributed in the combustor based on a weighting function. Thus, \( \dot{M} \), the mass loss from any computational cell, is obtained from the total mass loss rate using the following expression

\[
\dot{M} = \frac{\dot{m}}{V} C_d (\gamma - b/2)^6 \tag{3.55}
\]

where \( (\gamma - b/2)^6 \) is a sixth order polynomial serving as the weighting function (see Figure 3.8). Here, \( V \) is the combustor clearance volume and \( b \) is the combustor width in “y” direction (50.8 mm). The sum of mass loss rate from each cell is equal to the total mass loss rate, as expressed in Equation 3.56.

\[
\dot{m} = \int_0^b \dot{M} dy A \tag{3.56}
\]

\( C_d \) in Equation 3.55 is a coefficient to make LHS of Equation 3.56 equal to its RHS. “dy A” is the local cell volume. This formulation based on the weighting function is employed for two reasons: (1) the details and exact mechanisms of how mass leakage occurs are not known in the experimental system, and (2) resolving the sealing region to simulate the “exact” blow-down process through the governing equations is computationally expensive.
Figure 3.8: The mass loss weighting function, \((y - b/2)^6\), across the combustor width. y direction is (shown in x axis) is given in meters, corresponding to 50.8 mm.

The primary objective is to develop a model that will predict the estimated mass loss from the system (explained in the next chapter). As can be seen in Figure 3.8, most of the mass loss in the model happens near the boundaries and the bulk of the combustor in the middle section is effectively treated with no mass loss.

The effects of the local mass loss rate are included as source terms in the governing equations (chapter 2). These source terms are

\[
S_1 = M
\]

\[
S_{i+1} = u_i \dot{M}, \quad i=1,2,3
\]

\[
S_5 = HM
\]

where H is the enthalpy per unit mass and \(u_i\) is the velocity in “i” direction.

3.6 Modeling The Ignition Process

Details of ignition are not modeled. This would require an advanced chemistry mechanism and very fine computational cells. Instead, internal energy of \(r_i = 4\) mm radius zone is increased steadily over a period of \(t_{ign} = 300\) µsec after which a self sustaining flame is
obtained. Figure 3.9 shows the assumptions used in the modeling. In particular, the energy deposition rate per unit volume, $E_0$, is applied to every computational cell bounded by the ignition kernel region (Figure 3.9) with a weighting factor of the form

$$E_i = \frac{E_0}{1 + e^{r/r_i}}$$

(3.60)

which helps maintaining a smooth transition across the kernel to remove numerical instabilities. A plot of the weighting factor is given in Figure 3.9 (b). Total energy deposited in the combustor per unit time is $E_{tot} = \int_V E_i dV$. The amount of total energy, $E_{tot} = \int_{t_0}^{t_{ign}} E_{tot} dt$, deposited over the entire ignition period is on the order of 170 mJ.

3.7 Algorithm Summary

The numerical methodology developed in this study is shown in Figure 3.10. The first step is to initialize the algorithm, described by “Initialization” box, where all parameters of the problem are obtained from user input. This step also includes reading the fixed grid (which will need to be modified during the integration), creating the Parallel Domain Decomposition architecture used by MPI and dynamic allocation of arrays used for storing flow variables.

Each integration time step starts with determining the maximum allowed time step in the entire computational domain (Compute Time Step). The next task represented by
Piston Motion is central to the operation of the engine code. Several jobs are handled in this part: First, the piston position is determined along the piston trajectory based on the physical time and the time step. Depending on the velocity and the position of the piston, various control logics are queried to determine if the piston simply needs to be moved or if any other cell modification approach (i.e., cell creation or cell merging) needs to be enforced. Depending on the nature of cell modification, reinitialization of boundary cells and re-computation of MPI parameters (such as processor neighborhood and send/receive buffer lengths etc.) are carried out. Note that, during the cell merging and cell creation procedures, the indexing of the computational grid changes. In other words, the array sizes either decrease (cell merging) or increase (cell creation). This dynamic nature of the problem needs to be observed to efficiently use the computational memory. For example, some of the arrays are dynamically re-allocated and re-initialized during the computations to reflect these requirements. In addition, since the grid changes near the boundary, all grid parameters (such as volume, metrics, area vectors) are recomputed at regions close to
the piston boundary. Furthermore, various control parameters that affect the operation of other tasks in the engine methodology are determined here. These include ignition timing, exhaust port opening/closure timings and intake timing.

The integration step is described in **Predictor/Corrector**. Here, several important tasks are carried out. These include enforcing the boundary conditions (**Apply B.C.**), adding the ignition source term to affected computational cells (**Ignition Source**), determining the amount of mass loss over the time step (**Mass Loss**), the computation of fluxes (**Compute Fluxes**) and finally determining the new values of flow variables after the integration (**Update Time Level**).

Along the trajectory of the piston, the evolution of the flow variables is tracked by taking snapshots of the flow field at every 1 mm piston motion (**Statistics and Output**). Both the instantaneous and the time averaged (over the 1 mm interval) such snapshots are produced by the numerical methodology, facilitating the interpretation of the unsteady and periodic physics. The implementation of the feature that collects such output only at discrete spatial displacements (as opposed to fixed time intervals) is related to the periodic nature of the flow.

After the desired simulation time is reached, the computations are stopped (**Finalize**).

Typical simulation times are given in Table 3.5. In general, both models have comparable run times for similar grids.

<table>
<thead>
<tr>
<th></th>
<th>LES (Grid-1)</th>
<th>LES (Grid-2)</th>
<th>RANS (Grid-1)</th>
<th>RANS (Grid-2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1472</td>
<td>9744</td>
<td>1344</td>
<td>8736</td>
<td></td>
</tr>
</tbody>
</table>

**Table 3.5**: Single processor computational time (in hours) required for simulating a single cycle. All runs were completed on a parallel platform with 3.6 GHz Intel Xeon EM64T processors.
CHAPTER 4

ENGINE OPERATIONAL PARAMETERS

The present LES formulation has been successfully applied in a variety of flow conditions (both premixed and nonpremixed) in the past. In this thesis, the potential of LES in engine conditions is investigated. The geometry chosen for this is a spring driven engine concept as detailed in the experimental work of Disseau [19]. As will be discussed later in this chapter, some of the important boundary conditions and intake conditions are not unambiguously clear from the experimental work. Here, an effort is made to determine those conditions to proceed with more realistic operational parameters. Therefore, the numerical predictions presented here are necessarily dependent on these assumptions. Nevertheless, it will be shown that the assumptions are indeed realistic (i.e., as deduced from typical pressure-time data) and that the simulation results are able to recover those operational parameters in a cyclic manner.

4.1 Estimating The Operational Characteristics

A complete set of operational data is not available to make computational studies as close as possible to real engine run conditions. To establish a well posed problem, two important parameters, the mass trapped and the mixture temperature (average) at Exhaust Port Closure (EPC) on return stroke, are needed. However, these two quantities are not available. The pressure-volume signal over several cycles is the only experimental data for the combustor. Hence, in this thesis, an exact set of values will not be used. Instead, an analysis below is used to estimate important parameters to eliminate uncertainties as much as possible.

From preliminary CFD work, it was determined that the scavenging physics is very complex and it is only partially efficient at purging the burned mass from the previous cycle (about 10% of the total mass is burned products at EPC). This burned product volume is trapped in the center (approximately) of the combustor due to a tumbling motion. This
tumbling motion (as explained later) forms due to an impinging intake jet with the start of scavenging period. Hence, at EPC, the temperature should be somewhere between the inlet temperature (300 K) and the burned product temperature (which is not uniform, but found to be between 500-600 K). Experimental data [19] gives the exhaust temperature as 407 K. However, it must be mentioned that during scavenging, heat transfer from burned products to fresh reactants would elevate temperature of the latter. Hence, a simple weighting based on scavenging efficiency to determine a mean temperature at EPC is not trivial.

This problem can be approached by first assuming that from EPC to the ignition point, there is no appreciable mass loss. If we assume a certain temperature to be the average temperature at EPC, then from this point to the ignition point, the mass should be constant. Since the pressure and the volume is available experimentally at any given time during a typical cycle and the compression index is known from Figure 4.1, the temperature can be determined from this information by

$$T / T_{EPC} = (V / V_{EPC})^{1 - n_c}$$  \hspace{1cm} (4.1)$$

where the subscript “EPC” corresponds to conditions at EPC. The mass trapped then can be estimated from the equation of state (with a further assumption that an average gas
constant can be used, here we take $R_{\text{gas}} = 285 \text{ J/kg} \cdot \text{K})$. Results of such an analysis are shown in Figure 4.2 where four different initial conditions at EPC (400 K, 450 K, 500 K and 550 K) were used. The polytropic compression assumption works fairly well and the mass estimated is almost constant. Here, increasing pressure on the “x” axis corresponds to compression approximately from EPC to ignition.

Note that, it is only a matter of convenience to choose one of the temperature values at EPC for the purposes of the present study. Once $T_{EPC}$ is chosen, the impact of these EPC conditions on the peak pressures at TDC (assuming complete combustion) is shown in Figure 4.3. These results are obtained by invoking the equation of state at EPC and TDC (with appropriate values of the gas constant). Here, in addition to the temperature at TDC (which indirectly gives the effect of heat loss on the temperature obtainable at TDC), total mass loss is also included in the computations as a parameter. The EPC temperature range covered in these computations is typical of two-stroke engines. If there is no heat loss (i.e., adiabatic system), then the temperature at TDC would be the adiabatic flame temperature at constant volume. For propane-air flames (at equivalence ratio of 1), it corresponds to approximately 3050 K, with initial gas temperature of 500 K and specific heats for products computed at 1500 K. Also shown in the same figure is the window of the maximum and minimum pressures obtained from individual cycles in the experiment (closed
Figure 4.3: Peak pressure that can be obtained from a typical cycle as a function of $T_{TDC}$ and mass loss rate. Complete combustion is assumed. Experimental data (maximum and minimum values of several cycles) is shown with the closed rectangular box.

rectangular box). Results of this simple thermodynamic analysis seem to indicate that for all cases the mass loss from the combustor should be at least about 30% of the trapped mass at EPC. However, as reported elsewhere [19], the true extent of the mass loss is not known.

For the present study, the temperature at EPC is chosen to be $T_{EPC} = 500$ K. As noted before, this choice is somehow arbitrary and the temperature at EPC can be some other value. The parameters that can affect this value are primarily the efficiency of scavenging, the wall temperatures and the heat transfer between the product gas and the incoming charge mass. For instance, with perfect scavenging, all charge is composed of reactants with a temperature very close to the ambient condition. On the other hand, if the temperature of the combustor walls is larger than the ambient conditions, the charge will be heated to a higher temperature. Based on the simple analysis given above, the expected mass loss
Table 4.1: Assumed operational parameters of the experimental engine used in the present study. Note that $T_{EPC}$ and $m_{EPC}$ are somehow arbitrary, and their values are the result of the order of magnitude analysis as presented in this section.

<table>
<thead>
<tr>
<th>$T_{EPC} (K)$</th>
<th>$m_{EPC} (kg)$</th>
<th>$p_{EPC} (atm)$</th>
<th>$V_{EPC} (m^3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>$8.97 \times 10^{-6}$</td>
<td>1.54</td>
<td>$8.19 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

from the engine is about 30-40% of the trapped mass (at EPC). For clarity, the operational values for the real engine at EPC are given in Table 4.1.

4.2 Determining Operational Parameters

Numerical prediction of the engine pressure signal over multiple cycles (Figure 4.5) requires two critical aspects of the flow field to be accurately estimated. These are the EPC conditions (described above) and EPO conditions (in the expansion stroke). The requirement of accurate prediction of EPO conditions is obvious since it sets the dynamics (or initial conditions) of the next cycle.

The EPC conditions needs to be matched by adjusting the mass flow rate during the intake phase. The EPO conditions, on the other hand, can only be matched if the combustor pressure after ignition is accurately predicted. This can be achieved by reasonable levels of turbulence intensity near TDC (due to its effect on turbulent flame speed) and a close match of the mass loss rate in the combustor. The mass loss rate can be estimated by adjusting the mass loss coefficient using the formulation described in the previous chapter.

The strategy employed for this task can be summarized as follows: (1) Assume thermodynamic conditions at EPO to start the intake phase. Adjust mass flow rate to match EPC conditions as a result of this single cycle scavenging phase simulation. (2) Start computations at EPC based on conditions obtained in (1) and adjust mass loss rate to predict the peak pressure so that EPO conditions can be matched.

These two tasks are addressed in the next two subsections.
4.2.1 Inflow Conditions and Initialization at EPO

The computations are started at just before Exhaust Port Opening (EPO) (see Figure 4.1). At this instant, the mixture is assumed to be fully burned since unburned hydrocarbon (UHC) levels are usually small in typical SI engines [42]. Pressure is taken as 3 atm. (after inspection of the experimental pressure signal). Temperature is estimated to be about 1500 K at EPO using the polytropic relation (of the expansion phase, see also Figure 4.1). Velocities are set to zero. These conditions will be termed as the “starting solution”. With EPO, the assumed mass flow rate and turbulence levels are used to simulate the intake phase to create a combustible mixture to be burned near TDC.

The crucial step in this single cycle run to determine the realistic initial conditions was to reproduce high turbulence levels near TDC so that combustion can be completed and the return stroke of the piston can be reasonably predicted to successfully start the next cycle (of preliminary runs). Furthermore, the injection velocity should be determined to be able to reproduce the operational parameters. Hence, it is clear that the intake phase has a significant impact on the whole process.

In this study, the the mean injection velocity, \( U_{\text{mean}} \), is time dependent and selected to match the estimated trapped mass at EPC. Since the density at the inflow plane is computed as part of the solution, the mean injection velocity is computed at each instant from solving the following equation

\[
\int_S \rho U_{\text{mean}} dS = \dot{m}_{\text{flow}}
\]

where the integration is over the injection plane that represents the injection pipe (see Figure 3.2). After determining the mean injection velocity, turbulent fluctuations \( (U') \) of order 15% of the mean is added to obtain the injection velocity, \( U_{\text{inj}} = U_{\text{mean}} + U' \).

