Simulation of Turbulent Flames at Conditions Related to IC Engines

Golnoush Ghiasi
Department of Engineering
University of Cambridge

This dissertation is submitted for the degree of

Doctor of Philosophy

Robinson College       June 2018
Engine manufacturers are constantly seeking avenues to build cleaner and more efficient engines to meet ever increasing stringent emission legislations. This requires a closer understanding of the in-cylinder physical and chemical processes, which can be obtained either through experiments or simulations. The advent of computational hardware, methodologies and modelling approaches in recent times make computational fluid dynamics (CFD) an important and cost-effective tool for gathering required insights on the in-cylinder flow, combustion and their interactions. Traditional Reynolds-Averaged Navier-Stokes (RANS) methods and emerging Large Eddy Simulation (LES) techniques are being used as a reliable mathematical framework tools for the prediction of turbulent flow in such conditions. Nonetheless, the combustion submodels commonly used in combustion calculations are developed using insights and results obtained for atmospheric conditions. However, The combustion characteristics and its interaction with turbulence at Internal combustion (IC) engine conditions with, high pressure and temperatures can be quite different from those in conventional conditions and are yet to be investigated in detail. The objective here is to apply FlaRe (Flamelets revised for physical consistencies) model for IC engines conditions and assess its performance. This model was developed in earlier studies for continuous combustion systems.

It is well accepted that the laminar burning velocity, $S_L$, is an essential parameter to determine the fuel burn rate and consequently the power output and efficiency of IC engines. Also, it is involved in almost all of the sophisticated turbulent combustion models for premixed and partially premixed charges. The burning velocities of these mixtures at temperatures of $850 \leq T \leq 950$ decrease with pressure up to about 3 MPa as it is well known, but it starts to increase beyond this pressure. This contrasting behaviour observed for the first time is explained and it is related to the role of pressure dependent reaction for iso-octane and involving OH and the influence of this radical on the fuel consumption rate. The results
seem to suggest that the overall order of the combustion reaction for iso-octane and gasoline mixture with air is larger than 2 at pressures higher than 3 MPa.

The FlaRe combustion is used to simulate premixed combustion inside a spark-ignition engine. The predictive capabilities of the proposed approach and sensitivity of the model to various parameters have been studied. FlaRe approach includes a parameter $\beta_c$ representing the effects of flame curvature on the burning rate. Since the reactant temperature and pressure inside the cylinder are continually varying with time, the mutual influence of flame curvature and thermo-chemical activities may be stronger in IC engines and thus this parameter is less likely to be constant. The sensitivity of engine simulation results to this parameter is investigated for a range of engine speed and load conditions. The results indicate some sensitivity and so a careful calibration of this parameter is required for URANS calculation which can be avoided using dynamic evaluations for LES. The predicted pressure variations show fair agreement with those obtained using the level-set approach.

DNS data of a hydrogen air turbulent premixed flame in a rectangular constant volume vessel has been analysed to see the effect of higher pressure and temperature on the curvature parameter $\beta_c$. Since the reactant temperature and pressure inside the cylinder are continually varying with time, the mutual influence of flame curvature and thermo-chemical activities are expected to be stronger in IC engines and thus the parameter $\beta_c$ may not be constant. To shed more light on this, two time steps from the DNS data has been analysed using dynamic $\beta_c$ procedure. The results show that the effect of higher pressure and temperature need to be considered and taken into account while evaluating $\beta_c$.

When combustion takes place inside a closed vessel as in an IC engine the compression of the un-burnt gases by the propagating flame causes the pressure to rise. In the final part of this thesis, the FlaRe combustion model is implemented in a commercial computational fluid dynamics (CFD) code, STAR-CD, in the LES framework to study swirling combustion inside a closed vessel. Different values of $\beta_c$ has been tested and the need for dynamic evaluation is observed.
Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is my own work and contains nothing which is the outcome of work done in collaboration with others, except as specified in the text and Acknowledgements. This dissertation contains approximately 46,000 words including appendices, bibliography, footnotes, tables and equations and has 48 figures.

Golnoush Ghiasi
June 2018
Acknowledgements

I would like to express my gratitude to my supervisor, Prof. N. Swaminathan, for his kindness, help and support, especially during periods of difficult times. His patience and guidance throughout the course of this work contributed to the successful completion of this thesis. I will always be grateful to him for this great opportunity. What he has taught me goes beyond combustion science. Special thanks to Dr Yuri Wright and Mr Jann Koch from ETH Zurich for the STAR-CD setup and for providing the computational mesh used to simulate the internal combustion engine. Special thank to Dr Yuki Minamoto for providing the DNS data. The computing help I received from Mr Peter Benie is gratefully acknowledged. I would like to acknowledge KACST and Dr Omar Aljumaiah for funding and supporting this project.

Many others have contributed to the success of this work, including colleagues from the Hopkinson laboratory with whom I have had numerous interesting and fruitful discussions. Dr Irufan Ahmed thank you for all the generous help and useful suggestions, your patience and humble character helped me gain the confidence needed to start this project. Dr Ivan Langella and Zhi Chen, it was always refreshing having a discussion with you, your calm and collected approach towards various computational difficulties was always very inspiring. Anh Khoa Doan, thank you for all the great discussions, for being there with your endless positivity, drive and last but not least all the Belgian chocolates. I learnt a lot working along side you.

My dear friend Michael Panayi, I would like to thank you for standing by my side, in very difficult moments, when truly no one else was there. You held me up with all the kindness. Dear Doctor to be Marisa, thank you for listening to my endless nervous break downs, and repetitive questions, that you may never know the answers to, you are now qualified as a therapist.

Words can not explain my gratitude towards my parents, Mehran and Sedigh, whom made the very difficult decision of, sending me abroad at a young age, allowing and supporting me to experience life through my own eyes. I will forever be grateful for all the opportunities you have always provided me, with open arms. My dear, brothers Payam and Pouya, who were my very own "in-house" science teachers. You both have inspired me from day one, none of this would have been possible without you.
I look up to the stars and dream of a world that’s a better place. A world where dreams are reality. People living out their dream, not held back by their race or religion. This thesis is dedicated to all the ones who fight that prejudice daily, and never stop dreaming.
Table of contents

List of figures xv
List of tables xix
Nomenclature xxiv

1 Introduction 1
  1.1 Aim and Objectives ............................................. 3
  1.2 Outline .......................................................... 4

2 Background on premixed combustion related to IC engines 5
  2.1 Governing equations ............................................. 5
  2.2 Numerical paradigms ........................................... 7
    2.2.1 Direct numerical simulations ............................... 7
    2.2.2 Large eddy simulations .................................... 8
    2.2.3 Reynolds-averaged Navier-Stokes equations ............... 12
  2.3 Laminar premixed flames ....................................... 15
    2.3.1 Flame thickness ............................................ 15
    2.3.2 Flame speed $S_L$ ........................................... 16
  2.4 Turbulent premixed flames ..................................... 16
    2.4.1 Combustion regimes ......................................... 16
  2.5 Modelling of turbulent premixed combustion .................. 18
    2.5.1 The Eddy Break-up (EBU) model .......................... 18
    2.5.2 Bray-Moss-Libby (BML) modelling ......................... 20
    2.5.3 Flame surface density model .............................. 22
    2.5.4 G-equation approach ....................................... 23
    2.5.5 Artificially thickened flames ............................. 24
    2.5.6 Conditional moment closure (CMC) ......................... 24
    2.5.7 Transported pdf approach ................................. 25
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5.8 Presumed pdf approach</td>
<td>27</td>
</tr>
<tr>
<td>2.6 Engine simulations</td>
<td>29</td>
</tr>
<tr>
<td>3 Gasoline laminar flame behaviour at elevated temperature and pressure</td>
<td>35</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>35</td>
</tr>
<tr>
<td>3.2 Computational detail</td>
<td>37</td>
</tr>
<tr>
<td>3.3 Chemical mechanisms</td>
<td>38</td>
</tr>
<tr>
<td>3.4 Results and discussion</td>
<td>39</td>
</tr>
<tr>
<td>3.4.1 Validation cases</td>
<td>39</td>
</tr>
<tr>
<td>3.4.2 Flame speed and structure at elevated temperature and pressure</td>
<td>41</td>
</tr>
<tr>
<td>3.5 Sensitivity analysis</td>
<td>46</td>
</tr>
<tr>
<td>3.6 Summary</td>
<td>50</td>
</tr>
<tr>
<td>4 Spark-ignition engine simulation</td>
<td>53</td>
</tr>
<tr>
<td>4.1 Engine description</td>
<td>53</td>
</tr>
<tr>
<td>4.2 Numerical setup</td>
<td>55</td>
</tr>
<tr>
<td>4.2.1 Model implementation</td>
<td>55</td>
</tr>
<tr>
<td>4.2.2 Flamelet library generation</td>
<td>57</td>
</tr>
<tr>
<td>4.2.3 Chemical mechanisms</td>
<td>57</td>
</tr>
<tr>
<td>4.2.4 Computational mesh</td>
<td>57</td>
</tr>
<tr>
<td>4.2.5 Initial and boundary conditions</td>
<td>58</td>
</tr>
<tr>
<td>4.2.6 Computational details</td>
<td>59</td>
</tr>
<tr>
<td>4.2.7 Ignition treatment</td>
<td>59</td>
</tr>
<tr>
<td>4.3 Results and discussion</td>
<td>61</td>
</tr>
<tr>
<td>4.3.1 Influence of ignition treatment</td>
<td>61</td>
</tr>
<tr>
<td>4.3.2 Chemical mechanism effect</td>
<td>63</td>
</tr>
<tr>
<td>4.3.3 Unburnt temperature calculation</td>
<td>65</td>
</tr>
<tr>
<td>4.3.4 Combustion model comparison</td>
<td>66</td>
</tr>
<tr>
<td>4.3.5 Flame curvature induced effects</td>
<td>68</td>
</tr>
<tr>
<td>4.3.6 Effect of $\beta_c$</td>
<td>72</td>
</tr>
<tr>
<td>4.3.7 Change of speed and load</td>
<td>72</td>
</tr>
<tr>
<td>4.4 Summary</td>
<td>73</td>
</tr>
<tr>
<td>5 Model assessment using DNS data</td>
<td>77</td>
</tr>
<tr>
<td>5.1 Introduction</td>
<td>77</td>
</tr>
<tr>
<td>5.2 SGS combustion modelling investigated</td>
<td>80</td>
</tr>
<tr>
<td>5.3 DNS data</td>
<td>82</td>
</tr>
</tbody>
</table>
# Table of contents

5.4 Data processing .................................................. 85  
5.5 Results and discussion ........................................... 85  
5.5.1 SGS reaction rate closure ................................... 86  
5.5.2 Evaluation of $\bar{c}_v$ closure .............................. 91  
5.6 Summary ............................................................... 94  

6 Swirling combustion inside a closed vessel .................. 95  
6.1 Introduction ......................................................... 95  
6.2 Experimental test case ............................................ 96  
6.3 Numerical setup .................................................... 97  
6.3.1 Computational details ....................................... 97  
6.3.2 SGS combustion modelling .................................. 98  
6.3.3 Initialization .................................................... 99  
6.3.4 Spark treatment ............................................... 100  
6.4 Results and discussions ......................................... 100  
6.4.1 Cold flow validation ......................................... 100  
6.4.2 Reacting flow ................................................... 101  
6.5 Summary ............................................................... 110  

7 Concluding remarks ............................................... 111  
7.1 Summary of findings ............................................. 111  
7.2 Future work ......................................................... 112  

References ............................................................. 115
List of figures

2.1 Schematic of a laminar flame ................................................. 17
2.2 Turbulent premixed combustion regime diagram [143]. ............ 19

3.1 Comparison of measured and computed \( S_L \) for stoichiometric iso-octane-air mixtures at various reactant temperature, \( T_u \) and pressure. Results are shown for three mechanisms along with commonly used flame speed correlations: Cor1 is from [70], Cor2 is from [131]. ......................... 40

3.2 Flame and autoignition regions in \( T-P \) space predicted using Mech-2 (\( \times \)) and Mech-3 (circles) mechanisms for stoichiometric iso-octane and air mixture. The results are also shown for the gasoline surrogate mixture (open circles). Light blue rectangular region shows the mixture conditions explored. .... 42

3.3 Spatial variation of \( T \) and few selected species mole fractions across the flame for \( T_u = 900 \) K (top row) and 950 K (bottom) at 40 bar for Mech-3. .. 44

3.4 Variation of normalised burning rate mass flux with pressure for iso-octane and gasoline surrogate mixtures at three different temperatures. ......................... 45

3.5 Variation of normalised flame speed with pressure for stoichiometric iso-octane (left) and gasoline surrogate mixtures (right) at three different temperatures. The inset shows the variation of \( \beta \) with \( \ln(p/p_0) \). ......................... 46

3.6 Net rate of elementary reaction involving iso-octane, see Table 3.1, integrated across the flame. The results are shown for both gasoline surrogate and iso-octane mixtures at 4 pressures, 35, 40, 45 and 50 bar, with \( T_u = 850 \) (left set of frames) and 900 K (right). ......................... 48

3.7 Variation of net reaction rate with pressure for reactions 3226 to 3229 and 16. The reaction rates are integrated across the flame for the gasoline surrogate mixture at 900 K. The reaction 16 is \( \text{H}_2\text{O}_2 (+\text{M}) \leftrightarrow \text{OH} + \text{OH}(+\text{M}) \). .. 49
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.1</td>
<td>A schematic of a part of the symmetric computational volume along with boundary conditions used in the simulations. The outlet boundary conditions are shown for a case without backflow. The colour represents the velocity magnitude when the piston is at (BDC).</td>
</tr>
<tr>
<td>4.2</td>
<td>Flow chart showing the combustion model implementation in Star-CD.</td>
</tr>
<tr>
<td>4.3</td>
<td>Events sequence in the engine, which shows the valve movement plotted against the crank angle for Case 2.</td>
</tr>
<tr>
<td>4.4</td>
<td>Variation of heat release rate with $c$ for $T_u = 650$ K and $p = 10$ bar.</td>
</tr>
<tr>
<td>4.5</td>
<td>Ignition (a) power and (b) energy supplied for the two ignition treatments.</td>
</tr>
<tr>
<td>4.6</td>
<td>Pressure trace comparisons for two different ignition treatments using the mechanism of Hasse et al. [75].</td>
</tr>
<tr>
<td>4.7</td>
<td>(a) Heat release rate and (b) cumulative heat release for two different ignition treatments using the mechanism of Hasse et al. [75].</td>
</tr>
<tr>
<td>4.8</td>
<td>Pressure trace comparisons using chemical mechanism of Hasse et al. [75] and Mehl et al. [130].</td>
</tr>
<tr>
<td>4.9</td>
<td>Contours of heat release rate during combustion, $\dot{q}$, at different crank angles using mechanisms of (a) Hasse et al. [75] and (b) Mehl et al. [130].</td>
</tr>
<tr>
<td>4.10</td>
<td>(a) Heat release rate and (b) cumulative heat release using chemical kinetics of Hasse et al. [75] and Mehl et al. [130].</td>
</tr>
<tr>
<td>4.11</td>
<td>Sensitivity to $\tilde{c}$ threshold used to calculate $T_u$: (a) calculated $T_u$ and (b) corresponding pressure traces. Mechanism of Mehl et al. [130] is used for the simulations.</td>
</tr>
<tr>
<td>4.12</td>
<td>Pressure trace comparisons using the flamelet based combustion model (Hasse et al. [75] mechanism using 2 cells for ignition at a duration of $4^\circ$ CA) and $G$-equation with different values for the flame speed coefficient, $A$.</td>
</tr>
<tr>
<td>4.13</td>
<td>Variations of temperature (solid lines) and reaction rate (dashed lines) through flamelets having different reactant temperature and pressure.</td>
</tr>
<tr>
<td>4.14</td>
<td>Variations of $\nabla \omega$, $\nabla^2 c$, $\nabla c$ through the flamelets.</td>
</tr>
<tr>
<td>4.15</td>
<td>Variation of in-cylinder pressure and cumulative heat release rate with CAD for various $\beta_c$. The variation of percentage change in the peak pressure with $\beta_c$ is shown in (c).</td>
</tr>
<tr>
<td>4.16</td>
<td>Temporal evolution of $c = 0.1$ iso-surface coloured by temperature.</td>
</tr>
<tr>
<td>4.17</td>
<td>In-cylinder pressure trace comparison for the five operating conditions.</td>
</tr>
</tbody>
</table>
5.1 Visualisation of flame and flow features at $\hat{t} = 0.73$ (left) and 0.91 (right), where $\hat{t}$ is time normalised using the turbulence integral eddy turnover time. Blue isosurfaces represent $Q = \langle Q \rangle + 3 \sigma_Q$ and red iso-surface is for 60% of the maximum $\omega_c$. ................................................................. 83