A representative mass build-up in the combustor is shown in Figure 4.4 for several cycles of LES simulation. This computation corresponds to \( \dot{m}_{\text{flow}} = 1.46 \times 10^{-3} \) kg/sec. Accordingly, the computed values of \( U_{\text{mean}} \) are about 170 m/sec. Note that, at EPC (shown in the same figure) the trapped mass is predicted to be about \( 9 \times 10^{-6} \) kg, which very closely matches the targeted operational value in Table 4.1 and corresponds to the 500 K line in
Figure 4.4: A typical mass build-up (left axis, solid line) in the combustor as a function of time for LES simulation during Cycle-3 (see Figure 4.5). Piston trajectory (right axis, dot-dashed line) is also shown during this period.

Figure 4.5: Time history of the experimental pressure signal. The initial conditions for cycle 3 are obtained from the conditions of cycle 2 just before EPO. As a convention used in this study, a particular cycle is identified between two EPO positions.
4.2.2 Mass Loss Rate Estimation

The thermodynamic arguments in this chapter gave an indication on the order of mass loss in this research engine. The present LES method has an algorithm to predict this effect by a mass loss formulation (as described in Chapter 3), controlled by an adjustable coefficient, $C_d$. By successive simulations, this parameter can be found by interpolation from predicted pressure signal. However, the process can be too costly if good starting values of $C_d$ is not approximated. To efficiently estimate a value for this parameter a priori, the experimental signal can be used. Note that, the following equation holds between EPC and EPO

$$m = m_0 - C_d \int_{t_{EPC}}^{t_{MLR}} (\dot{m}/C_d) dt$$

(4.3)

where $m$ is the instantaneous mass, $m_0$ is the mass at EPC and $\dot{m}$ is the mass loss rate (Equation 3.53 or 3.54). Manipulating this expression gives MLR (percentage loss relative to $m_{EPC}$) as a function of an integral expression

$$\frac{100}{m_0} \times C_d \int_{t_{EPC}}^{t_{MLR}} (\dot{m}/C_d) dt = \frac{m_0 - m}{m_0} \times 100 = MLR$$

(4.4)

from which $C_d$ is obtained as

$$C_d = \frac{MLR \cdot m_0}{100 \times \int_{t_{EPC}}^{t_{MLR}} (\dot{m}/C_d) dt}$$

(4.5)

In the numerical results, this formulation is used between EPC and $t_{MLR}$. Here, $t_{MLR}$ is the time at the expansion stroke 1 msec after the TDC. Evaluating this expression for MLR=35 gives a value of $C_d = 6.5 \times 10^{-2}$. Results of model simulations with this value closely matched experimental peak pressure. However, determination of the final value used in the present study is deferred to the next section.

4.3 Final Parameters and Initialization

The single cycle simulation described above is carried out several times until the assumed operational parameters can be consistently recovered with reasonable accuracy at EPC and EPO. As a result of this process, initial conditions that will be used for the detailed analysis of numerical predictions are expected to be better represented. In other words,
Figure 4.6: Predicted pressure development in the combustor using LES model. Mass loss coefficient selected as $C_d = 7.1 \times 10^{-2}$.

Computations of several cycles (4 of them were conducted here) are assumed to relax some of the limitations of the starting solution (zero velocity, assumption of fully burned products, and assumptions of $T=1500$ K and $p=3$ atm).

Consequently, the conditions of the fourth cycle (of preliminary simulations) at EPO are used for the real initial conditions of the third cycle (see Figure 4.5). The first two cycles of the experimental signal is not used in the quantitative comparisons presented later due to uncertainty caused by transient start-up phenomena in the experiments. The remaining 3 cycles are simulated in this work, as detailed in the next chapter.

During these multiple preliminary runs, mass loss coefficient is further adjusted. The final value that best represents the third cycle was $C_d = 7.1 \times 10^{-2}$ for LES and $C_d = 7.0 \times 10^{-2}$ for RANS. Result of LES simulation with the final value of the mass loss coefficient is shown in Figure 4.6. Corresponding pressure curve with RANS analysis is shown in Figure 4.7.

The computational results predict all features of the measured signal in good agreement,
with subtle differences around TDC. The compression stroke and expansion stroke closely follow the measured data. It is obvious that especially these parts of the pressure-volume curve is very dependent on the earlier parts of the cycle. For instance, an inconsistent pressure rise following the combustion (a function of mixture composition) in computations would give a different compression and expansion curve.

The presented numerical pressure-volume diagrams establish that the numerical algorithm (i.e., the LES/RANS method, mass loss formulation, ignition details etc.) is able to give a very close picture of the complete engine cycle, including the ignition and scavenging phases. As mentioned in the beginning of this section, the assumptions used to obtain Figure 4.6 and Figure 4.7 are the final parameters for the detailed numerical analysis of the engine in the remainder of the present study.

The methodology described above for the initial conditions, while not ideal, is simple enough to make both set of computations (i.e., LES and RANS) consistent with each other.
CHAPTER 5

ANALYSIS OF THE HIGH AR ENGINE

In this part of the present work, a more detailed analysis of the engine cycle described in the previous chapter is carried out. The results presented are based on the assumed operational parameters described earlier.

There are several objectives that need to be realized. Having established that the numerical methodology is able to predict pressure variation (previous chapter) in the combustor across several cycles with reasonable accuracy, the underlying physics and flow development need to be studied. This aspect of the high aspect ratio combustor has not been studied before and a physical understanding is urgently needed. Among topics of interest are the physics of the scavenging phase, the efficiency of the scavenging, the nature of turbulence, the mixture strength near TDC, flame propagation, and causes of cyclic changes.

5.1 Observations on Flow Development

The evolution of the flow field during a typical cycle (full two-stroke) is given for LES in Figure 5.1 and for RANS in Figure 5.2. In what follows, the scavenging period is to be understood as the time interval between EPO and EPC.

The streamline pattern in these figures reveals clearly main pathways and interaction regions between incoming reactants and burned products. The sequence starts at the time of EPO and evolves one cycle. Figure 5.1 (a) is the exhaust blowdown period. This is a fairly fast process, taking about 1 msec. In the next snapshot (b), the fuel is introduced by an inclined jet (35 degrees with the lower wall) which impinges on the facing wall (right wall) and starts to form a recirculating region in the middle of the combustion chamber.

The incoming reactants have two routes to follow, i.e., the top and bottom port openings which serve as exhaust regions. The inlet jet is a high velocity stream and immediately establishes several vortical structures in the combustor. These regions are wall dominated
Figure 5.1: Streamline pattern for a complete cycle as simulated by LES model using Grid-1. Each subfigure is accompanied by the information of piston distance to TDC ($x_{TDC}$) in (mm). Piston is on the left, and ports are in the lower and upper sides of each frame, situated at 25.4 mm from the right wall. Tics are located every 8 mm intervals on the horizontal axis, and every 10 mm on the vertical axis.
Figure 5.2: Streamline pattern for a complete cycle as simulated by RANS model using Grid-1. Each subfigure is accompanied by the information of piston distance to TDC ($x_{TDC}$) in (mm). Piston is on the left, and ports are in the lower and upper sides of each frame, situated at 25.4 mm from the right wall. Tics are located every 8 mm intervals on the horizontal axis, and every 10 mm on the vertical axis.
separation regions in the lower wall and the right wall near the stagnation region. In most
snapshots of the scavenging period (subfigures (c), (d), (e) and (f)), the dominant feature is
the center recirculation region, which has a rotation vector normal to the piston direction.
This type of motion is generally called a “tumbling motion” and used in traditional engines
with canted valves as a means of enhancing turbulent state of the flow prior to ignition. It
should not be confused with swirl, which has a rotation vector parallel to the axis of motion.

In the present engine, the tumbling motion is a necessary consequence of the geometry.
It also traps some of the burned products from the previous cycle and, hence directly affects
the efficiency of the scavenging process. The prediction of the numerical simulation results
on charging efficiency will be quantified later.

With the piston approaching to EPC (25.4 mm from TDC), part of this recirculating
region is pushed through the ports, as evidenced in Figure 4.4 where the mass in the
engine is decreasing. However, most of this loss is actually due to incoming reactants short-
circuiting the tumble region and escaping through the opposite port (cross scavenging). This
is due to reduced engine volume, leaving little space for the reactants to sustain the tumble
recirculating region as evidenced in the return part of the scavenging phase (Figure 5.1 (e)
and (f)) where the other escape route (bottom port) is progressively closed by the piston.
Since the tumbling motion is dynamic, it does not cease to exist immediately. Rather it
starts to disintegrate slowly, deformed by the highly strained flow, leading to fine scale
turbulent motion after EPC (Figure 5.1 (g)). Figure 5.1 (h) is a snapshot of the ignition
period. The last snapshot (i) is after the combustion is complete and the piston is in the
expansion stroke.

Because of the high momentum of the incoming reactants, the bottom port is very
active in maintaining a viable engine. This somehow confusing result is due to the fact
that it increases the residence time of the incoming reactants in the engine by providing an
alternate route (loop scavenging). Since this engine is very small with a very high-velocity
incoming jet, it is important that a mechanism be present to help achieve an optimum
residence time. Without this, the efficiency parameters of the engine would be worse since
the sequence of events would follow the return part of the scavenging period (which clearly
Figure 5.3: Experimental visualization of scavenging. Shadowgraph (a) and its sketch (b) shows a vortical region adjacent to the lower wall and the exit way for reactants through the upper port. Reproduced from [19].

shows an inefficient scavenging by short-circuiting) from the beginning of the scavenging phase, not in the second half of it. However, the tumbling motion also acts as an inefficiency source (i.e., the trapped products by the tumble motion). The discussion also reveals that the present form of this engine would be less efficient with a smaller stroke.

The RANS predictions in Figure 5.2 show the same mechanisms in the engine, in terms of scavenging characteristics. In particular, the formation of the tumble vortex is predicted by RANS, in qualitative agreement with LES. However, in RANS closures all scales are modeled, and therefore they are very dissipative. This is obvious in the RANS streamlines where intense smearing of flow structures is clearly seen. LES, with its account of turbulent viscosity by use of dynamically computed model coefficients, exhibited an unsteady picture of the flow. For example, there is a small recirculation zone right next to injection port with the wall as predicted by LES (Figure 5.1 (f)). A similar zone is not observed in RANS results due to excessive dissipation. Experimental visualization (Figure 5.3) reveals a flow field at this instant fairly close to LES.

What eddy viscosity accounts for in LES is not the same as in RANS. LES eddy viscosity only computes scales smaller than sub-filter level and accordingly a significant part of the turbulent spectrum is already computed explicitly. An indication of these arguments is manifested in the volume averaged turbulent viscosity for each model as shown in Figure 5.4. Consistent with the underlying averaging procedure (spatial for LES and ensemble-time for RANS), LES gives much smaller turbulent viscosity, hence less dissipation. RANS gives turbulent viscosity levels an order of magnitude larger than LES.
Figure 5.4: The volume averaged ratio of model predicted turbulent viscosity to molecular viscosity obtained from LES solution and RANS for GRID-1. Also shown is the piston position in (mm).

Figure 5.5 shows the variation of fuel mass fraction and mean temperature in the combustor as a function of time and position. The TDC positions of streamline snapshots can be compared to piston trajectory of Figure 5.5 to find the average quantities across the combustor. For example, inspection shows that 46.4 mm from TDC (Figure 5.1 (c)), the average temperature and the fuel mass fraction are about 700 K and 0.03, respectively. Fuel mass fraction prediction (Figure 5.5) shows that LES prediction is larger than the RANS prediction. A possible reason is that the trapped mass (burned) predicted by RANS may be larger due to less efficient scavenging. This is related to the efficiency of large scale mixing. If the tumble vortex continues to exist (without much disintegration), an obvious consequence would be reduced large scale mixing. Hence, ultimately, the success of scavenging predictions is related to how well the fluid mechanics is predicted. Instantaneous snapshots (shown later) of mass fraction close to and after EPC might relate the observed mass fraction behavior (between models) and the tumble vortex structure. For example, comparison of Figure 5.1 (g) and Figure 5.2 (g) already implies that the interaction would
Both models predict similar global features, with reservations noted above. However, detailed analysis of scalar quantities (i.e., temperature or fuel mass fraction) and velocity field will give more insight about the success of either one of the simulation models. Modern understanding of flame propagation in premixed systems suggests that mixture preparation as well as its underlying flow structures need to be properly captured by any model for a successful simulation. For example, a model should be able to predict flame extinction as result of high stretch rates. Therefore, how realistically velocity field and its properties are computed does matter. This is indeed the main requirement, assuming that a reasonable success in the mixture preparation is achieved. Moreover, upon flame initiation, mixing of
cold reactants and burned products are essential, again implying dependence on velocity field. The implications of these topics are deferred to later parts of this work.

5.2 Description of the Scavenging Phase

5.2.1 Unsteady Flow Features

Instantaneous snapshots that describe the evolution of velocity, temperature and fuel mass fraction are presented next. Since the flow is periodic, a sequence of such snapshots is necessary to identify how the flow is developing.

The development of reactant jet is given in Figure 5.6 for LES and Figure 5.7 for RANS. As established in the streamline pattern, the tumble vortex is created as a result of the interaction between the fuel jet and combustor facing wall (right side in each figure). In the beginning of the scavenging period, there is no coherent flow structure in the combustor. This is revealed in Figure 5.6 (a) where the reactant jet has just been introduced. The maximum flow velocities in the jet core are on the order of 180 m/sec. This number is determined from mass flow rate considerations as developed in the previous chapter. The Reynolds number based on the mean jet velocity and the injector pipe diameter is 43750. Therefore, the jet development is expected to be turbulent. It takes about 10 mm from EPC for the tumble vortex to form, as can be seen in the second snapshot (b). At this instant, the jet has deflected from facing wall and the upper wall. The tumble vortex core is beginning to form between incoming jet and the deflected jet. In the third frame (Figure 5.6 (c)), the vortex is fully established. At this instant, velocity values confirm the observation made during the interpretation of streamline pattern that the flow is mostly recirculating and the jet has both upper ports and lower ports as exit routes. This picture starts to change in the return part of the scavenging phase as shown in the fourth frame (d). The flow is compressing and the immediate effect of this is to decrease the relative importance of the lower port. This establishes the upper port as the only exit route.

As described in the previous chapter, the actual efficiency of the lower port during the expansion part of the scavenging phase (frames (a), (b), and (c)) is not known. The port width is 12.7 mm and the injector tube is located slightly off the combustor inlet plane. Its
Figure 5.6: Instantaneous velocity magnitude field predicted by LES. Snapshots start from EPO and end at EPC. Main flow structure is the tumble vortex, as can be identified at the center of the combustor. Results are for the center combustor plane at half the combustor thickness.
Figure 5.7: Instantaneous velocity magnitude field predicted by RANS. Snapshots start from EPO and end at EPC. Results are for the center combustor plane at half the combustor thickness.
diameter is about 3 mm. The jet is assumed to have a larger diameter at the combustor inlet plane due to the fact that the jet develops between the exit plane of the injector tube and combustor inlet plane. The exact value for the off-set distance, however, is not known. Nevertheless, half of the lower port is used as an exit port in the present study when the inflow starts. Therefore, in the return part of the scavenging phase just before EPC (frame (e)), the short-circuiting of the incoming jet becomes very dominant since exhaust segment of the lower port is progressively closed by the piston.

The developments of temperature and fuel mass fraction are shown in Figure 5.10 and Figure 5.8 for LES. Both fuel mass fraction and temperature fields essentially show similar evolution through the entire cycle. High temperature regions are associated with burned products and low temperatures are associated with fresh reactants. It is obvious that both displacement of burned products and mixing between the cold gases and hot gases are occurring at the same time. Because of the tumble vortex, however, there is a portion of the burned products trapped in the middle of the combustor, revealed both in the temperature and fuel mass fraction figures. At the time of port closure in the return stroke (Figure 5.10 (f) and Figure 5.8 (f)) there is non-homogeneity in the mixture composition.

RANS predictions of velocity, temperature and fuel mass fraction are presented in Figure 5.7, Figure 5.11 and Figure 5.9, respectively. Main vortex structure is also predicted to be developing similar to LES predictions, as revealed in the RANS velocity plot. One difference, however, is the fact that vortex is less diffused when compared to LES results. This is due to the fact that viscosity is much higher (quantified previously) in RANS and large scale vortices that result in entrainment between cold and hot gases are damped. This is clearly seen in RANS temperature and fuel mass fraction results where the trapped burned products continue their existence during the entire scavenging phase. It is also revealed that at EPC, the vortex in LES predictions starts to lose its coherence while for RANS predictions no such observation can be made. The presence of a still strong vortex might have a strong influence on the combustion period. Ideally, its decay is desired from combustion perspective since it will promote more mixing and homogenization of the mixture (after EPC) and corresponding increase in turbulence intensity.
Figure 5.8: Instantaneous fuel mass fraction field predicted by LES. Snapshots start from EPO and end at EPC. The effect the tumble vortex (see Figure 5.6) on burned product trapping is clearly seen. Implications on efficiency are discussed in the text. Results are for the center combustor plane at half the combustor thickness.
Figure 5.9: Instantaneous fuel mass fraction field predicted by RANS. Snapshots start from EPO and end at EPC. The effect of the tumble vortex on the burned product trapping is more dramatic compared to LES results (c.f. Figure 5.8). Results are for the center combustor plane.
Figure 5.10: Instantaneous temperature field predicted by LES. Snapshots start from EPO and end at EPC. See also the corresponding mixture strength in Figure 5.8. Results are for the center combustor plane at half the combustor thickness.
Figure 5.11: Instantaneous temperature field predicted by RANS. Snapshots start from EPO and end at EPC. Results are for the center combustor plane.
Note that the results for development of flow variables are shown here for a single cycle simulation. Therefore, the sequence of events described above may or may not repeat itself in terms of achieving similar (or exact) flow patterns. Therefore, these need to be compared to realizations from other cycles so that a better quantitative interpretation can be obtained. This would reveal model performance and its sensitivity in modeling cyclic behavior. These aspects related to cyclic variability are discussed later in this work.

5.2.2 Mean Flow and Turbulence Statistics

Development of turbulence statistics and mean flow has practical significance for design. For example, identifying regions of high shear and turbulence intensity may help evaluate their efficiency in obtaining favorable turbulent flow conditions during subsequent stages of the cycle. For this task, first and second moments of velocity are computed (time-averaged in time intervals corresponding to 1 mm of piston displacement).

Figure 5.12 shows the mean velocity distribution, $\bar{u}$, $\bar{v}$ and $\bar{w}$ at a position 48 mm from TDC. Corresponding RANS plots are given in Figure 5.13. Comparing the mean velocity field of both models with their instantaneous counterparts (Figures 5.7 and 5.6, middle row, right), it is immediately clear that averaging does not alter the main characteristics of the flow field. In particular, the location of the tumble vortex and the jet development look reasonably similar. Moreover, the mean LES velocity field is very similar to the RANS prediction except in the recirculation region (lower right corner). Moreover, the tumble vortex is stationed in the middle of the combustor (approximately) for both models (LES and RANS).

Figure 5.14 and 5.15 show the mean velocity components through the center of the vortex. This indicates clearly that the vortex structure is that of solid body rotation type. In this case, a tangential velocity of the form $V = \omega r$ can be defined with respect to the vortex center, where $r$ is the distance to the vortex center and $\omega$ is the angular velocity (rotation rate). The rotation rate in the RANS simulation is computed to be about $\omega \approx 2270$ (rad/sec). The LES prediction of the rotation rate is about $\omega \approx 2470$ (rad/sec). The corresponding frequencies are 362 and 393 Hertz, respectively. When compared with
Figure 5.12: Spatial distribution of the mean velocity and its rms statistics (LES solution). The fields are extracted from center combustor plane. Distance to TDC is 48 mm. Also shown in subfigure (b) are the two stations (A and B) that are used for turbulence budget analysis.
Figure 5.13: Spatial distribution of the mean velocity and its rms statistics. The fields are extracted from center combustor plane. Distance to TDC is 48 mm. RANS solution.
Figure 5.14: Variation of mean velocity components along the vortex center as obtained from LES solution.

The above discussion indicates that the mean flow field can be predicted with reasonable similarity with either of the models. However, the same can not be said about higher order statistics. For example, LES prediction of RMS quantities reveals a region of high turbulent activity at the lower right corner of the combustor due to high mean flow gradients created by the interaction of the recirculating region with the developing jet. The recirculating region is formed between the opposite wall (right side), lower wall (right bottom) and the reactant jet. The structure of the flow is very complex and have similarities with jet in cross flow and backward facing step. Turbulence generated in this region will have a significant effect on TDC turbulence levels after the intake phase is over.

On the other hand, turbulence statistics by RANS as given in Figure 5.13 show a very different picture. The recirculation region is strongly damped and shear stress production is very limited, confined to the injection port region. This observation strongly suggests the well known limitations of $k-\varepsilon$ model (i.e., failure to account for streamline curvature and
normal stress anisotropy etc.) as the underlying reason for the poor performance.

In any shear layer, the distribution of normal and shear stress components of Reynolds stress tensor depends on their interaction with the mean velocity gradients \[59\]. In tensor notation, the production expression is

\[
P(\tau_{ij}) = -\tau_{ik} \frac{\partial U_i}{\partial x_k} - \tau_{jk} \frac{\partial U_j}{\partial x_k}
\]

where repeated indices imply summation. In order to facilitate the interpretation, production terms of $\bar{w}$, $\bar{u}^2$ and $\bar{v}^2$ are written explicitly as:

\[
P(\bar{w}) = -\bar{w} \frac{\partial U}{\partial y} - \bar{u}^2 \frac{\partial V}{\partial x} - \bar{w} \left( \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} \right) - \bar{u} \frac{\partial V}{\partial z} - \bar{v} \frac{\partial U}{\partial z}
\]

\[
P(\bar{u}^2) = -2\bar{w} \frac{\partial U}{\partial y} - 2\bar{u}^2 \frac{\partial U}{\partial x} - 2\bar{w} \frac{\partial U}{\partial z}
\]

\[
P(\bar{v}^2) = -2\bar{w} \frac{\partial V}{\partial x} - 2\bar{v}^2 \frac{\partial V}{\partial y} - 2\bar{w} \frac{\partial V}{\partial z}
\]
Figures 5.16 and 5.17 show LES solution of each individual term in the budget expressions at 2 locations characterizing the recirculation region (A) and the stagnation region (B). The locations of these two stations are shown in Figure 5.12. Inspection of Figure 5.12 reveals that lower edge of the jet (bordering the recirculation region) has higher $u^2$ levels. Line plots at station A indicates that the normal stress profile is influenced by all three terms in Equation 5.3. However, the degree of this interaction is a function of the wall-normal distance. The contribution of the normal stress to itself is positive until its eventual decay ($y > 0.005$ in Figure 5.16). This term is not effective in simple shear layers like flat plate boundary layer flows. Then, the observed peak is determined mainly by the competition between the remaining two terms. Cross-stream (i.e., spanwise) components $uw$ and $\partial U/\partial z$ acts as a sink when both of them are positive. This region corresponds to approximately $0.035 < y < 0.055$. In this region, the contribution of the first term ($-2\overline{w}\overline{U}/\partial y$) is positive. Note that the second and third terms are usually neglected in simple shear flows (e.g., flat plate boundary layer) because they are either zero or very small. The fact that all three have an impact demonstrates the complexity of the shear layer dynamics.

Analyzing other normal stress terms ($u^2$ and $v^2$) indicates that there is significant normal stress anisotropy, as expected from shear layer flows. In particular, $u^2 > v^2$ and $u^2 > w^2$ for $y < 0.005$. The observed peak of $v^2$ at the upper edge of the jet (Figure 5.16) is clearly seen in Figure 5.16. The last term in Equation 5.4 is negligible in the production of $v^2$. However, the remaining shear stress term is very effective in promoting larger $v^2$. If the streamwise direction is taken as “x”, then it is obvious that $\partial V/\partial x$ is an indication of streamwise curvature (secondary strain). This term is positive on the upper edge of the jet. Nevertheless, this is counterbalanced by the sink effect of $v^2\partial U/\partial y$.

At the stagnation region (station B), the turbulence intensities are smaller (Figure 5.17). Analysis of each term will not be carried out here, but several remarks are due. This region can be considered as the relaxation region, similar to the topology seen in backward facing steps following the reattachment point. Hence, anisotropy levels between the individual normal stress components (Figure 5.17) are less pronounced. Typical values for each are about 300-400 $m^2/s^2$. RANS model prediction in this region is characterized by anomalous
normal stress values (Figure 5.19). This is due to the spurious kinetic energy production seen in eddy viscosity closures at stagnation point flows [59]. This can be seen when Equation 5.1 is summed over the normal stress components to obtain the kinetic energy (k) production (in 2D):

\[ P(k) \approx -\mu^* \frac{\partial U}{\partial x} - \nu^* \frac{\partial V}{\partial y} - \frac{\partial}{\partial y} \left( \frac{\partial U}{\partial x} + \frac{\partial V}{\partial x} \right) \]  
(5.5)

In actual situations, the signs of the first two terms involving normal stresses would be opposite to each other (due to continuity) and therefore overall production rate would be determined by the competition between these two terms and the shear stress term. Hence, both positive and negative production rates are possible. However, with RANS closure where Reynolds stresses are modeled as

\[ u_i u_j = 2\eta T S_{ij} - \frac{2}{3} \eta S_{kk} \delta_{ij} \]  
(5.6)

first and second terms in Equation 5.5 would be proportional to \( \nu_T (\partial U/\partial x)^2 \) and \( \nu_T (\partial V/\partial y)^2 \), respectively, leading to positive contributions and higher production rates. Since, turbulent viscosity (in RANS) is proportional to turbulent kinetic energy, this phenomenon would translate into higher viscosity levels. In LES, the situation is different, because normal stresses would have both large scale (unsteady) and small scale (subgrid) components. For example, the streamwise normal stress component is obtained from \( \mu^* = \overline{UU} - \overline{U}^2 + (2/3)k^{gs} \). Hence, capturing the normal stress anisotropy is possible in LES. As a result, the production rate of turbulent kinetic energy will be predicted more realistically, which may lead to smaller turbulent production rates.

In the above discussion, an explanation of turbulence generation mechanisms is attempted by a representative stage in the high aspect ratio combustor. Consequently, it might be expected that quantitative numbers reported for stress levels and their structure might be changing significantly with time because of the unsteady and transient nature of the flow. However, a close inspection of different stages in the intake phase (not shown here) has not produced major differences that would alter the general description given above. Thus, it is considered to be an adequate description. This also shows that once the main structures are established in the combustor, the nature of turbulence will be less sensitive.
to piston motion during the intake phase. This is because the turbulence in the combustor is a forced system where in the majority of the intake phase the dissipation of turbulence is balanced (roughly) by the turbulence generation mechanism provided by the jet. In the absence of the forcing (i.e., intake jet), however, the details of turbulence evolution is expected to be different and more sensitive to interactions with the bulk flow. This is the case during the compression phase (after the intake port closure).

5.2.3 Preliminary Assessment of Model’s Performances

The fundamental differences discussed above also imply different model performance in realistic flow problems that strictly require well resolved wall layers. The present geometry presents a challenge in this respect, because both heat transfer and flow near the wall need to be resolved. Furthermore, the intake ports should be adequately resolved to accurately model the development of the high-Re number intake jet. Meeting this requirement is computationally very expensive (a discussion is given later when discussing heat transfer effects). Therefore, a model that can capture flow physics even with a coarser grid would be a tremendous help in understanding complex engineering flows.

One observation noted before was the experimentally visualized corner recirculation region. When both models employ the main investigation grid (Grid-1), only LES is able to predict this recirculation region. Grid-1 is a relatively coarse grid that does not adequately resolve the wall. One direct consequence of this is that the turbulent kinetic energy peak near the wall can not be captured, leading to overshoots in kinetic energy and turbulent viscosity. Hence, already dissipative nature of the RANS closures can be even more dissipative than designed when coarse grids are used. As a result, the accuracy of the model to produce a realistic ensemble-averaged picture of the flow field is seriously compromised. For example, one negative effect can be an underestimation of the reattachment length. In some cases, separation may be entirely prevented due to excessive shear [69].