5.2 Temporal variation of mean pressure ($\circ$) and reactant temperature ($\square$) inside the vessel is shown on the left. The picture on the right compares the $P_a-T_a$ map from the DNS (symbols) to that of isentropic theoretical curve (line). ................................................................. 84

5.3 Contours of filtered reaction rate from the DNS (left column) for $\Delta^+ = 0.5$, 1 and 2 (from top to bottom) at $\hat{t} = 0.73$ and the corresponding modelled reaction rate (right). The reaction is normalised using $\rho_u, s_L$ and $\delta_{th}$. ........... 87

5.4 Contours of filtered reaction rate from the DNS (left column) for $\Delta^+ = 0.5$, 1 and 2 (from top to bottom) at $\hat{t} = 0.91$ and the corresponding modelled reaction rate (right). The reaction is normalised using $\rho_u, s_L$ and $\delta_{th}$. ........... 88

5.5 Typical variation of normalised filtered reaction rate from the model (look-up table in the top row) and the DNS values (bottom) for $\Delta^+ = 0.5$. The results are shown for two different times $\hat{t} = 0.73$ (left column) and 0.91 (right). ........... 89

5.6 Joint pdf, $\mathcal{P}$, of normalised DNS and modelled filtered reaction rate for $\hat{t} = 0.73$ (left) and 0.91 (right). The results are shown for $\Delta^+ = 0.5$. The colour scale is for $\log(\mathcal{P})$. ................................................................. 90

5.7 Comparison of DNS and modelled SGS scalar dissipation rate at $\hat{t} = 0.73$ (left) and 0.91 (right) for $\Delta^+ = 0.5$. The modelled value is obtained using Eq. (5.5) with $\beta_c = 0.6$ and 0.3 respectively for $\hat{t} = 0.73$ and 0.91. ........... 91

5.8 Pdf of $\beta_c$ (solid line) and $\beta_c^*$ (dashed) evaluated using Eqs. (5.9) and (5.10) for a filter width of $\Delta^+ = 0.5$. The left frame is for $\hat{t} = 0.73$ and the right is for 0.91. ................................................................. 92

5.9 Joint pdf of modelled and DNS values of SDR, normalised using $s_L$ and $\delta_{th}$ appropriately. The results are shown for $\hat{t} = 0.73$ (top row) and 0.91 (bottom) for $\beta_c$ obtained using Eq. (5.9) (left column) and $\beta_c^*$ from Eq. (5.10) (right). 93

6.1 Schematic of the experimental test case with the representative computational domain used for the simulations. A schlieren picture is also shown. ........... 96

6.2 Numerical domain considered for the simulations. The red sphere represents the sparking region. ................................................................. 97

6.3 Variation of filtered reaction rate for stoichiometric propane-air mixture at $T = 400$ K for (a) $p = 8$ bar and (b) 20 bar pressures. ................................................................. 99

6.4 Contours of (a) radial, (b) azimuthal and (c) transverse velocities computed in the LES. The results are shown in the mid $x$-$y$ plane at about 10 ms. ....... 102
6.5 (a) Radial variation of the azimuthal velocity in the mid $x$-$y$ plane at two different times and the corresponding variation of turbulence intensity is shown in (b). ............................................. 103
6.6 Contours of computed velocity magnitude in the mid $x$-$y$ (top row) and $x$-$z$ (bottom) planes at 4.2 (left column) and 9 ms (right) after the ignition. .... 104
6.7 Iso-surface of $\tilde{c} = 0.7$ coloured with $\overline{\omega_c}$ (in kg/m$^3$ $-$ s) at 4.2 (top) and 9 ms (bottom) ................................................................. 105
6.8 Contours of $\tilde{c}$ in the mid $x$-$y$ (top row) and $x$-$z$ (bottom) planes at 4.2 (left column) and 9 ms (right). ................................................. 106
6.9 Contours of $\overline{\omega_c}$ (kg/m$^3$ $-$ s) in the mid $x$-$y$ (top row) and $x$-$z$ (bottom) planes at 4.2 (left column) and 9 ms (right). ................................. 107
6.10 Contours of SGS dissipation rate, $\tilde{\epsilon}_c$ (s$^{-1}$), in the mid $x$-$y$ (top row) and $x$-$z$ (bottom) planes at 4.2 (left column) and 9 ms (right). ................. 108
6.11 Variations of (a) filtered reaction rate and (b) SGS dissipation rate with $\tilde{c}$ at 4.2 and 9 ms. The scatter is from LES and the lines are the corresponding conditional averages. .............................................. 109
6.12 Comparison of measured (dashed line) and computed flame propagation for $\beta_c = 6.0$ (blue line), 6.7 (red), 7.5 (green). ................................. 109
6.13 Pressure rise prediction ................................................................. 110
### List of tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>First 15 most important reactions involving $iC_8H_{18}$</td>
<td>47</td>
</tr>
<tr>
<td>4.1</td>
<td>Engine parameters[96]</td>
<td>54</td>
</tr>
<tr>
<td>4.2</td>
<td>Engine operating conditions</td>
<td>55</td>
</tr>
<tr>
<td>4.3</td>
<td>Wall temperatures used to specify the BCs</td>
<td>59</td>
</tr>
</tbody>
</table>
Nomenclature

Acronyms/Abbreviations

*BM*EP  Break mean effective pressure
*C*CV  Cycle-to-cycle variation
*C*FD  Computational fluid dynamics
*DI*  Direct Injection
*D*N*S*  Direct numerical simulation
*ED*  Energy deposition
*EGR*  Exhaust gas recirculation
*FlaRe*  Flamelet revised for physical consistencies
*F*SD  Flame surface density
*HCCI*  Homogeneous charge compression ignition
*IC*  Internal combustion
*LES*  Large eddy simulation
*LHS*  Left hand side
*P*CCI*  Premixed Charge Compression Ignition
*PDF*  Probability density function
*RANS*  Reynolds averaged Navier-Stokes
*RHS*  Right hand side
Nomenclature

SDR  Scalar dissipation rate
SGS  Subgrid scale
TI   Turbulent intensity
TKE  Turbulent kinetic energy
URANS Unsteady-RANS
WOT  Wide open throttle