A more refined grid (Grid-2) is used to investigate the effect of the grid resolution on model performance. The solution of Grid-1 is interpolated to Grid-2 and computations are carried out for both LES and RANS. Combustion results of Grid-2 and its comparison with
Figure 5.16: Budget terms in the production of normal stresses at position A (see Figure 5.12). LES solution. $Y$ is the wall normal distance in (m).
Figure 5.17: Budget terms in the production of normal stresses at position B (see Figure 5.12). LES solution. $Y$ is the wall normal distance in (m).
Figure 5.18: Budget terms in the production of normal stresses at position A (see Figure 5.12). RANS solution. Y is the wall normal distance in (m).
Figure 5.19: Budget terms in the production of normal stresses at position B (see Figure 5.12). RANS solution. Y is the wall normal distance in (m).
Grid-1 is given in the next section. Figure 5.20 shows the instantaneous streamlines at the return stroke of the combustor for both models and both grids. LES predictions reveal a separated corner in both cases, with Grid-2 showing more intense vortical structures. Nevertheless, overall topology in both cases is reasonably similar. However, only the refined grid (Grid-2) RANS solution shows a separation (recirculation) region in the corner. This is expected since the RANS model is a low-Re number variant of the popular $k - \varepsilon$ model and its possible improvements over the typical high-Re number variants would only materialize with adequate grid resolution.

In other aspects, both LES and RANS simulations do not show major sensitivity to grid refinement. In particular, the flow structure established by the tumble vortex is similar in coarse and refined grids. However, a major influence of grid resolution that is not substantiated at this stage of the present work is its effect on the heat transfer prediction. This aspect would be investigated further when the combustion process is analyzed.

5.2.4 Characterization of Charging Efficiency

Combustion power is proportional to mass of the gas burned and in each cycle introducing as much mass as required by the design conditions is essential. This is accomplished by purging burned products from the previous combustion cycle and introducing fresh reactants for the next combustion period. In four-stroke engines, there are two separate strokes, exhaust and intake, used for this. In two-stroke engines, both processes are happening either simultaneously or there is a significant overlap in the time interval in which they are effective. Therefore, achieving a mixture that is homogeneous and composed entirely of reactant species is very difficult because of the mixing between gases as well as the burned products being trapped in the combustor due to fluid mechanics effects. This is a characteristic of two-stroke engines and its effect must be minimized in order to have desired power output. However, this is generally difficult to obtain because, unlike four-stroke engines, scavenging strategies are more geometry dependent. Therefore, significant effort is spent in the design process to achieve optimum geometry and port/valve locations.

In the present engine, all of these complications exist. In addition to mixing between
Figure 5.20: Instantaneous streamlines at the corner of the combustor from both models. Effect of grid resolution.
the gases, the presence of the tumble vortex is shown to have a significant impact on
flow development and the final scavenging efficiency at the time of EPC. The extent of
scavenging process can be characterized by the trapping efficiency ($\eta_{tr}$) and the scavenging
efficiency ($\eta_{sc}$) defined as

$$\eta_{tr} = \frac{\text{mass of delivered mixture retained}}{\text{mass of delivered mixture}} = \frac{M_r}{M_i} \quad (5.7)$$

$$\eta_{sc} = \frac{\text{mass of delivered mixture retained}}{\text{mass of trapped engine charge}} = \frac{M_r}{M_r + M_p} \quad (5.8)$$

where $M_r$ is the mass of delivered mixture retained, $M_i$ is the mass of delivered mixture and
$M_p$ is the residual gas from the previous cycle [94]. The efficiency parameters of typical two-
stroke engines are $0.7 < \eta_{sc} < 0.9$ and $0.6 < \eta_{tr} < 0.8$ [94]. As an example, these efficiency
parameters are computed during cycle 4 (see Figure 4.5). Total mass injected over the entire
intake phase can be computed from

$$M_i = \int_{IPO}^{EPC} \dot{m}_{flow} dt = \int_{IPO}^{EPC} 1.46 \times 10^{-3} \, dt = 1.46 \times 10^{-3} (t_{EPC} - t_{IPO})$$

$$= 1.46 \times 10^{-3} \times 14.06 \times 10^{-3}$$

$$= 20.5276 \times 10^{-6} \, \text{kg} \quad (5.9)$$

where subscript “IPO” denotes intake port opening, which is different than EPO. $M_r$ and
$M_p$ can be determined at the time of EPC if the composition and mass of the mixture
are known. Total mass of the engine at EPC is about $8.8 \times 10^{-6}$ kg, which is equal to
$M = M_r + M_p$. To compute the efficiency parameters, $M_r$ needs to be computed. Since, from
CFD, all species are predicted as a result of the simulation, a simple integration of reactants
in the combustor yields

$$M_r = \sum_{\text{reactants}} \int V \rho Y_m = 7.492 \times 10^{-6} \, \text{kg} \quad (5.10)$$

In the computation of $M_r$, the reactants are $C_3H_8$, $O_2$, and $N_2$. At the time of EPC, the
$C_3H_8$ and $O_2$ concentrations are due to the injected mass only (since it was observed that
there are no unburned hydrocarbons during the exhaust stage). However, $N_2$ concentration
at EPC is due to both the injected mass and the unscavenged $N_2$ from the previous cycle.
Hence, $N_2$ is determined from its mass fraction in the stoichiometric $C_3H_8+N_2+O_2$ system. Repeating the same computations in other cycles results in similar numbers.

Using the values of $M_i$, $M_r$, and $M$ for this example cycle, the efficiency parameters are computed as follows:

$$\eta_{tr} = \frac{M_r}{M_i} = \frac{7.492 \times 10^{-6}}{20.5276 \times 10^{-6}} \frac{\text{kg}}{\text{kg}} = 0.365$$

$$\eta_{sc} = \frac{M_r}{M_r + M_p} = \frac{7.492 \times 10^{-6}}{8.8 \times 10^{-6}} \frac{\text{kg}}{\text{kg}} = 0.851$$

While the scavenging efficiency can be considered relatively high and therefore desirable, this is only achieved by using high amounts of fresh gases introduced into the engine. This results in a small trapping efficiency. Therefore, the present engine does not have good fuel economy standards. The primary reason for the small efficiency is the small residence time of the reactant jet. This, in turn, is caused by the high AR effect, since the geometry is more like a 2D shape and therefore the flow direction exhibits a simple pattern. This is dictated by the fact that there is less room for the jet to evolve in the chamber since the wall (geometry) is felt at all times.

### 5.3 Description of Combustion Phase

#### 5.3.1 Mixture Conditions Between EPC and Ignition

The complete engine cycle is successful only if the required power output is obtained from combustion. Therefore, charge preparation has a significant effect on the cycle performance. Important mechanisms in the flow that determine the charge preparation is described previously. The subsequent period between EPC and ignition is also important in determining the combustion efficiency. It can be argued that scavenging period before EPC imposes the global flow structures that will exist during ignition while the pre-ignition period determines their final form.

The distribution of fuel mass fraction in the pre-ignition period is shown in Figure 5.21 during a typical cycle. It is clearly seen that LES shows a more homogeneous mixture. In the case of RANS, strong non-homogeneity still exists even at the last frame (just before ignition). The tumble vortex is essentially an inviscid phenomenon and the mixing with the surrounding fluid will only happen if it disintegrates. It will be shown in Figure 5.24 that
even at the end of combustion period the tumble vortex keeps its form. The reason that LES gives a more homogeneous mixture is clearly explained by the fact that after EPC the tumble vortex starts to decay. This brings increased interaction between the core of the vortex and its periphery which results in higher rates of mixing.

Of course, it can be argued that because of the increased mixing in LES the mixture strength is reduced. This can be seen by contrasting with RANS results. LES produces a mixture that has an average fuel mass fraction of $Y_F = 0.05$. A perfectly homogeneous and undiluted stoichiometric propane mixture has a fuel mass fraction value of $Y_F = 0.06$. RANS predictions show that a major portion of the combustor has values very close to $Y_F = 0.06$, except in regions where the tumble vortex is located. In the core of the vortex, RANS has fuel mass fraction values as low as $Y_F = 0.04$.

Therefore, although mixture strength is reduced locally in LES, global distribution of fuel is more favorable for a successful ignition since initial stages of ignition will be less dependent on the position of the vortex core. This is not the case in RANS and it can be expected that depending on the cyclic changes in the tumble vortex structure, initiating combustion will be more difficult because of the distribution of fuel around the spark plug. The situation in RANS is almost like the reverse stratification where regions away from the spark plug have more favorable mixture composition. This has implication of for design studies. For example, a design methodology that solely depends on RANS for guidance will most likely attempt to place the spark plug to a new position with less dilution. However, LES shows that this may not be necessary.

### 5.3.2 Ignition and Flame Development

Typical pressure development in the combustor is shown in Figure 4.6. Compression ratio is about 2. The shape of experimental pressure-volume diagram at the end of compression phase reveals that heat release rate can no longer support a pressure increase since $dP/dV$ is negative. This means that either combustion is over or heat transfer rate is too high. Numerical prediction of pressure, temperature and oxidizer mass fraction during combustion is shown in (Figure 5.22) for LES. It can be seen that combustion is effectively over
Figure 5.21: Instantaneous fuel mass fraction at PRE-IGNITION stage predicted by LES (top) and RANS (bottom) during a typical cycle. Results are shown for the center combustor plane.
by TDC since mass fraction of the oxidizer decreases to very small values. Both the experiment and the numerical prediction have the same trend where pressure starts to decrease just before TDC, although numerical prediction slightly overpredicts rate of pressure increase near TDC. Since this engine configuration has no fixed TDC (i.e., it is a function of spring kinematics where rate of deceleration near TDC is proportional to rate of pressure increase), the fact that TDC and maximum pressure roughly correlate is expected. However, in most other engines the maximum pressure occurs after TDC to obtain maximum brake torque (MBT) from the cycle. This is done by adjusting spark timing for design conditions (intake flow rate, turbulence level, mixture stoichiometry etc.) to get MBT from the cycle. In the present engine, spark timing is 11 mm before top dead center (BTDC).

In the expansion stroke, it can be shown that Temperature in Figure 5.22 follows equation of state (5.13) by the polytropic expansion (approximate), with $n_e = 1.58$ (see also Figure 4.1).

$$T = \frac{(PV_{n_e})_{\text{ref}}}{mR_{\text{mix}}V_{n_e-1}}$$

Although this is an approximate analysis regarding temperature variation, it seems that combustion parameters are predicted with reasonable accuracy. The maximum temperature in the system is about 2700 K. In addition, the temperature is about 1550 K at EPO. Experimental pressure at EPO is about 3 atm and the present numerical predictions are able to capture this. To simulate multiple cycles, it is important that these numbers closely reproduce experimental data since ensuing scavenging phase is strongly influenced by initial conditions (i.e., conditions at EPO). Any significant deviation from the expansion curve in Figure 5.22 would result in a mismatch with the operational parameters described in Table 4.1. For instance, if the pressure is higher at the time of EPO, the blowdown process (initial stages of exhaust) would change. This would cause the details of reactant jet development to be different than “real conditions”. Eventually, the sequence of events during the scavenging phase would lead the flow to have a different state (i.e., different turbulence levels, stoichiometry, temperature etc.) at the return stroke when the ports are closed (EPC).
Figure 5.22: Variation of Pressure, Temperature and $O_2$ mass fraction (normalized by its value before combustion) during the combustion period. Also shown is the temperature estimated from Equation 5.13 (square symbols).

The predicted flame development is shown in Figure 5.23 through temperature iso-surface (1500 K) and streamline pattern. Ignition is carried out by progressively heating a 4 mm diameter region at the center of the combustor (Figure 3.2) until temperature in the ignition zone reaches 1900 K (locally). The first frame describes the initial stages of flame development after ignition is completed. Wrinkling effect of turbulence has just started to take place since at this time the flame kernel size became large enough to be influenced by the flow. The corresponding streamline pattern (first frame in the second row) shows a highly directional (counter-clockwise) bulk flow due to the tumbling motion. This bulk recirculating flow motion convects the flame to the upper surface after the ignition. At the same time, the lower left portion of the flame is convected by the downward motion of the flow. Second and third frames are showing the stretch effects since certain parts of the flame front are elongated mainly in the direction of the local flow. These are less obvious in the last two frames since the flame size now occupies a sizable portion of the cylinder volume. This is also evident in the last two frames of the streamline pattern, since
Figure 5.23: LES prediction of the combustion period at center engine plane (z=3.125 mm) as revealed by temperature contours and the streamline pattern using Grid-1.

the strongly directional form of the vortex is now weaker due to increased dissipation after elevated temperature levels.

RANS prediction of the flame evolution following the ignition is shown in Figure 5.24. Here, the dominant effect of the bulk flow is more obvious. The flame kernel is essentially first convected upwards, and accordingly flame propagation is entirely characterized by the local structure and strength of the vortex near the ignition zone. Consistent with this explanation, then, it is seen that lower part of the combustor is burned at the final stages of the combustion period. In the corresponding streamline snapshots, the stages of the flame convection can be approximately followed by identifying dense regions. The directional form of the vortex is still obvious in the final stages of the combustion, although diminished in strength. This is attributed to the fact that RANS vortex is stronger than its counterpart in LES. The total duration of the 5 snapshots is about 2.5 msec.
Figure 5.24: RANS prediction of the combustion period at center engine plane (z=3.125 mm) as revealed by temperature contours and the streamline pattern using Grid-1.
Similar patterns exist in the case of 3D flame propagation snapshots, shown in Figure 5.25 for LES and RANS. Real 3D flame propagation is exhibited only in LES. Generally speaking, contrasting the 3D iso-surfaces with their 2D counterparts (at the center combustor plane, Figure 5.23 and Figure 5.24), it is obvious that RANS results are essentially the same across the combustor thickness. LES results show strongly convoluted and wrinkled flame surfaces. Therefore, 2D snapshots of RANS are indicative of the overall flow topology. However, the same is not true for LES and the center plane snapshot may only give a loose average of the flame iso-surfaces across the combustor thickness.

The flame surface area (as computed from the outer envelope of the iso-surface) for the combustion period is shown in Figure 5.26 for both models. As expected, LES exhibits larger flame surface areas due to turbulence enhanced wrinkling effects while RANS predicts smaller surface areas since the wrinkling is absent due to strong dissipation. Note that both models predict approximately the same amount of reactant mass to be burned. Also, experimental pressure curve is reasonably predicted by both models. This means that the overall consumption rate of fuel must be approximately the same. This can only happen if the turbulent flame speed of the RANS solution is larger. Indeed, in the numerical work presented here, the EBU coefficient of RANS is larger by a factor of about 3.

The combustion model used in this study computes the reaction rate as the minimum of the Arrhenius reaction rate and the mixing controlled rate. This assumption essentially recognizes the fact that the reaction will only take place if cold reactants are brought into contact with the hot burned products. This requires a simulation model that realistically predicts TDC turbulence in order to compute this mixing rate with reasonable accuracy. This combined methodology, therefore, assumes that turbulent burning rate (or flame speed) is proportional to turbulent fluctuation levels in the high Damköhler number limit where flamelet assumptions hold.