Greek Symbols

\( \Delta \)  Filter width
\( \delta \)  Flame thickness
\( \delta_{ij} \)  Kronecker delta
\( \dot{\omega} \)  Reaction rate
\( \varepsilon \)  Dissipation
\( \eta_k \)  Kolmogorov’s scale
\( \gamma \)  Thermal diffusivity
\( \Lambda \)  Integral length scale
\( \mu \)  Dynamic viscosity
\( \mu \)  Kinematic viscosity
\( \rho \)  Density
\( \tau \)  Heat release
\( \tau_{ij} \)  Reaction rate
\( \tilde{\varepsilon}_c \)  Subgrid scale scalar dissipation rate of \( c \)

Non-dimensional Numbers

\( Da \)  Damköhler number
\( Ka \)  Karlovitz number
$Le$  Lewis number
$Re$  Reynolds number
$Re_T$  Turbulent Reynolds number
$Sc_T$  Turbulent Schmidt number

**Roman Symbols**

$\Delta h_f^0$  Enthalpy of formation
$\bar{c}''$  Variance of $c$
$c$  Progress variable
$C_p$  Heat capacity constant
$C_s$  Smagorinsky constant
$h$  Total enthalpy (sensible+chemical)
$k$  Turbulent kinetic energy
$N_c$  Scalar dissipation rate of $c$
$p$  Pressure
$R_0$  Universal constant of ideal gases
$S_L$  Laminar flame speed
$T$  Temperature
$t$  Time
$u$  Velocity vector
$V_{k,i}$  Diffusion velocity of species $k$
$W_k$  Molecular mass of $k$-th species
$x, y, z$  Spatial coordinates
$Y_k$  Mass fraction of species $k$
Subscript

$\Delta$  Subgrid scale

$b$  Burnt

$s_{gs}$  Subgrid scale

$u$  Unburnt
Chapter 1

Introduction

The global energy consumption has been on an increasing trend from the beginning of the industrial revolution in Europe up to the current decade. The exhaustible natural fossil fuel resources supply a significant proportion of this global energy consumption, contributing to 81% of the global energy consumption in 2010 [46].

In fact, according to the latest International Energy Agency (IEA) oil market report 2017, the world energy consumption will grow by 28% between 2015 and 2040. In their recent report, even though IEA2017 expects the non-fossil fuels (renewables and nuclear) to grow faster than fossil fuels, the latter still accounts for more than three-quarters of world energy consumption through 2040.

Furthermore, the IEA forecast anticipates further increase in oil demand, which may reach about 110.1 million barrels per day in 2030. This forecast is based on fundamental factors such as the increase in global population, and the fact that most of the oil consumption is in the areas of transports and petrochemical industries, which are sectors that are not expected to change in the foreseeable future. Oil refined products such as gasoline and diesel have been the preferred energy sources in the transport sector and remains to be the major source in the anticipated future, 93% of fuels used for transport in 2010 is based on fossil fuels and it is predicted to account for 83% share in 2035. This is due to several factors, most important of which is the high energy to weight ratio of these fuels, and the challenge in energy storage for alternative energy sources [82]. This increase in demand is not expected to be matched by the amount of proven oil reserves which currently stand at about 1.64 billion barrels [46].

Other logistical factors such as energy supply chain, and the replacement cost of existing systems, suggest that even if an alternative source of energy is considered, it is safe to assume that oil based products will remain the main source of energy for transport in the coming decades. On the other hand, combustion products such as: carbon dioxide (CO$_2$), carbon
monoxide (CO), sulphur dioxide (SO₂), nitrogen oxides, and un-burnt hydrocarbons (UHC) have been identified as a contributing cause to the climate change problem and greenhouse effect. Therefore, current and past combustion systems adopted in the transport sector are monitored and evaluated continuously. Collaborative governmental and international efforts results in increasingly stringent pollution control measures. Thus existing engines technology needs significant efforts to improve efficiency and meet ever demanding environmental pollution control limits. The engine research is commonly conducted using experimental, analytical, and numerical approaches. While experimental research makes a significant proportion of current activities, analytical research provide limited insight into the combustion phenomena. Nonetheless, numerical studies have the potential to reduce the cost in capital and time associated with experimental studies. However, the development of sophisticated and high fidelity models capable of delivering the required level of details in engine research is an active area in itself. This effort is geared towards improving existing combustion models commonly used in engine simulations.

Two modes for combustion of gaseous fuel are identified: non-premixed, in which fuel and oxidiser enter the combustion chamber separately, and premixed, in which fuel and oxidiser are mixed homogeneously before combustion begins [137]. Fuel-air mixing is incomplete in practical combustion systems, leading to partially premixed combustion. Recently, premixed combustion with lean condition (low fuel-to-air ratio) has attracted industries interest, as its promising potential for achieving high thermal efficiency and low pollutant emissions simultaneously [137]. Future spark-ignited IC engines are expected to burn lean, as it will lead to significant improvement in thermal efficiency and reduction in green house gas emissions. The combustion process in IC engines is characterised by complex turbulent-chemistry interactions, which can span multiple combustion regimes, hence careful design is required because of the inherent difficulty of achieving stable lean combustion [187].

In response to the aforementioned factors, combustion scientists have focused their efforts on developing more advanced combustion systems. Some of the promising systems focusing on utilising combustion regimes commonly referred to as Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) technology with low NOx emission and about 10 to 15% improvement in fuel efficiency are promising alternatives to current IC engine combustion technologies [85]. They may pave the way for a new generation of transport engines delivering substantially better standards for emissions and efficiency. Nonetheless, significant research needs to be carried out to make the full potential of these techniques deployable at industrial scale levels [187].
1.1 Aim and Objectives

The advent of computational hardware, methodologies and modelling approaches in recent times make computational fluid dynamics (CFD) an important and cost-effective tool to gather the required insights on in-cylinder flow, combustion and their interactions. Direct Numerical Simulations (DNS) in which all-spatial and temporal scales are resolved, is still unaffordable for complex geometries such as IC engines, hence it is used as an investigation tool for developing closures for Reynolds Averaged Navier-Stokes (RANS) and Large Eddy Simulations (LES) methodologies [134].

Reynolds-Averaged Navier-Stokes (RANS), in which the equations describing the mean flow field are solved, is the current industry standard for simulations of reacting flows in IC engines. Nonetheless, Large Eddy Simulations (LES) resolving the large eddies with models for the smaller scales can improve the accuracy of these simulations. LES methodology is computationally more expensive than RANS, however with the increase in computational power in the recent years, it is gathering popularity for engine simulations. Furthermore, LES can be used to study cycle-to-cycle variability in IC engines, which is not possible in RANS calculations [76, 162]. This work, by pushing the limits in CFD modelling of reacting flow in engine and engine like setups would ultimately lead to an improvement in future generations of engines in terms of their efficiency and harmful emissions. Thus improving the consumption rate of the valuable and exhaustible fossil fuel, which will become even more valuable in future generations, and help to mitigate the harmful impact on the environment caused by current engine technologies.

1.1 Aim and Objectives

The overall aim of this work is to apply the existing modelling framework, the FlaRe (Flamelets revised for physical consistencies) model, developed by Kolla and Swaminathan [99], under IC engines conditions and assess its performance. For this approach to be useful in designing IC engines, it needs to be accurate, robust, and computationally economical. Therefore, the objectives of this study are:

1. To investigate whether there is a monotonic decrease of $S_L$ with $p$ for stoichiometric mixture of Gasoline-air and iso-octane-air at conditions relevant for next generation of internal combustion engines, by performing laminar flame computations using the state-of-the art comprehensive chemical mechanisms, validated well in previous studies. In particular, to understand if the commonly used correlations for $S_L$ with $p$ can be used at elevated pressure and temperature conditions of interest for modern engines;
2. To test the FlaRe model for an SI engine calculation (URANS) and to determine its sensitivity to spark ignition treatment, chemical kinetics, and engine operating conditions (changes in engine load and speed), these two key engine parameters influences the flow and thermo-chemical conditions inside the cylinder and thereby affects the turbulence combustion interaction (TCI) which governs one particular parameter $\beta_c$, of this model. Thus, the sensitivity to this parameter is investigated;

3. To test the unstrained flamelet closure for the SGS reaction rate and to investigate the behaviour of $\beta_c$ and its dynamic evaluation using DNS data of isochoric combustion [200, 201].