The overall reaction rate predictions and its mixing controlled component is given in Figure 5.27. In this scatter plot, 6 snapshots describe the time history of the overall reaction rate for both models (LES and RANS). $y = x$ line in each plot constitutes the upper limit on the reaction rate (Arrhenius rate). The first snapshot in the series is just before the ignition.
Figure 5.25: Evolution of flame iso-surface (1500 K) as predicted by LES (a) and RANS (b). Front Y-Z plane is the piston surface. Piston is moving in the +X direction, towards the TDC.
Figure 5.26: Flame surface area predicted by LES and RANS during combustion

In the second and third frames for LES, both kinetic rate and the mixing controlled rate influence the overall reaction rate, although the dominance of mixing controlled regime is evident. However, the scatter of the rates in the second and third frames is distributed both at high reaction rates and low reaction rates. The corresponding frames for RANS, however, show entirely mixing controlled regime for high reaction rates and entirely kinetic controlled rate for low reaction rates. In Figure 5.28, the overall reaction rate (red) and reaction rate when it is equal to kinetic rate are plotted in scatter plot mode with respect to temperature. This is essentially similar to the previous plot with temperature effect made obvious. In both plots, the variance of the mixing controlled reaction rate is bigger for LES, indicating overlaps in the reaction rate space. In RANS results, reaction rate is always mixing controlled and will be only Arrhenius controlled if the EBU constant is progressively made larger. This is also based on the fact that turbulence related integral quantities at TDC are both larger and more uniform for RANS. In other words, EBU is effective either globally or nowhere. Therefore, locally capturing or mimicking the real flame structure is impossible with RANS while, with more realistic prediction of integral quantities, LES is able to locally capture this. For instance, mixing controlled regime for
LES predominantly occurs after the second frame where the flame develops to be larger than the integral scales of turbulence.

As indicated previously, RANS is able to predict pressure curve. This happens, however, with EBU constant of 2.3 versus 0.7 for LES. This indicates that overall the time scales are predicted to be larger for RANS (see also Figure 5.30) and by increasing the EBU constant for RANS we are decreasing the time scale of mixing.

5.3.3 Engine Heat Transfer

5.3.3.1 Issues in the High AR engine

The energy balance for the engine chamber can be written as (Appendix C)

\[
\frac{c_v}{v} \frac{dT}{dt} = -\frac{1}{v} \sum_{k=1}^{N_k} \frac{dY_k}{dt} + q_w \frac{S}{V} - \frac{P \, dV}{v \, dt} \tag{5.14}
\]

where \(q_w\) is the wall heat transfer rate per unit area, defined as \(q_w = -k(dT/dn)\) and evaluated at the wall. \(n\) indicates the wall-normal direction. \(S\) is the total surface area of the chamber across which heat transfer takes place. \(m\) is the mass of the gas in the chamber, related to chamber volume through \(V = m \nu\). Possible mass losses in the chamber are absorbed into the pressure work term.

A basic conclusion from this expression is that the engine pressure (or temperature) will be mainly controlled by heat release and heat loss terms. Furthermore, the effect of the heat loss term strongly depends on the ratio \(S/V\), defined previously as aspect ratio (AR). Since the piston is moving, AR is changing with the stroke, but its value near the combustion timing is more critical. Traditional engines are usually characterized by low AR. For example, an engine with a bore of 100 mm would have a AR of about 140 (1/m) at 20 mm clearance distance (to the cylinder head). In the present engine, AR is computed to be 453 (1/m) prior to ignition. This comparison imply that the dynamics of the combustion process in the high AR combustor may be very different than traditional engines, a conclusion that has been shown in recent experimental studies [19, 23]. In particular, the combustion process in high AR engines are strongly modified from the beginning of the combustion phase in contrast to low AR combustors for which only later stages are strongly affected. Hence,
Figure 5.27: Scatter plot representing overall reaction rate and mixing controlled reaction rate at 6 successive stages of the combustion period. Left column for LES and right column for RANS. Time from ignition increases from top to bottom in each column.
Figure 5.28: Scatter plot representing overall reaction rate (square symbol-red) and the overall reaction rate when it is equal to the kinetic rate (circle symbols-blue) with respect to local temperature at 6 successive stages of the combustion period. Left column for LES and right column for RANS. Time from ignition increases from top to bottom in each column.
from design perspective, the correct quantification of heat transfer rates is important to optimize the cycle.

5.3.3.2 Computation of Heat Transfer

The correct prediction of the heat transfer in IC engines depends on two major factors: (a) the requirement for resolving the wall and, (b) the need for using advanced mechanisms to correctly capture the flame structure. Both of these directly impact the temperature gradient at the wall. In most cases, however, neither of these two factors is addressed in the engine literature. This is related to the physics of the heat transfer problem near cold walls, characterized by very small thermal quenching distances on head-on configurations (typically on the order of 0.1 mm for hydrocarbon flames). Furthermore, depending on the wall temperature, the need for advanced mechanisms becomes even more acute since the location of the flame near the wall can only be determined unambiguously by using chemistry mechanisms involving minor species and if those species are resolved on the numerical grid. For example, Popp et al. [80] computed wall heat fluxes of methane flames using a 17 species mechanism and a wall resolution of just several micrometers. A similar work by Hasse et al. [37] investigated cold wall quenching of iso-octane flames using three mechanisms (26, 29 and 56 species) and very fine grid at the wall (less than a micrometer). Because of this enormous computational load, both of these studies were conducted in 1D configurations.

Two characteristic dimensions can be used to put the grid resolutions into a perspective. The first one is the thermal quench distance \( \delta_q \) and the second one is the flame thickness. The flame thickness can be computed from \( \delta = 2\alpha/S_L \) [96]. At 1500 K, \( \alpha \) (thermal diffusivity) is computed as \( 78 \times 10^{-6} \text{ m}^2/\text{sec} \) using the Sutherland Law and the definition of Prandtl number. Assuming the unburned mixture temperature is 600 K, the laminar flame speed at 5 atm is \( S_L = 0.86 \text{ m/sec} \) (from Equation 2.46). This approximate analysis then gives \( \delta \approx 181 \mu\text{m} \). Note that the flame thickness is only approximate. At conditions other than the reference value used here, a first order estimate of flame thickness scale with pressure as \( \delta \propto \exp(P^{-0.84}) \) [96]. With typical chamber pressures varying in the range 2-12 atm during combustion, it is reasonable to expect flame thickness values on the order of 100
\(\mu m\). The quench distance can be defined as the distance from the wall at which the flame temperature is 1500 K. Temperature iso-surface values as a marker of flame position have been successfully used by many authors \([37, 100]\). A typical finding of quenching studies is that in most conditions the quench distance is about half the flame thickness \([81, 37]\). Furthermore, significant concentration levels of intermediate species are reported between the wall and the flame half thickness by Popp et al. \([81]\) during propane premixed flame quenching. Hence, it is clear that grid spacing on the order of several micrometers is necessary if the intermediate species are to be resolved by at least 20 grid points.

These observations also explain the major problem of fully addressing heat transfer in the high AR engine through the use of credible chemistry mechanisms and fine grids. Prior to the ignition period, the dimensions of the present combustor are \(20 \times 50.8 \times 6.35\) (in mm). Note that all six walls of the closed chamber need to be resolved if the computation of heat transfer rates is to be given high priority. Furthermore, the most critical dimension (spanwise) severely influences the selection of spacing since the accuracy requirements of numerical scheme dictates a maximum stretching rate (less than five percent). From typical resolution quotations of several micrometers (see above, Popp et al.\([80]\)), it is straightforward to conclude that a typical high AR combustion simulation would convincingly overwhelm available resources.

As a result of these constraints, and because of the motivation to fully simulate several cycles, some simplifications to relax these stringent conditions were necessary. In particular, a global 1 step reaction is used to model the heat release. As discussed above, this prevents resolving the inner structure of the flame. Furthermore, overshoots in the predicted heat transfer rates can be expected. The other aspect of the heat transfer problem, wall resolution, however, is addressed by two grids. In Grid-1 (the main investigation grid), the uniform spacing corresponds to a wall resolution of 0.26 mm. In Grid-2 (the fine grid), the minimum wall distance is 57 \(\mu m\). Note, however, that the nearest distance of any flow variable in the computations corresponds to exactly half of the cited spacing for both grids, since variables are stored in the center of each numerical cell in the present finite volume scheme.
Predicted wall heat fluxes of the present work by LES and RANS during the combustion period is shown in Figure 5.29. Also shown is the corresponding pressure response of the models with grid refinement. Several observations can be made regarding heat transfer behavior and grid impact on the solutions. For example, both LES and RANS predict an increased heat transfer rate when the grid is refined. Moreover, for a fixed grid, both models predict similar values for heat fluxes. In all cases, maximum heat flux occurs when the combustion is complete, as revealed by maximum pressure timing. Typical heat flux values in LES are 0.7 \( MW/m^2 \) for Grid-1 and about 1.1 \( MW/m^2 \) for Grid-2. Similar values apply to RANS predictions as well. According to Popp et al. [81], typical values of propane quenching at 500 K wall conditions are 0.8-0.9 \( MW/m^2 \). The larger predictions in the present methodology are most likely due to the use of a global mechanism since it is well known that global mechanisms overpredict heat transfer rates. The predictions of Popp et al. [81] were obtained by detailed chemistry mechanisms, with both inert and reacting wall conditions.

One distinct difference is the slower combustion in the case of RANS with Grid-2. Note that both models are calibrated for several cycles using Grid-1 (see Section 5.4 for a discussion of multi-cycle behavior of models). Once model parameters are determined for Grid-1 (mass loss coefficient and combustion model coefficient \( C_{EBU} \)), they are used for Grid-2 without any change. Hence, fluid mechanics properties of solutions might be changing with grid refinement. To verify this, time scale predictions of both models in the form of probability density function (PDF) are plotted in Figure 5.30 just before the ignition timing. Time scale is a key quantity in the present combustion model, and a vastly different distribution will be reflected on the solution. This is because the reaction rate is inversely proportional to the time scale. LES predictions of time scale pdf’s are very similar, with the finer grid having slightly wider distribution. The mean value of LES predicted time scales are 0.121 msec with Grid-1 and 0.125 msec with Grid-2. RANS predictions of time scale pdf’s, however, are not similar, with mean value of 0.255 msec with Grid-1 and 0.506 msec with Grid-2. This implies that when the refined grid is used with RANS, the EBU coefficient will have to be increased to match the experimental pressure curve.

These results indicate that in the case of LES, reasonable predictions can be obtained.
However, RANS is more grid dependent. On the other hand, the performances of both models in terms of heat transfer estimates depend on the grid resolution. This is shown in Figure 5.31 where LES and RANS temperature profiles at 10 mm from TDC on a y-z plane at y=40 mm. This spanwise profile is selected only to be representative of many locations close to end of the combustion period where most of the charge is expected to be already burned. Grid-1 is coarse and almost a flat temperature profile is observed (both LES and RANS). Grid-2 is still coarse when compared to typical values reported in the literature but high temperature regions are resolved much better than Grid-1. An almost linear temperature profile can be detected. However, as explained before, without proper chemistry treatment these results are not very accurate. Results by other researchers indicate that as far as temperature is concerned, the resolution requirement dictated by resolving the minor species may not be that strict. For example, Andrae et al. [4] reported temperature and propane mass fraction profiles at the time of quenching for stoichiometric conditions at 400 K and 10 atm. Inspection of that graph ([4]) implies that temperature profile can be approximated as linearly changing from the wall at engine conditions (cold walls and high pressures). Given the fact that wall heat fluxes are close to reported values in the literature, it can be argued that Grid-2 might reasonably approximate possible real-life conditions for heat transfer purposes.

In chapter 4, a thermodynamic analysis was presented to estimate the order of mass leakage from the combustor. The estimates given by that analysis depend on the assumptions employed for EPC conditions. In particular, the analysis suggested that total mass loss from the system (based on the available experimental pressure signal) will be smaller at higher EPC temperatures. For example, inspection of Figure 4.3 shows that total mass loss of a system that has EPC conditions at $T_{EPC} = 550$ K may be in the range 25-45 %, depending on the assumed TDC temperatures (for the range 2600 K - 3200 K). For the present conditions based on $T_{EPC} = 500$ K, it seems that total mass loss would be on the order of 30-50 %. However, in practice, the maximum mass loss estimates from the thermodynamic analysis would materialize only if there is negligible heat transfer from the system. This would result in higher temperatures, perhaps very close to adiabatic values at constant
volume. In other cases, the mass loss would be rather closer to lower range of the given estimates.

The heat transfer analysis presented in this chapter, however, suggests that there is intense heat losses, and the maximum temperature in the combustor would be much less, close to 2600 K. Figure 5.32 shows LES predictions of the combustor mass, pressure and temperature from both grids. At EPC, Grid-1 predicts the trapped mass to be about $8.8 \times 10^{-6}$ kg and the mixture temperature to be about 504 K. Grid-2 predictions for the mass and temperature are $8.7 \times 10^{-6}$ kg and 510 K, respectively. Hence, for practical purposes, the conditions at EPC from both grid predictions can be considered to be the same. Also, note that Figure 4.3 shows the mass to be about $8.97 \times 10^{-6}$ kg at $T_{EPC}=500$ K. The numerical predictions underestimate this value by about 2 %. Figure 5.32 shows that maximum temperature from Grid-1 would be about 2700 K, while that of Grid-2 would be about 2600 K. This 100 K difference in temperature prediction is also manifested in the pressure prediction. For example, Grid-1 predicts the maximum pressure to be 11.63 atm while Grid-2 predicts the maximum pressure to be 10.72 atm. The difference, about 0.9 atm, is mostly due to the higher heat transfer since the mass burned and mass lost from both grids are within 2 % of each other. For example, inspection of Figure 5.32 shows that mass losses from Grid-2 and Grid-1 are about 39 % and 40.9 %, respectively. If the mean temperature of Grid-1 were 100 K less than the prediction (2700 K), this would translate into a mass increase of about 4 % for the same pressure conditions (i.e., peak pressure corresponding to Grid-1 predictions). This is computed from the relation $PV/R = mT$ at TDC. For example, assume $m_1$ and $T_1$ are the Grid-1 predictions of mass and temperature. Here, $m_1 = 8.8 \times 10^{-6}$ kg and $T_1 = 2700$ K. If the temperature were 2600 K ($T_2$), the mass loss would be less. In other words, for the same pressure conditions, the mass ($m_2$) corresponding to $T_2$ would be higher. The mass ratio is $m_2/m_1 = T_1/T_2$, which is 2700/2600. This is about 4 % increase.