4. To implement the FlaRe combustion model in LES context in a commercial CFD code, STAR-CD and test its performance.

These objectives are achieved by conducting simulations of laminar flames, SI engines and by using DNS data. The LES implementation is also tested and validated. The LES experimental and numerical data for the validations are selected carefully and are discussed in later chapters.

1.2 Outline

The background literature on engine simulations along with turbulent combustion model are described in Chapter 2. The first objective of this work is addressed in Chapter 3. The results from IC engine URANS calculations for objective 2 are discussed in Chapter 4. The analysis of DNS data to find answers for the thesis objective is discussed in Chapter 5. The simulations of swirling flames inside a closed vessel are discussed to address the fourth objective indicated above for this thesis.
Chapter 2

Background on premixed combustion related to IC engines

2.1 Governing equations

The common Navier-Stokes equations for constant-density flows require some special treatments for turbulent combustion. Species react chemically and their rate of reaction requires special modelling. Detailed thermodynamic and transport data for a multicomponent gas is required as a result of this complexity. A number of assumptions are required. The reacting fluid is considered to be a mixture of Newtonian perfect gases. Fickian diffusion is assumed for molecular diffusive flux. Combustion is assumed to be adiabatic with the gravitational and external forces on gases are neglected. Using the above common assumptions, the governing equations for instantaneous mass, momentum, species mass fractions and total enthalpy are given as follows [143, 149]:

- conservation of mass:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0, \quad (2.1)
\]

where \(u_i\) is the velocity component in spatial direction \(x_i\), \(t\) is time and \(\rho\) is the fluid mixture density.

- conservation of momentum:
Background on premixed combustion related to IC engines

\[ \frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} \tag{2.2} \]

where \( p \) is the pressure and

\[ \tau_{ij} = \mu \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} \tag{2.3} \]

is the viscous stress tensor, \( \mu \) and \( \delta_{ij} \) being kinematic viscosity and the Kronecker delta respectively;

- Species Conservation:

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial [\rho (u_i + V_{k,i}) Y_k]}{\partial x_i} = \dot{\omega}_k, \quad k = 1, 2, \ldots, N \tag{2.4} \]

where \( Y_k \) is the mass fraction of species \( k \), in a mixture containing \( N \) number of species and \( V_{k,i} \) is the diffusion velocity of species \( k \) in the direction \( i \), and \( \dot{\omega}_k \) is the chemical reaction rate of the species \( k \), which is expressed using Arrhenius equation, see for example [197] for more details.

- conservation of total enthalpy (sum of sensible enthalpy, \( h_s \), and enthalpy of formation, \( \Delta h^0_f \)).

The energy conservation equation can be presented in many different forms. In most combustion modelling cases, the form involving total enthalpy of the mixture, \( h \) per unit mass is usually preferred for low-speed flows:

\[ \frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = -\frac{\partial q_i}{\partial x_i} + \frac{Dp}{Dt} + \tau_{ij} \frac{\partial u_i}{\partial x_j} \tag{2.5} \]

where \( Dp/Dt \) is the substantial derivative of pressure \( p \). The heat flux in the direction \( x_i \) is modelled as:
\[ q_i = -\lambda \frac{\partial T}{\partial x_i} + \rho \sum_{k=1}^{N} h_R Y_k V_{k,i} \]  

(2.6)

where \( \lambda \) and \( T \) are the thermal conductivity and temperature respectively. The last term in Eq. 2.5 is the viscous dissipation term, which is typically small for low speed reacting flows. The Eqs. (2.1), (2.2), (2.4) and (2.5) constitute a system of equations for reacting flows with \( N+5 \) dependent variables, \( N \) species, density, 3 velocities, temperature and pressure. There are \( N+4 \) equations and the fifth equation is the equation of state for the mixture, which is:

- state equation

\[ p = \rho R_0 T \sum_{k=1}^{N} \frac{Y_k}{W_k} \]  

(2.7)

where \( R_0 = 8.314 \text{ J/mol} \) – \( k \) is the universal gas constant and \( W_k \) is the molecular mass of the \( K \)-th species. The above equations can be solved, in principle, with numerical methods approximately. However, three different paradigms can be employed depending on the research objective.

## 2.2 Numerical paradigms

Turbulent combustion numerical simulations are broadly classified into three different types. Direct Numerical Simulations (DNS), Large-Eddy Simulations (LES), and Reynolds Averaged Navier-Stoke (RANS) simulations. Each of these have their own advantages and disadvantages, and the common practice to choose a technique depends on the balance between the level of details required and the computational power available.

### 2.2.1 Direct numerical simulations

Direct numerical simulations (DNS) directly solves the full instantaneous Navier-Stokes equations without any model for turbulent motions. In DNS, all turbulence scales are resolved and their effects on combustion are captured without models for turbulent-chemistry interactions. Thus, this method is computationally very demanding and typically limited to
simplified geometries and low Reynolds numbers. It is sometimes referred to as numerical experiments as it does not involve any empirical constants and it can reveal physical insights into various processes involved in turbulent combustion. The increase in computational power in recent years has allowed some advancement in the ability to simulate moderate Reynolds number flows using DNS [32]. Hence, DNS is very useful for model/hypothesis testing and for developing new models for turbulence-chemistry interaction. Nonetheless, simulating reacting flows in practical engines using DNS does not appear to be feasible in the near future. Therefore, it has become the standard to use either RANS (averaged) or LES (filtered) paradigms for practical application. These approaches are explained briefly below.

2.2.2 Large eddy simulations

The large eddy simulations (LES) resolve the large dynamic scales of turbulence, while the small scales and their effects are modelled using subgrid closure. This technique is widely used for non-reacting flows, see for example [51] and [145]. In terms of computational expenses this technique is cheaper than DNS but more expensive than RANS [155]. The opportunities of LES in analysing in-cylinder flows have been reviewed in [162] and it explains that IC engines are good applications for LES analysis as the flows are inherently unsteady due to moving geometries (piston and valves), dynamics of large-scale flow structures are important the Reynolds number values in IC engine are modest around 10000 to 30000, and lastly the domain of interest is confined and moderate in size. Past engine simulations using LES are discussed further in section 2.6.

LES Filtering

The governing equations for large eddy simulations are obtained by filtering the instantaneous balance equations discussed in section 2.1, using a filtering operation. The filtered value of a quantity $f$ is defined as [155]:

$$\tilde{f}(x) = \int f(x')F(x-x') \, dx'$$  \hspace{1cm} (2.8)

where $F$ is the spatial filter function, which depends on space and the filter width, $\Delta$. Eq. (2.8) was written for simplicity for the one-dimensional case. The filter width establishes the accuracy of the LES calculations as it defines which scales are resolved and which are modelled [155]. While several choices for the filter are available, the Gaussian filter is defined as [155]:
2.2 Numerical paradigms

\[ F(x) = \left( \frac{6}{\pi \Delta^2} \right)^{3/2} \exp \left[ -\frac{6x^2}{\Delta^2} \right] \]  

(2.9)

Extension to a three-dimensional case is straightforward and can be found in the literature. The filter given above is integrated to unity as:

\[ \int_{-\infty}^{+\infty} F(x) \, dx = 1 \]  

(2.10)

For flow with variable density, a mass-weighted (Favre) filtering is used and the Favre filtering is defined as:

\[ \overline{\rho f}(x) = \int \rho f(x') F[(x - x')] \, dx' \]  

(2.11)

Although the filter operation described above is conceptually simple, it hides some issues and should carefully be conducted:

- Deriving the balance equations for the filtered quantities require the exchange of both filter and derivative operators. This filter is only valid under restrictive assumptions. Ghosal and Moin [61] have investigated this in detail. Moureau et al. [136] states that for example in piston engines, time commutation errors must also be accounted for.

- Filtered value of the fluctuation is not zero ie \( \overline{f} \neq 0 \) and also \( f \neq f \).

Filtered equations

Governing equations for large eddy simulations are obtained by filtering the instantaneous equations given in Eqs. (2.1) to (2.5).

\[ \frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho \tilde{u}_i}}{\partial x_i} = 0 \]  

(2.12)

\[ \frac{\partial \overline{\rho \tilde{u}_i}}{\partial t} + \frac{\partial \overline{\rho u_i u_j}}{\partial x_j} + \frac{\partial \overline{p}}{\partial x_i} \frac{\partial \overline{\tau_{ij}}}{\partial x_i} = \frac{\partial}{\partial x_i} (\overline{\tau_{ij}} - \overline{\rho (u_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j)}) \]  

(2.13)
Background on premixed combustion related to IC engines

\[
\frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{Y}_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ V_{k, i} \tilde{Y}_k - \rho \left( u_i \tilde{Y}_k - \tilde{u}_i \tilde{Y}_k \right) \right] + \tilde{\omega}_k
\]  

(2.14)

\[
\frac{\partial \tilde{h}}{\partial t} + \frac{\partial \tilde{u}_i \tilde{h}}{\partial x_i} = \frac{D\rho}{D\tilde{t}} + \frac{\partial}{\partial x_i} \left[ \frac{\lambda}{\partial x_i} - \rho (u_i \tilde{h} - \tilde{u}_i \tilde{h}) \right] + \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N} V_{k, i} Y_k h_k \right)
\]  

(2.15)

where

\[
\frac{D\rho}{D\tilde{t}} = \frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho}{\partial x_i}
\]  

(2.16)

The equations presented above are in order the mass, momentum, chemical species and total enthalpy of the mixture. These are essentially the equations used to solve the reacting flow-field. The species mass fraction equations are typically replaced using a transport equation for a reaction progress variable, \( c \) to describe the thermo-chemical state of the mixture in premixed combustion. This equation will be discussed later. In the above equations, the following unclosed quantities must be modelled:

- Unresolved Reynolds stresses \( \overline{\rho(\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j)} \), requiring a subgrid scale turbulence model.
- Unresolved species fluxes \( \overline{\rho(u_i \tilde{Y}_k - \tilde{u}_i \tilde{Y}_k)} \) and enthalpy fluxes \( \overline{\rho(u_i \tilde{h} - \tilde{u}_i \tilde{h})} \).
- Filtered laminar diffusion fluxes for species and enthalpy. These molecular fluxes may be modelled through a simple gradient assumption.
- Filtered chemical reaction rate \( \overline{\dot{\omega}_k} \).
- The pressure velocity term \( \overline{u_i \frac{\partial p}{\partial x_i}} \) is usually approximated by \( \tilde{u}_i (\partial \overline{p}/\partial x_i) \).

**Modelling unresolved fluxes**

Modelling approach for the above unclosed terms in LES equations may follow similar concepts developed for RANS approaches, such as using the subgrid scale turbulent kinetic energy model.
2.2 Numerical paradigms

energy and its dissipation rate. However, in large eddy simulations, an additional information is available as large scale turbulent motions are numerically resolved. Closure models may be based on similar assumptions, using the known largest structures to estimate the effects of the smaller ones. The Smagorinsky sub-grid model is widely used because of its simple formulation. In this model, unresolved momentum fluxes or subgrid stresses are expressed using the Boussinesq approximation [180]:

\[
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} = -\nu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = -2\nu_t \bar{S}_{ij},
\]  

(2.17)

where \(\nu_t\) is a subgrid scale eddy viscosity, modelled writing

\[
\nu_t = (C_S \Delta)^2 |\mathbf{\bar{S}}| = (C_S \Delta)^2 \sqrt{(2\bar{S}_{ij}\bar{S}_{ij})},
\]

(2.18)

In the case of homogeneous isotropic turbulence, the model constant \(C_S\) is estimated to be \(C_S \approx 0.2\) and the value of \(C_S\) depends on flow configurations. This model is known to be too dissipative, especially close to walls and so it is improved using the Germano dynamic model [59], through an automatic determination of the model constant \(C_S(x,t)\) depending on time and space. This model has shown good efficiency in a wide range of applications [59] and was extended to compressible turbulence, however the computational cost, because of the dynamic evaluation of \(C_s\) is significant compared to the classical Smagorinsky model. Other sub-grid scale models also have been developed in the past and are reviewed in [180] and [190]. Similar to RANS, the unresolved scalar fluxes are also described using a gradient transport assumption:

\[
\bar{u}_i \bar{\phi} - \bar{u}_i \bar{\phi} = -\nu_t \frac{\partial \bar{\phi}}{\partial x_i},
\]

(2.19)

where \(Sc \approx 0.4\) is the sub-grid scale Schmidt number for scalar \(\phi\) and the turbulent viscosity is calculated by Eq. (2.18) [147]. Validation of LES against experiments are to be performed using statistics and not using snapshots. This is because LES does not resolve instantenious quantities but filtered values of the quantities. However, a qualitative rough comparison can be made using snapshots from LES and experiments. LES has the ability of describing the large scale turbulent flow features with acceptable computational cost and thus it has been widely used for non-reacting flows [51, 145]. However, it is still under development for
turbulent reacting flows. The main challenge for combusting flows come from modelling of combustion and its interaction with turbulence which are subgrid scale processes. This modelling is discussed in section 2.4.

2.2.3 Reynolds-averaged Navier-Stokes equations

Reynolds Averaged Navier Stokes (or RANS) computations have historically been the first possible approach to turbulence modelling. RANS techniques were developed to solve the mean values of all quantities and variation of some quantities of interest (turbulent kinetic energy, for example). The balance equations for Reynold or Favre averaged quantities are obtained by averaging the instantaneous equations described in section 2.1. The averaged equations require closure models. A turbulence model to deal with the flow dynamics in combination with a turbulent combustion model to describe chemical species conversion and heat release. Solving these equations provide averaged quantities corresponding to averages over time for stationary flows or averages over different realizations (or cycles) for periodic flows like those found in piston engines. RANS simulations are computationally the least expensive out of the three paradigms, but it only provides averaged quantities. Quantity $f$, is decomposed into its mean and fluctuating values written as \[ f = \bar{f} + f'. \] By substituting the decomposition into the instantaneous transport equations, the RANS equations can be derived. This Reynolds, averaging introduces many other unclosed correlations between $f$ and density fluctuations $\rho f'$ in flows with density variations as in combusting flows. To avoid this difficulty, mass weighted average called Favre averages are usually preferred, which is defined as \[ \bar{f} = \rho \bar{f} / \bar{\rho}. \] Therefore, when there is no body force acting on the fluid, the RANS equations from Eqs. (2.1)- (2.4) and (2.5) can be written as \[ 149]:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho \bar{u}_i}{\partial x_i} = 0, \]  

\[ \frac{\partial \bar{\rho} \bar{u}_j}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{u}_j}{\partial x_i} = - \frac{\partial \bar{\rho}}{\partial x_j} + \frac{\partial}{\partial x_i} \left( \bar{\tau}_{ij} - \bar{\rho} u'_i u'_j \right) \]  

\[ \frac{\partial \bar{\rho} \bar{Y}_k}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{Y}_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial \bar{Y}_k}{\partial x_i} - \bar{\rho} u'_i \bar{Y}_k \right) + \bar{\omega}_k \]
\[ \frac{\partial \tilde{h}}{\partial t} + \frac{\partial \tilde{h} u_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\mu}{\sigma} \frac{\partial \tilde{h}}{\partial x_i} - \rho u''_i h'' \right) + \frac{\partial u_i}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N} V_{k,i} Y_k h_k \right) \] (2.23)

where \( \mu \) is the dynamic viscosity, \( \sigma \) is the mixture Prandtl number, and \( D \) is the molecular diffusion coefficient.