The combined analysis suggests that about 35-40 % mass loss from the system can be expected at conditions corresponding to 500 K EPC conditions. This expected mass loss would decrease substantially if the EPC conditions are selected to be higher than 500 K.
Figure 5.29: Time history of the predicted heat flux by numerical methods. Also shown are predictions of pressure by both models (LES and RANS) and the experimental signal (symbols).

Figure 5.30: Probability Density Function of Time scale prior to ignition timing as a function of grid resolution.

Hence, it is clear that optimization of the present engine will be highly dependent on the EPC conditions. Therefore, the experimental verification of EPC conditions will greatly improve the overall understanding of the high AR engine.
Figure 5.31: Temperature profile as a function of spanwise dimension.

Figure 5.32: Time histories of LES predicted mass, pressure, and mean temperature in the engine from Grid-1 (solid line) and Grid-2 (dashed line).
5.3.4 Flame Structure

The flow structure characterized by integral scale properties (i.e., turbulence intensity, length scale) interact with the premixed flame front and modify the flame propagation. The extent of the interaction needs to be predicted so that appropriate chemistry closures can be used in numerical simulations.

Borghi [9] was the first to develop a diagram to describe this interaction with scalings based on flame and turbulence properties. Later, it was modified by other researchers (for instance, Peters [74]). More specifically, the velocity ratio (turbulence RMS velocity to flame speed $u'/S_L$) and the length scale ratio ($l_t/l_f$) are used as the parameters governing this characterization. These parameters define also other important quantities, like the turbulent Reynolds number ($Re_t$), Damköhler number (Da) and the Karlovitz number (Ka):

\[ Da = \frac{l_t}{l_f} \left/ \frac{u'}{S_L} \right. \]  
\[ Re_t = \frac{l_t}{l_f} \frac{u'}{S_L} \]  
\[ Ka = \frac{t_f}{\eta} = \left( \frac{l_f}{\eta} \right)^2 \]

Here, $l_f$ is the flame thickness, $l_\delta$ is the inner layer thickness, and $\eta$ is the Kolmogorov length scale. In addition, a second Karlovitz number can be defined based on the inner layer thickness:

\[ Ka_\delta = \left( \frac{l_\delta}{\eta} \right)^2 \]  

In the regime diagram due to Peter’s, 5 separate regions can be identified (Fig. 5.33). For example, $Re_t = 1$ line is the limit for laminar flame propagation. Below $u'/S_L = 1$ is the wrinkled flame region and between $u'/S_L$ and $Ka = 1$ line corrugated flamelet regions can be identified. Thin reaction zone (TRZ) is between $Ka = 1$ and $Ka_\delta = 1$ and the broken reaction zone (BRZ) is above the $Ka_\delta = 1$ line. In the wrinkled flamelets regime, the flame front is very thin and since $u' < S_L$, the turbulent fluctuations can not modify flame propagation to any significant degree. Therefore, the turbulent flame propagates much like a laminar flame front. In the corrugated flamelets regime, the smallest flow scale $\eta$ is larger than the flame thickness and the inner structure of the flame (including the preheat and reaction zone)
Figure 5.33: Combustion regime diagram proposed by Peters [74]. Present RANS prediction of the combustion regime is shown with symbols.

is not modified. Hence, the flame can still be considered laminar. The boundary for the existence of corrugated flamelets (Ka=1) is also known as the Klimov-Williams criterion above which the flame thickness is larger than the Kolmogorov scale. This is the classical flamelet limit.

In the thin reaction zone regime where \( l_f > \eta > l_\delta \), the turbulent eddies are able to penetrate into the preheat zone but still larger than the reaction zone. Peter’s argued that since the reaction zone (where the reactions take place) is not disrupted, the flame structure is still laminar and the flamelet regime can be extended to \( Ka_\delta = 1 \) line. However, the local burning speed is now different than laminar flame speed since in the preheat zone the transport processes are modified by turbulence. As a result, the flame thickness is broadened.

The combustion model used in this study [88] assumes the model is applicable in the flamelet regime. In engine literature, the flamelet regime is typically used for wrinkled and corrugated flamelet regimes. This regime is characterized by small turbulence fluctuations and integral length scales much larger than laminar flame thickness, \( l_f \).

To determine the operating point on the diagram, the ratios \( u'/S_L \) and \( l_f/l_f \) need to be computed. In \( k-\varepsilon \) model, the length scale is proportional to \( k^{3/2}/\varepsilon \). These parameters
are computed for RANS during flame propagation on the flame surface (by locating 1500 K iso-surface of temperature) and shown in the diagram as symbols (Figure 5.33). The scatter plot indicates that all points are in the TRZ regime.

The regime diagram by Peters is more suitable for RANS since the parameters are all physical quantities. Recently, another diagram that uses similar arguments is proposed by Pitsch [77] to predict combustion regimes in LES applications. This is shown in Figure 5.34. In this diagram, integral length scale is replaced by the LES filter size. The regime diagram is constructed to relate the length scale ratio ($\Delta/l_f$) to Karlovitz number. Karlovitz number is defined [77] as

$$Ka = \frac{l_f^2}{\eta^2} = \left( \frac{u'^3 l_f}{S_f \Delta} \right)^{1/2}$$  \hspace{1cm} (5.19)$$

where $u'$ now is the subgrid velocity scale that can be computed from subgrid kinetic energy. When the new parameters are computed on the flame surface for LES, the scatter plot in the combustion regime diagram (Figure 5.34) shows that wrinkled, corrugated and TRZ regimes exist in the combustor.

Temperature contours can be used to verify if the predictions of both models with respect to combustion regimes are physically occurring. The information that the preheat zone is thickened in TRZ regime will be used to choose contour levels to reflect this. At this stage, the unburned zone temperature is about 600 K. The flame location is identified with $T=1500$ K. The start of preheat zone is taken as $T=700$ K. By using 3 contour levels, two intervals of equal magnitudes will fall between 700-1500 K.

Figure 5.35 shows the temperature contours at clearance distance of 16.5 mm for RANS solution. The reaction zone thickness is clearly broadened as can be seen in subfigure (b) at a representative flame front. The line plot gives the variations of temperature ($T$), Reaction Rate (RR) and Fuel Mass Fraction ($Y_F$).

A similar plot is given for LES predictions in Figure 5.36. A quick inspection of the contour plot indicates that contour intervals are not uniform. A detail view of the middle section of the combustor clearly shows regions of very thin flame structure. Consistent with the LES combustion regime predictions (Figure 5.34), broadened contour intervals are also present in the combustor. Similar line plots (Figure 5.37) across two cuts (Figure 5.36 (b))
indicate that flame thickness is broadened in the preheat zone at cut B.

The regime diagrams showed that the combustion modeling assumption (EBU) can be justified based on the expected flame structures. The experimental data on SI engine flame structure seems to indicate that engines under most conditions operate in the flamelet regime. For example, zur Loye et al. [104] made shadowgraph measurements of stoichiometric propane flame propagation in SI engines to deduce flame thicknesses and topology. They found that at low engine speeds (below 600 rpm), the flame is simply connected with moderate wrinkling. With higher engine speeds (above 1200 rpm), the flame structure is increasingly fragmented and wrinkled. Similarly, Smith [93] showed that wrinkled flames occur in the flame zone. Thickened flame zones were also observed. According to Bracco [11], at high engine speeds, $l_f/\eta$ is on the order of 1. These experimental observations and the fact that laminar flame thicknesses of about 100 $\mu$m or less are typically found in engine applications seem to indicate that the occurrence of wrinkled as well as wrinkled-thickened zones are very possible flame topologies most likely to be found in the present engine of 2400 rpm. This means that present LES predictions are more reasonable with experimental observations presented in the literature. Nevertheless, a direct verification of this conclusion is still required from experiments in the high aspect ratio combustor.
Figure 5.35: Flame structure and temperature contours of RANS solution at clearance distance of 16.5 (mm). (a) Combustor view, (b) Variation of flow variables across the cut (A) in subfigure (a). A very broad flame zone is evident. $T$ is temperature, $RR$ is the reaction rate normalized by 0.1 and $Y_F$ is the fuel mass fraction. See also Figure 5.33.
Figure 5.36: Temperature contours of LES solution at clearance distance of 16.5 (mm). Detail view (b) is the middle part of the Combustor view (a). Both thin flame fronts (e.g., cut A) and thickened flame fronts (e.g., cut B) can be clearly seen. See also Figure 5.34.

Figure 5.37: Flame structure obtained at cut A and B of Figure 5.36 (b). $T$ is temperature, $RR$ is the reaction rate normalized by 0.1 and $Y_F$ is the fuel mass fraction. See also Figure 5.33.
5.4 Cyclic Variability in the High AR engine

The most important indicator of CCV in an IC engine is the power output. Experimental data on the high AR engine reveals that there are significant variations in the peak pressures, as shown in Figure 5.38, where LES predicted signal is also plotted. Corresponding RANS prediction is given in Figure 5.39. Only 5 cycles are available from experimental data [19]. Cycles 6 and 7 data are essentially equivalent to Cycles 3 and 4, and appended to the experimental data after the fifth cycle to extend the simulation in real time. These additional cycles also serve in showing the importance of the initial conditions at the beginning of the exhaust blowdown period for any cycle on the engine output. Computations start at the expansion stroke of cycle 2, which constitutes the initial conditions for cycle 3. The first 2 cycles are not used since it was determined that the rate of pressure increase during the combustion period is somehow different than the remaining cycles. This difference is attributed to transient start-up phenomenon.

The LES results show that the predictions at cycles 3, 4 and 5 follow experimental trends closely. RANS predictions, however, give essentially the same pressure output at cycles 3, 4 and 5. Theoretically, this behavior from both models is expected since the averaging of the time accurate Navier-Stokes equations is different in LES and RANS. In RANS, ensemble averaging is used in the averaging procedure. Accordingly, a RANS computation would typically give the ensemble-average of many realizations. LES, on the other hand, employs spatial averaging and as a result, the time dependency of the original Navier-Stokes equations is retained more rigorously. Thus, it can be expected that both models would respond differently to statistically equivalent initial conditions. In particular, one expects LES to be more sensitive to initial conditions than RANS. An indication of this is observed in the prediction of cycles 6 and 7. Since cycles 6 and 7 are not real measured signal, the numerical predictions should fail to capture these cycles. This is because end of cycle 5 is not really the initial conditions for cycle 6. LES correctly captures this, predicting a different peak pressure than the “assumed” cycle 6. RANS, however, predicts a pressure response very similar to cycle 3. If the RANS prediction is contrasted with previous cycles, it is clear that RANS results show little difference between different cycles.
Figure 5.38: Time history of the LES predicted pressure output (solid line) and the experimental signal (symbols) over several cycles.

Figure 5.39: Time history of the RANS predicted pressure output (solid line) and the experimental signal (symbols) over several cycles.
The underlying origins of the observed variations in the present engine output needs to be studied and quantified so that cyclic variability can be minimized and design conditions can be adjusted based on the most probable engine cycle. In other words, the standard deviation of the peak pressure should be small. The extensive literature in the past has generally identified the mean flow structures near TDC as one of the major causes of the cyclic changes. The conditions existing near TDC is geometry dependent and therefore their topology vary from one engine to another. However, it is generally possible to classify those motions as simple recirculating regions or more organized structures (such as tumble or swirl) that usually result from the intake phase of the cycle. Hence, the nature of the mean flow structures specific to a particular engine as well as their effects on the engine output should be identified.

Both LES and RANS simulations have revealed that the dominant structure in the flow is the tumble vortex. This large scale structure is significantly affected by the interaction with the wall and the fuel jet [66]. As a result, the vortex center would move in the combustor in an unsteady manner.

A specific effect of the unsteady vortex center movement in IC engines is the significant variations in the mixture conditions observed close to TDC. These variations are one of the major causes of cycle-by-cycle variations in the engine pressure signal [5]. These variations are also evident in the high AR engine. For example, LES results predict significantly different distribution of temperature and fuel fraction for three consecutive cycles as shown in Figures 5.40 and 5.41. Corresponding RANS predictions (shown in the same figures) suggest little change between cycles.

In order to visualize the extent of vortex center movements, the instantaneous vortex center and its time evolution should be quantified. There are several methods in the literature [33] for vortex center identification. In the present study, a method based on finding the maximum angular momentum in the domain is used [33], as described in Figure 5.42. In the first step, an instantaneous 2D velocity field is extracted from the CFD solution.

1A tabulated list of present understanding on the origins of cyclic variations is given in Chapter-1
Figure 5.40: Visualization of temperature field at EPC for three cycles, shown for LES (top) and RANS (bottom).
Figure 5.41: Visualization of Fuel mass fraction at EPC for three cycles, shown for LES (top) and RANS (bottom).
Then, the following expression

\[ f(P) = \frac{1}{(2N+1)^2} \sum_{i} \frac{r_i \times u_i}{|r_i||u_i|} \] (5.20)

is computed for a point P, surrounded by N=10 layers of neighboring points. The number of layers is determined based on numerical experiments that give adequate resolution of vortex cores. 10 layers approximately correspond to 6mm² resolution. The computations are carried out until a maximum is found. An example of the computed vortex center with this method is shown in Figure 5.42. In this randomly selected 2D field, the present algorithm is able to correctly predict the location of the vortex core. To verify if the accuracy of the method is prevailing over the entire cycle, several vector fields are inspected visually and numerically. It was observed that there was a single dominant vortex in the extracted 2D fields during the scavenging phase. In that case, it is straightforward to identify this maximum angular momentum with the tumble vortex center. However, during the late compression phase, there appears several vortical structures with varying degrees of strength. In some instances, these multiple structures might have nearly equal magnitudes. An example to this case can be seen in Figure 5.41 for RANS solution. In such cases, only the strongest vortex is considered the center. For statistical purposes, however, it is sufficient to study vortex center movements until EPC. Later stages of compression take place under vortex breakdown, and EPC structures serve as initial conditions for this phase.

The method is applied over 170 individual 2D vector fields (spanning 4 consecutive cycles) to track the distribution of the vortex motion. Figure 5.43 shows this in a scatter plot, contrasting LES and RANS predictions. The locations of the vortex cores are non-dimensionalized with appropriate scales to reflect their relative positions in the clearance volume (i.e., between the piston and TDC). The RANS solution predicts the vortex center at the middle of the combustor in the majority of the individual realizations. LES, however, tends to give a more random distribution, spanning larger distances with respect to the geometrical center. Note that implicit in this plot is the displacement of the vortex core with respect to time in the horizontal axis since in each case the piston is actually moving. While the scatter plot indicates that there might be significant variations of the vortex
Figure 5.42: The schematic of the vortex center computation algorithm (left) and the result of the algorithm as applied to a 2D velocity field during scavenging (right).

Figure 5.43: Scatter plot of the tumble vortex center locations over 4 cycles obtained from LES (left) and RANS (right) predictions. Horizontal axis is the relative position of the vortex center with respect to distance between the piston and TDC. Vertical axis is normalized by the width of the combustor (50.8 mm).
center (especially in the case of LES), a definitive conclusion about cyclic changes is not obvious. A more direct approach would have been to directly compute the vortex center at a particular piston position over hundreds of cycles and create statistical measures of this change, such as its $RMS$ or pdf. However, this is computationally not feasible at the present.

Another way of inspecting these changes between individual cycles is to plot vector fields and visually determine if the methodologies (RANS and LES) have variations in their predictions. Then the degree of cyclic changes can be quantified based on the difference between the individual cycles and their ensemble averaged mean.

The level of CCV is studied for LES in Figure 5.45 by plotting 5 individual cycles vector fields $U$ and their ensemble average $<U>$ before ignition timing. In each vector field, the vortex center is also shown. These snapshots reveal that LES tends to predict a truly unsteady flow field. Moreover, the topology of the flow field is only globally similar, with a counter-clock-wise tumble vortex constituting the main bulk flow. The center of this structure is changing substantially between cycles. Finer details of the flow field also show differences, with smaller structures appearing at different locations. Comparing these individual vector fields with the ensemble averaged field indicates that this engine has significant cycle-by-cycle variations.

A similar study of RANS predictions at exactly the same piston position over 4 individual cycles leads to strikingly opposite conclusions. Figure 5.45 indicates that all four individual cycles have almost the same overall topology as well as the same tumble vortex structure. Each cycle predicts slightly different locations for the vortex center. However, this is an artifact of the vortex center identification method as explained before since the tumble vortex is elongated in RANS. Moreover, after comparing the individual cycles with the ensemble averaged field, it is apparent that there is no significant CCV.

There are implications of these findings. Since the combustion period is strongly influenced by the mean flow, it is reasonable to associate the cyclic changes in the power output with the variations in the mean flow. The mechanism of the mean flow effect on CCV is the convection of the initial flame kernel by the mean flow. As a result, the flame propagation
would take place under different mixture compositions, temperature and strain rate, among other important parameters. Figure 5.40 and 5.41 underscore these aspects, detailing the nature of expected mixture composition for both LES and RANS. In particular, the scalar fields globally follow the observed behavior deduced from the vector fields. Therefore, an LES solution is expected to exhibit CCVs. RANS engine power output, however, is less likely to experience CCVs.

The cyclic change levels can be quantified analyzing for a particular point using the concepts given in Appendix B. This analysis is conducted for the probe point 32 (Figure 3.4) because it is close to TDC and very critical for combustion development. Various flow variables are sampled over 4 cycles in this analysis to compute ensemble average of the signal. After this step, based on a cut-off frequency (of 1 Khz), a cycle mean is computed. Then the RMS of the low-frequency cyclic variations in the flow variable is computed based on the ensemble average of the difference between the cycle mean and the ensemble average of the flow variable (Equation B.15). The relation between the cycle mean, ensemble average and the low-frequency cyclic change is given in Equation B.14.

Figure 5.46 show the ensemble average and the cyclic change level (RMS) in the model coefficients of LES. For example, $C_n$ has an average of about 0.045 and RMS of about 0.01. Inspection of the dissipation model coefficient indicates that it has an average of about 0.5 and RMS of about 0.1. Because of the periodic nature of the flow, however, these values are changing through the cycle. In high Reynolds number applications of the present LES method with constant coefficients, the model coefficients assume values of about 0.067 for $C_v$ and 0.916 for $C_e$. This shows that present engine might be exhibiting significant cyclic changes in the model coefficients, a conclusion that is in agreement with TDC vector/scalar fields as well as pressure signal.

Low-frequency cyclic changes in temperature is shown in Figure 5.47 for both models. Consistent with the physics of the flow, major changes are observed near TDC. But LES exhibits much larger cyclic changes compared to RANS. These quantitative values clearly support the view presented before that LES is more prone to cyclic changes in its predictions.
Figure 5.44: Instantaneous 2D LES vector fields (at center plane) for 5 consecutive cycles and their ensemble averaged mean.
Figure 5.45: Instantaneous 2D RANS vector fields (at center plane) for 4 consecutive cycles and their ensemble averaged mean.
Figure 5.46: The ensemble average and low frequency cyclic changes (RMS) of model coefficients, $C_v$ (top) and $C_\varepsilon$ (bottom), are shown for a complete cycle.
Figure 5.47: The ensemble average and low frequency cyclic changes (RMS) of temperature at P32 are shown for both models, LES (top) and RANS (bottom), over a complete cycle.
CHAPTER 6

CONCLUSIONS

This study investigated the potential of LES in the study of a small scale research engine. This was based on the motivation that the study of such small devices is difficult by experimental techniques and often unreliable by traditional RANS closures. Therefore, as argued in chapter 1, the theoretical strengths of LES may be crucial in providing an accurate picture of flow processes in small devices. An increased understanding of such small scale devices by any investigative tool (numerical or experimental) would contribute to efficient designs of portable power sources.

To numerically simulate such IC engines with simple geometries, a second-order accurate (in time and space) predictor-corrector time-stepping scheme is extended to handle piston motion of IC engines with rectangular geometries. The methodology is parallelized using domain decomposition paradigm with MPI to reduce the duration of simulations. When applied to the analysis of model engines, the resulting methodology has the capability to conduct scaling studies or to investigate effect of different boundary conditions in a design cycle. Based on this, a small scale research engine with high AR is simulated using the developed methodology and assumed operational parameters.

Main contributions of this work can be summarized as follows:

(1) The findings of the study enabled full characterization of physical processes occurring in the combustor. This work is the first CFD study that attempts to analyze this engine. It is also the first detailed analysis of scavenging period and mixture formation. As argued in chapter 4, no experimental information on cycle details of the simulated engine is available. Therefore, the present investigation has successfully advanced the existing knowledge of the studied engine.

(2) Validation of the assumed operational parameters by the numerical methodology provided an approximate yet a complete set of realistic conditions. As indicated in chapter
these assumed operational parameters for the simulations were estimated with the help of a simple thermodynamic analysis. This was necessitated by the fact that a well defined experimental quantification of the operating conditions did not exist. Hence, the success in the validation provided by the numerical methodology facilitated estimates of engine efficiency parameters that were not available previously.

(3) Scavenging and mixture preparation are found to be highly influenced by the tumble vortex in the investigated engine. In chapter 5, it was argued that a mechanism is necessary to induce longer residence times since such small devices are necessarily characterized by small residence times. It is found that the tumble vortex provided such a mechanism, at least in the first part of the scavenging period (expansion stroke), to help maintain a long residence time by providing an alternative route (through part of the bottom port) to the upper port. The present study has also demonstrated that the upper port promotes cross-scavenging while the lower port (intake port) promotes loop scavenging. It has been found that the cross scavenging process is very active in the return stroke, whereby, the piston starts to compress the flow and pushes the combustor mass out of the upper port. Consequently, the importance of the loop scavenging is progressively reduced. Findings imply that the scavenging physics of scaled down (in the spanwise direction) engines would exhibit a similar behavior since scaling down strengthens the two-dimensional nature of the bulk flow structures.

(4) It is also demonstrated that tumble vortex leads to some inefficiency because of the trapped burned mass in the vortex core. The overall scavenging efficiency of the engine is found to be % 85. This aspect of tumble vortex formation is different than 4-stroke traditional engines with valves (since very little unscavedeng product mass exists during the intake) and therefore realistic prediction of the tumble vortex dynamics are important for a successful combustion period. Chapter 5 demonstrated that LES provides a more physical interpretation of the tumble vortex evolution during late compression period, leading to more homogeneous and less directed mean flow structures. This is due to vortex decay and in the process, the trapped burned mass is mixed with the remaining charge much more vigorously. RANS, on the other hand, showed a vortex much less diffused than its LES
counterpart. Therefore, as argued in chapter 5, a design methodology that solely depends on the RANS technique will most likely lead to wrong conclusions. This shows that design methodologies based on LES have the advantage over RANS based methods.

(5) Qualitative observations (from experiments) in the high AR engine on mass and heat losses [19] are quantified. The accuracy and uncertainty aspects of the numerical predictions (in quantifying these losses) are discussed and their effect on engine performance (for assumed operational conditions) is presented (in chapter 4 and 5). Similar to (1), the present understanding of the engine has been advanced by being able to quantify these two performance impacting factors [19] in small scale engines.
CHAPTER 7

RECOMMENDATIONS FOR FUTURE WORK

Experimental work The success of the methodology in predicting observed pressure signal indicates that the findings of the present numerical study may be used in furthering the understanding of the high aspect ratio combustor. This conclusion assumes that the selected operational parameters are realistic conditions and the subsequent unsteady flow physics revealed by the numerical procedure are the most likely physical realization of the flow. Despite the difficulties of conducting detailed experimental measurements, these aspects related to mixture characteristics as well as turbulent flow structures need to be quantified. This task can be carried out even in limited sense provided some experimental understanding is obtained. For example, LDV measurements can be done to predict scales of turbulence near TDC in a time resolved manner so that numerical understanding can be complemented and compared. In addition, spatial structure of the flow field needs to be measured by PIV so that numerically revealed tumble vortex structure can be compared to experimental instantaneous flow field. These are the minimum requirements if the predictive capability (i.e., providing full 3D field information) of the numerical method will be realized.

Advanced Chemistry Mechanisms The correct prediction of the flame-wall interaction can only be addressed if mechanisms that include minor species are employed. For this task, a more refined grid should also be used. Use of advanced mechanisms will also result in a more realistic capture of the flame propagation even at locations away from the walls. In a parallel effort, this strategy should be supported by techniques that speed-up the chemical source term estimations. Two methods that have shown promise in this sense are In Situ Adaptive Tabulation (ISAT) and Neural Network Estimation techniques.

More Realistic Combustion Models The limitations of the EBU model should be studied by employing more consistent models. For example, since the simulations revealed
that combustion might be taking place in the flamelet regime, a $G$ equation flamelet model can be used to incorporate chemistry and unsteady strain effects. The use of LEM as a combustion subgrid model does not assume any flame regime and may contribute to better predictions in terms of flame propagation. These modern aspects of combustion analysis can actually be conducted only during the late combustion, leading to significant savings in computing time of the simulations. This is because the present work indicates very similar mean flow structures between the coarse and the fine grids. Hence, the solution of the coarse grid can be interpolated into the fine grid at the time of port closure in the return stroke. Consequently, this interpolated grid will be integrated with more advanced combustion models, with possible improvements in predictions.

**Lower Order Models** The detailed flow field information of the present methodology also provides variations of mean quantities such as temperature and fuel mass fraction over the entire cycle. This knowledge of flow variables can be used to construct lower order predictive tools to speed-up the design work.
APPENDIX A

LOCALIZED DYNAMIC $K^{SGS}$ MODEL (LDKM)

Model coefficients are determined by the Localized Dynamic $k$-equation Model (LDKM) of Kim [51]. The model has been successfully tested, for example, in reacting flows ([53],[52]) and non-reacting flows([68]). The model is local and does not need any spatial averaging. This gives the model flexibility and robustness required for simulating complex geometries. The model assumes that smallest resolved scales and largest unresolved scales are related in the representation of the stress tensor. A justification for this assumption is provided in the experimental free jet studies by Liu et al.[63]. In the implementation of these ideas, a second (and larger) test filter, denoted by $\tilde{\alpha}$, is used to extract the smallest resolved scales. The test filter is taken as twice the LES filter size [51].