The last term in the RHS of Eq. (2.21) is known as the Reynolds stresses, which leads to the closure problem. The objective of turbulence modelling is to provide closures for the unknown quantities found in the above equations [195]. The Reynolds stresses may be closed using turbulence models. Most turbulent models are based on an equation for turbulent kinetic energy, defined as \( k = \frac{1}{2} (u'_i u'_i) \), where \( u'_i \) is the fluctuation of velocity \( u_i \). Following the Boussinesq approximation [157], the Reynolds stress is modelled as:

\[ \rho g u''_i u''_j = -\mu_t \sigma_t \frac{\partial \tilde{h}}{\partial x_i} - 2 \frac{\partial}{\partial x_i} \left( \frac{\rho}{3} \delta_{ij} \tilde{k} \right), \] (2.24)

There are also some other approaches to close the Reynolds stresses. For instance, [112] developed a method to avoid the Boussinesq approximation but to solve additional modelled transport equations for each individual component of Reynolds stresses. The turbulent scalar fluxes \( u''_i \phi'' \) are generally closed using a classical gradient approximation:

\[ \tilde{u}''_i \phi'' = -\mu_t \frac{\partial \tilde{\phi}}{\sigma_t \partial x_i}, \] (2.25)

where \( \mu_t \) is turbulent eddy viscosity and \( \sigma_t \approx 0.7 \) is the turbulent Schmidt number [180]. In most turbulence modelling practices, a two-equations \( k - \varepsilon \) model developed by Jones and Launder [111] has been widely used as it is simple, cost effective and has proven to give acceptable prediction for a wide range of turbulent flows. The symbol \( \varepsilon \) is the dissipation of \( k \). Additionally, it provides turbulent time scale estimate for both integral \( k/\varepsilon \) and Kolmogorov \( \sqrt{\varepsilon/\nu} \) scales which are useful for turbulent combustion modelling.

In this approach, the turbulent viscosity, \( \mu_t \), that appears in Eq. (2.24) and (2.25) is estimated as:

\[ \mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon}, \] (2.26)
where the coefficient $C_\mu = 0.09$ is commonly used. The turbulent kinetic energy $\tilde{k}$ and its dissipation rate $\tilde{\varepsilon}$ are described using their balance equations:

\[
\begin{align*}
\frac{\partial \rho \tilde{k}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{k}}{\partial x_i} &= \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{Sc_k} \right) \frac{\partial \tilde{k}}{\partial x_j} \right] + P_k - \bar{p} \tilde{\varepsilon} \quad (2.27) \\
\frac{\partial \rho \tilde{\varepsilon}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{\varepsilon}}{\partial x_i} &= \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{Sc_\varepsilon} \right) \frac{\partial \tilde{\varepsilon}}{\partial x_j} \right] - C_{\varepsilon_1} P_k - C_{\varepsilon_2} \bar{p} \tilde{\varepsilon}^2 \quad (2.28)
\end{align*}
\]

\[
P_k = -\rho u''_i u''_j \frac{\partial u_i}{\partial x_j} - u''_i \frac{\partial \bar{p}}{\partial x_i} + \rho' \frac{\partial u''_i}{\partial x_i} \quad (2.29)
\]

where the Reynolds stresses $\rho u''_i u''_j$ are determined using Boussinesq approximation in Eq. (2.24) and the model constants are typically: $Sc_k = 1.0$, $Sc_\varepsilon = 1.3$, $C_{\varepsilon_1} = 1.44$ and $C_{\varepsilon_2} = 1.92$. These constants may require some calibration when modelling different turbulent flow configurations [63, 151].

In computations of turbulent flames, the problem can become tractable by describing the thermochemistry via few representative scalars instead of solving for all the reactive species. A reaction progress variable, $\alpha$, is the most appropriate scalar for this purpose in premixed combustion. The progress variable can be defined using temperature or scalar mass fraction, or a combination of scalar mass fractions. For example, if one uses the mass fraction of water vapour, $Y_{H_2O}$ then $\alpha = Y_{H_2O}/Y_{H_2O}^b$, where the superscript $b$ denotes burnt mixture value, and it is a monotonic function taking a value of 0 in the fresh reactants and 1 in the fully burnt products. Alternative definitions of progress variable have also been proposed in [10]. The transport equation for the Favre averaged progress variable, $\tilde{\alpha}$, is:

\[
\begin{align*}
\frac{\partial \rho \tilde{c}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{c}}{\partial x_i} &= \frac{\partial}{\partial x_i} \left( \rho D_c \frac{\partial \tilde{c}}{\partial x_i} - \rho u''_i \tilde{c}''_i \right) + \tilde{\omega}_c \quad (2.30)
\end{align*}
\]

The above equation is the same for LES also by interpreting the various terms accordingly. The use of RANS and/or LES require combustion modelling to provide a closure model for the mean chemical source term that appear in the averaged or filtered equations. These source terms are not usually described using averaging techniques because of the strong non-linearity
2.3 Laminar premixed flames

Study of laminar premixed flames is a pre-requisite and the first step for the study of turbulent premixed flames. Elaborate discussion on the laminar flames can be found in [143, 149, 172] and [197]. Two important characteristics, which are required for turbulent flame conditions, are discussed briefly below.

2.3.1 Flame thickness

Defining the flame thickness $\delta$ is a necessary requirement for numerical calculation of combustion problems, since it can be used as a reference length scale for the flame, and gives an estimation for the computational domain and the required numerical mesh size resolution [149]. From the scaling laws, the thickness of the laminar premixed flame can be obtained as [66], also known as Zel’dovich thickness;
Background on premixed combustion related to IC engines

\[ \delta = \frac{\lambda}{\rho C_p S_L} \]  

where all the values are estimated according to the unburnt gas mixture, \( S_L \) is the unstretched laminar flame speed, which is used as a reference speed for premixed combustion studies [180]. When the Prandlt number, \( Pr = \nu/\alpha \) and the Schmidt number, \( Sc = \nu/D \), are equal to unity and the reactive scalars have the same diffusion coefficient, \( D \), the flame thickness can be written as \( \delta = D_{th}/S_L \). The flame thickness based on temperature variation, called thermal thickness, can be written as [172]:

\[ \delta_L = \frac{T_b - T_u}{\text{Max} \left( \frac{\partial T}{\partial x} \right)} \]  

when \( T_b \) is the burnt mixture temperature and \( T_u \) is the reactant temperature. The definition in Eq. (2.31) is known to be too approximate to be used for mesh determination as it underestimates the flame thickness. While the definition in Eq. (2.32) gives an overestimation of the flame thickness, and it requires the knowledge of the solution and the temperature profile. However \( \delta_L \) is the most commonly used thickness for premixed flame analysis and this thickness is used in this study.

2.3.2 Flame speed \( S_L \)

The flame speed is the velocity at which the flame propagates into the reactants relative to the flow in the direction normal to the flame itself. It controls the consumption rate and the heat release. If the flame is unstretched, the laminar flame speed [26] is a thermochemical property of the mixture [172]. A simple schematic in Fig. 2.1 shows \( S_L \) and \( \delta_L \) diagrammatically.