A.1 Computation of $C_V$

The closure expression of the exact subgrid stress tensor is reproduced here from Equation 2.29

$$\rho \tau_{ij}^{sgs} = \bar{\rho} (u_i u_j - \bar{u}_i \bar{u}_j) = -2 \bar{\rho} C_v \sqrt{k^{sgs}} \Delta \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij}, \quad (A.1)$$

where $C_v$ is the model coefficient that needs to be determined. All other terms on the RHS of A.1 is known from the resolved scale. The exact computation of the LHS is only possible if a DNS solution is post-processed. However, in the context of LES, the subgrid stress tensor can be computed at the test filter level

$$\rho \tau_{ij}^{sgs,test} = \bar{\rho} \left( \tilde{u}_i \tilde{u}_j - \frac{\tilde{u}_i \tilde{u}_j}{\bar{\rho}} \right) \approx -2 C_v \Delta \bar{\rho} \left( \frac{\tilde{u}_i \tilde{u}_j}{2\bar{\rho}} - \frac{\tilde{u}_i \tilde{u}_j}{2\bar{\rho}} \right) \delta_{ij} + \frac{1}{2} \left( \tilde{\rho} \tilde{u}_k \tilde{u}_k - \frac{\tilde{u}_k \tilde{u}_k}{\bar{\rho}} \right) \delta_{ij}, \quad (A.2)$$

where the subgrid kinetic energy term in Equation A.1 is replaced by its formal definition since only resolved variable and their test-filtered forms are used. Here, the strain rate at
the test filter level, $\tilde{S}_{ij}$, is defined as,

$$\tilde{S}_{ij} = \left\{ \frac{\partial}{\partial x_i} \left( \frac{\tilde{u}_j}{\tilde{\rho}} \right) + \frac{\partial}{\partial x_j} \left( \frac{\tilde{u}_i}{\tilde{\rho}} \right) \right\}$$  \hspace{1cm} (A.3)

Equation A.2 is a over-determined tensorial system with 6 equations and one unknown ($C_v$). A method to determine the model coefficient from these expressions is proposed by Lilly [61]. The method is based on minimizing the subgrid tensor modeling error with respect to $C_v$. The modeling error, $E_{ij}$, can be defined on the test filter level as [61],

$$E_{ij} = \left( \frac{\tilde{u}_i \tilde{u}_j}{\tilde{\rho}} - \frac{2}{3} \left( \frac{\tilde{u}_i \tilde{u}_k - \tilde{u}_k \tilde{u}_i}{\tilde{\rho}^2} \right) \right) \delta_{ij} + 2C_v \Delta \tilde{\rho} \left( \frac{\tilde{u}_i \tilde{u}_j}{\tilde{\rho}^2} - \frac{\tilde{u}_k \tilde{u}_j}{\tilde{\rho}^2} \right) \frac{1}{2} \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right)$$ \hspace{1cm} (A.4)

In more compact form, the modeling error can be expressed by

$$E_{ij} = L_{ij} + 2C_v D_{ij}.$$ \hspace{1cm} (A.5)

where $L_{ij}$ is the exact test-filter subgrid tensor

$$L_{ij} = \frac{\tilde{u}_i \tilde{u}_j}{\tilde{\rho}} - \frac{1}{3} \left( \frac{\tilde{u}_i \tilde{u}_k - \tilde{u}_k \tilde{u}_i}{\tilde{\rho}^2} \right) \delta_{ij}$$  \hspace{1cm} (A.6)

and $2C_v D_{ij}$ is modelled test-filter subgrid stress tensor,

$$D_{ij} = 2C_v \Delta \tilde{\rho} \left( \frac{\tilde{u}_i \tilde{u}_j}{\tilde{\rho}^2} - \frac{\tilde{u}_k \tilde{u}_j}{\tilde{\rho}^2} \right) \frac{1}{2} \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right)$$ \hspace{1cm} (A.7)

In the final step of the procedure, the following expression for the minimization of the rms error is solved:

$$\frac{\partial E_{ij} E_{ij}}{\partial C_v} = 4D_{ij} L_{ij} + 8C_v D_{ij} L_{ij} = 0.$$ \hspace{1cm} (A.8)

Since all terms are known at the LES level, the model coefficient can be easily obtained from Equation A.8:

$$C_v = -\frac{L_{ij} D_{ij}}{2D_{ij} D_{ij}}.$$ \hspace{1cm} (A.9)

### A.2 Computation of $C_\varepsilon$

An approximate expression for the subgrid kinetic energy dissipation ($\varepsilon$) has been obtained by Nelson [73] in the limit of high Reynolds number flows with low compressibility effects
in the following form:

$$\varepsilon \approx \hat{\mu} \left( \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_j}{\partial x_i} \right) \approx \rho \epsilon^{(k_{gs})} \frac{\epsilon^{(k_{gs})}}{\Delta} \quad (A.10)$$

Similar to the procedure used for computing $C_v$, a test filter level expression of Equation A.10 can be written as

$$\varepsilon \approx \hat{\mu} \left[ \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{\partial \bar{u}_j}{\partial x_i} \left( \frac{\bar{p} \bar{u}_j}{\bar{p}} \right) \frac{\partial \bar{u}_j}{\partial x_i} \left( \frac{\bar{p} \bar{u}_j}{\bar{p}} \right) \right] \approx \rho \epsilon^{(k_{gs})} \frac{\epsilon^{(k_{gs})}}{\Delta} \left( \frac{\bar{p} \bar{u}_j \bar{u}_k}{2\bar{p}} - \frac{\bar{p} \bar{u}_k \bar{u}_k}{2\bar{p}} \right) \quad (A.11)$$

This final expression is rather simple and all terms are available from the resolved field.

Therefore, the model coefficient $C_\epsilon$ can be obtained as

$$C_\epsilon = \frac{\hat{\mu} \Delta}{\bar{p}} \left[ \frac{\partial \bar{u}_j}{\partial x_i} \frac{\partial \bar{u}_j}{\partial x_i} - \frac{\partial \bar{u}_j}{\partial x_i} \left( \frac{\bar{p} \bar{u}_j}{\bar{p}} \right) \frac{\partial \bar{u}_j}{\partial x_i} \left( \frac{\bar{p} \bar{u}_j}{\bar{p}} \right) \right] \left( \frac{\bar{p} \bar{u}_j \bar{u}_k}{2\bar{p}} - \frac{\bar{p} \bar{u}_k \bar{u}_k}{2\bar{p}} \right)^{\frac{1}{2}} \quad (A.12)$$
APPENDIX B

DEFINITIONS ON ENGINE TURBULENCE

Since a major characteristic of IC engines is the turbulent nature of the flow, some definitions relevant for turbulent flow analysis need to be explored. This would also help quantify cyclic change levels in the combustor. Reynolds averaging has been an important tool for both theoretical and experimental studies in turbulent flows. It assumes that the local instantaneous velocity at a point in space can be split into two components

\[ U(t) = \overline{U} + u(t) \]  
\[ \overline{U} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_{t_0}^{t_0+\tau} U(t)dt \]

where \( \overline{U} \) is the mean value and \( u(t) \) is the fluctuating component \[42\]. From a practical point of view, the determination of how much the instantaneous velocity deviates from the mean is very important. In the following definition

\[ u' = \lim_{\tau \to \infty} \left( \frac{1}{\tau} \int_{t_0}^{t_0+\tau} u'^2(t)dt \right)^{1/2} \]

\( u' \) is a statistical measure of this deviation and called as root mean square (RMS) value of turbulence. It is frequently used in characterizing turbulent flows, for example when referring to turbulent scales, since it provides a very good approximation to typical kinetic energy values (\( \approx u'^2 \)) of the most energetic scales.

B.1 Ensemble Averaged Decomposition

Definitions given above are applicable in principle for any flow. However, in periodic flows as seen in IC engines, the determination of the mean flow has difficulties because of variations in the flow from one cycle to another. Cyclic variations are manifested, for example, in the engine power output and common to all engines, with varying levels. It is usually accepted that the reason for these cyclic changes are the fluid motion, more specifically
the strength and location of large scale structures in the engine [86]. These structures are
very sensitive to inflow conditions, which are necessarily not the same from cycle to cycle.
Therefore, while on average certain patterns can be observed for the characteristics of large
scale structures (e.g., recirculation zones), their details for individual cycles are different.
Hence, corresponding ensemble averaged definitions where the averaging time interval is
replaced by another quantity more representative of the degree of flow development are
more appropriate. In the engine literature, this is the crank angle ($\theta$) and in the notation
of Heywood [42], the instantaneous velocity can be written as

$$U(\theta, i) = \bar{U}_{EA}(\theta) + u(\theta, i) \quad (B.4)$$

where the index “i” shows a particular cycle out of many such cycles obtained, for example,
in experimental measurements. The ensemble averaged velocity is defined as

$$\bar{U}_{EA}(\theta) = \frac{1}{N_c} \sum_{i=1}^{N_c} U(\theta, i) \quad (B.5)$$

and provides a single characteristic value for the mean velocity similar to steady flows. In
this definition, $u(\theta, i)$ is the fluctuating component and its RMS can be computed from

$$u_{F, EA}(\theta) = \left\{ \frac{1}{N_c} \sum_{i=1}^{N_c} [u(\theta, i)]^2 \right\}^{1/2} = \left\{ \frac{1}{N_c} \sum_{i=1}^{N_c} [U(\theta, i)^2 - \bar{U}_{EA}(\theta)^2] \right\}^{1/2} \quad (B.6)$$

**B.2 Cycle-Resolved Decomposition**

Engine flows may exhibit large cyclic differences. When there are large variations in the
mean flow between cycles, the fluctuating component defined in the context of ensemble-
averaged mean will erroneously give large turbulence values. This difficulty can be avoided
if it is recognized that a specific mean value for a particular cycle can be defined by filtering
$U(\theta, i)$ such that

$$U(\theta, i) = \bar{U}(\theta, i) + u(\theta, i) \quad (B.7)$$

Note that the fluctuating components have different meanings in Equations B.4 and B.7.
Obviously if there is no cyclic change, $\bar{U}_{EA}$ and $\bar{U}(\theta, i)$ will have the same value. In any
other case their relation can be defined as

$$\bar{U}(\theta, i) = \bar{U}_{EA}(\theta) + \hat{U}(\theta, i) \quad (B.8)$$
which expresses the fact that individual cycle mean is the sum of the ensemble mean and a fluctuating component, \( \hat{U}(\theta, i) \). This is a convenience and provides a formulation for determining cycle-by-cycle variation in the mean flow. Using Equation B.8 in Equation B.7, an expression similar to Equation B.4 can be obtained:

\[
U(\theta, i) = \overline{U}_{EA}(\theta) + \hat{U}(\theta, i) + u(\theta, i)
\]  

(B.9)

In this last expression (Equation B.9), it is clear that the turbulent fluctuation term in Equation B.4 is split into a low (\( \hat{U}(\theta, i) \)) and a high frequency (\( u(\theta, i) \)) fluctuating components.

### B.3 Numerical Implementation

The formulation presented above assumes that data is available at a specific point in a continuous manner. In experimental or numerical techniques for flow problems, the signal is obtained at discrete time intervals. In this case, the “instantaneous” signal, \( U(\theta, i) \), is the discrete signal from the measured data. If these discrete signals are grouped into a crank angle interval around a specific mean angle \( \theta \), such that \( N_j \) samples would be contained in the interval \( \theta \pm \Delta \theta \), a cycle mean can be determined for the crank angle interval

\[
\overline{U}(\theta \pm \Delta \theta, i) = \frac{1}{N_j} \sum_{j=1}^{N_j} U_{i,j}
\]  

(B.10)

where the index “i” refers to a particular cycle while the index “j” refers to the samples in the interval. Here, it is implicitly assumed that the experimental signal frequency is larger than the frequency of traveling the crank angle interval. This would ensure that the interval in Equation B.10 would contain at least 1 sample (i.e., \( N_j = 1 \)). \( U_{i,j} \) is the discrete signal for the interval at a specific cycle. Averaging Equation B.10 would give the ensemble averaged velocity at a particular crank angle, similar to Equation B.4:

\[
\overline{U}_{EA}(\theta) = \frac{1}{N_i} \sum_{i=1}^{N_i} \overline{U}(\theta \pm \Delta \theta, i)
\]  

(B.11)

A fluctuating component can be defined for the interval \( (\theta \pm \Delta \theta, i) \) for “j” samples by:

\[
U_{i,j} = \overline{U}_{EA}(\theta) + u_{i,j}
\]  

(B.12)
This definition includes the cyclic variations in the mean flow (i.e., low frequency fluctuations) and is not very suitable. Following Equation B.8, the cycle-by-cycle variation in mean velocity is

\[
\hat{U}(\bar{\theta} \pm \frac{\Delta \theta}{2}, i) = U(\bar{\theta} \pm \frac{\Delta \theta}{2}, i) - \overline{U_{EA}(\bar{\theta})} \tag{B.13}
\]

Equation B.9 can be rewritten as:

\[
U_{i,j} = \overline{U_{EA}(\bar{\theta})} + \hat{U}(\bar{\theta} \pm \frac{\Delta \theta}{2}, i) + u_{i,j} \tag{B.14}
\]

Equation B.14 is the discrete equivalent of Equation B.9 and separates low frequency fluctuations in the cycle from the high frequency fluctuations. In the literature, this is called cycle resolved turbulence analysis [22]. A measure of cyclic variation for a particular crank angle can be obtained by defining the RMS of low frequency cyclic variations:

\[
U_{RMS}(\bar{\theta}) = \left\{ \frac{1}{N_i} \sum_{i=1}^{N_i} [\hat{U}(\bar{\theta} \pm \frac{\Delta \theta}{2}, i)]^2 \right\}^{1/2} \tag{B.15}
\]

In the present study, since the engine motion is linear, the crank angle (\(\theta\)) is replaced by the distance to TDC, \(x_{TDC}\).
ENERGY BALANCE IN THE CHAMBER

The observed pressure increase in the chamber depends mainly on the heat release rate through chemical reactions and energy losses in the form of heat transfer across the chamber surfaces. The energy balance for the engine chamber can be written as

$$\frac{dE}{dt} = Q + W + \dot{m}h$$

where rate of internal energy change is expressed as a function of heat loss rate ($Q$), system boundary work ($W$) and enthalpy loss ($\dot{m}h$) in the case of mass leakage. $Q$ can be expressed as $Q = q_wS$ where $q_w$ is the wall heat transfer rate per unit area, defined as $q_w = -k(dT/dn)$ and evaluated at the wall. $S$ is the total surface area of the chamber across which heat transfer takes place. Internal energy is defined as $E = mu$. Here, $m$ is the mass of the gas in the chamber, related to chamber volume through $V = mv$, and $u$ is the internal energy per unit mass, defined as $u = \sum_{i=1}^{Ns} u_k Y_k$. After manipulation, Equation C.1 becomes

$$m \frac{du}{dt} = q_wS - p \frac{dV}{dt} + \rho \frac{dm}{dt}$$

(C.2)

Using the chain rule expression

$$m \frac{d\rho}{dt} + \rho \frac{dm}{dt} = \frac{dV}{dt}$$

(C.3)

the energy equation becomes

$$m \frac{du}{dt} = q_wS + \rho m \frac{d\rho}{dt}$$

(C.4)

Differentiating the internal energy per unit mass expression and using the chain rule

$$du_k/\frac{dt} = (du_k/dT)(dT/\frac{dt})$$

(C.5)

the rate of internal energy change per unit mass can be obtained as

$$\frac{du}{dt} = c_v \frac{dT}{dt} + \sum_{i=1}^{Ns} e_k \frac{dY_k}{dt}$$

(C.6)
Inserting this expression in Equation C.4 and dividing by volume, the final relation is obtained:

$$\frac{c_v}{\nu} \frac{\partial T}{\partial t} = -\frac{1}{\nu} \sum_{k=1}^{N_s} e_k \frac{dY_k}{dt} + q\omega \frac{S}{V} - \frac{P d\nu}{\nu dt} \tag{C.7}$$

Here, the ratio $S/V$ is the previously defined aspect ratio (AR) and its impact on the energy balance directly comes through the heat transfer term. Possible mass losses in the chamber are absorbed into the pressure work term and can be extracted through the following relation:

$$m \frac{d\nu}{dt} + \nu \frac{dm}{dt} = \frac{dV}{dt} \tag{C.8}$$
REFERENCES