2.4 Turbulent premixed flames

2.4.1 Combustion regimes

Turbulence is characterised as fluctuations of all local properties and occurs for sufficiently large Reynolds numbers. One of the milestones of turbulent flows is the idea of the energy cascade. It was firstly introduced by Richardson [158], and assumes that energy is transferred from large to small scales, where it is eventually dissipated because of fluid viscosity. The
The dissipation rate per unit mass, $\bar{\varepsilon}$, and the kinematic viscosity, $\nu$, the small-scale turbulence is defined using micro scale defined for the length scale and $\eta_k = (v^3/\bar{\varepsilon})^{1/4}$ for the time scale [155]. Damköhler described how the large-scale turbulence acts to wrinkle the flame without changing its internal structure, whereas the small-scale eddies affect the transport processes within the flame. Diagrams defining regimes of premixed turbulent combustion in terms of velocity and length scale ratios have been proposed in past studies [12, 140]. This regime diagram involves Damköhler, Karlovitz and Reynolds numbers. These non-dimensional numbers are defined as:

$$ Da = \frac{\Delta S_L}{\delta u'} \quad Ka = \frac{\tau_c}{\tau_{eta}} = \left( \frac{\delta}{\eta_k} \right)^2 \quad Re_t = \frac{u' \Lambda}{S_L \delta} $$

The Damköhler number (2.34) corresponds to the ratio of the integral time scale $\tau_i = \Lambda/u'$, to the chemical timescale, $\tau_c = \delta/S_L$. The Karlovitz number $Ka$ is the ratio of the chemical time scale to the Kolmogorov time $\tau_{eta}$. The turbulent Reynolds number, $Re_t$, given above may also be expressed as, $Re_t = u' \Lambda/\left( \delta S_L \right)$. The definitions given above yields $Re_t = Ka^2 Da^2$. 

Fig. 2.1 Schematic of a laminar flame
Using $Re_t$, $Da$ and $Ka$ numbers, various combustion regimes may be identified in terms of velocity ratio, $u'/S_{L}$, and length scale ratio, $\Lambda/S_{L}$. The regime diagram introduced by Peters [140], which is shown in Figure 2.2, includes four different regimes of premixed combustion.

- **Flamelet** ($Ka < 1$ and $Da > 1$): Chemical times are shorter than the integral turbulence time scale and the flame thickness is smaller than any turbulence scale. For $u' < S_{L}$, turbulence is unable to affect the inner flame structure which remains close to a laminar flame. The corrugated flame regime, in which $u' > S_{L}$ and turbulence enters the preheat zone, forming pockets of fresh and burnt gasses.

- **The thin reaction zone regime** ($\tau_k < \tau_s < \tau_t, Ka > 1, Da > 1$): The turbulent integral time scale is still larger than the chemical time scale but the Kolmogorov scales are smaller than the thermal thickness.

- **Well-stirred reactor regime** ($Da < 1$). The chemical time is larger than turbulent times. The overall reaction rate is controlled by chemistry as the reactants and products are mixed by turbulence. Turbulence enters and modifies the preheated zone but not the reaction zone. as a result the reaction zone keeps a quasi-laminar structure.

- **Broken reaction zone regime** ($Ka > K_{a8}$). Both preheat and reaction zone are affected. The effect of the strain can cause local extinction. There is no laminar structure.

### 2.5 Modelling of turbulent premixed combustion

The main objective of turbulence combustion modelling is to provide closure for the mean reaction rate, $\bar{\omega}$, appearing in Eq. (2.30). Various approaches have been developed in the past and these models are briefly reviewed in the discussion below. Specific details regarding aspects relevant to IC engine simulations are provided in section 2.6.

#### 2.5.1 The Eddy Break-up (EBU) model

This model proposed by Spalding [172] is based on phenomenological analysis assuming high Reynolds ($Re_t >> 1$) and Damköhler ($Da >> 1$) numbers. Spalding [173] proposed that the rate of consumption of the reactant depends more on the rate of breakup of lumps of unburned fuel/air mixture. The rate of breakup of these lumps is controlled by turbulence and the reaction rate is:
Fig. 2.2 Turbulent premixed combustion regime diagram [143].
\[ \bar{\omega}_c = -C_{EBU} \bar{p} \frac{E}{k} \sqrt{c^{\prime \prime}^2} \]  

(2.35)

where \( C_{EBU} \) is the model parameter. For combustion with thin flame and very fast reaction, (large values of \( Re_t \) and \( Da \)) the variance \( \tilde{c}^{\prime \prime} = \tilde{c}(1 - \tilde{c}) \). Although the Eddy Break-Up model offers the simplest expression of the reaction rate, it excludes the effects of chemical kinetics. A variant of this approach, called the eddy dissipation concept, is developed to include complex chemical kinetics [49, 67]. This model was first developed for RANS, and has been extended to LES. The subgrid scale version can be written as [190]:

\[ \bar{\omega}_c = -C_{EBU} \bar{p} \frac{1}{\tau_{SGS}} \tilde{c}(1 - \tilde{c}) \]  

(2.36)

where \( \tau_{SGS} \) is a subgrid turbulent time scale, estimated as:

\[ \tau_{SGS} \approx \frac{l_\Delta}{u'_{SGS}} \approx \frac{\Delta}{\sqrt{k_{SGS}}} \]  

(2.37)

Where \( l_\Delta \) is a subgrid length scale, taken to be the filter size \( \Delta \) and \( u'_{SGS} \) a subgrid turbulent velocity.

### 2.5.2 Bray-Moss-Libby (BML) modelling

This flamelet model is based on a reaction progress variable and its statistics for thermo-chemical closure [20, 22, 89], is discussed elaborately in many books, for example [137]. The main assumption for this approach is that the turbulent flame is thin and the turbulent scales do not disturb the flame structure. The probability density function (pdf) of the progress variable, \( c \) at a given location \( x \) is expressed as sum of contribution from fresh, fully burnt and burning gases. This pdf is written as:

\[ p(c, x) = \alpha(x) \delta(c) + \beta(x) \delta(1 - c) + \gamma(x) f(c, x) \]  

(2.38)

where \( \alpha, \beta \) and \( \gamma \) respectively denote the probability to have, at location \( x \), fresh gases, burnt gases and reacting mixture. \( \delta(c) \) and \( \delta(1 - c) \) are respectively the Dirac delta functions
corresponding to fresh gases \((c = 0)\) and fully burnt mixture \((c = 1)\). Since the flame front is taken to be thin, the probability to be in the burning gases is low, \(\gamma << 1\). Hence, the pdf becomes:

\[
p(c; x) = \alpha(x)\delta(c) + \beta(x)\delta(1 - c)
\] (2.39)

The coefficients \(\alpha\) and \(\beta\) can be determined as a function of Favre-averaged progress variable, \(\tilde{c}\), using [20, 22, 89]:

\[
\alpha = \frac{1 - \bar{c}}{1 + \tau \bar{c}}; \quad \beta = \frac{(1 + \tau)\bar{c}}{1 + \tau \bar{c}}.
\] (2.40)

where \(\tau = (T_b - T_u/T_u)\) is the heat release parameter. Thus, the thermochemical state of the mixture is determined by \(\tilde{c}\) which can be obtained from its transport equation, Eq. (2.30). The turbulent scalar flux term, \(u''c''\) appearing in Eq. 2.30 can be expressed as:

\[
\bar{\rho}u''c'' = \bar{\rho}\bar{c}(1 - \bar{c})(\bar{u}_b - \bar{u}_u),
\] (2.41)

where \(\bar{u}_u\) and \(\bar{u}_b\) are the conditional mean velocities in fresh and burnt gases respectively. As the burnt gases have lower density, velocity increases towards the burnt gas \((\bar{u}_b > \bar{u}_u)\). Therefore, \(u''c''\) is positive implying counter gradient flux, however the conditional mean velocity needs to be modelled. The BML model is able to predict the counter gradient diffusion phenomena, which has been observed both experimentally [118] and numerically [189].

The above analysis does not provide the mean reaction rate \(\bar{\omega}_c\), and alternative modelling approaches are required to close this term. For the closure of \(\bar{\omega}_c\), since it is zero everywhere outside the reaction zones, its mean value can be determined by [137]:

\[
\bar{\omega}_c = \gamma(x, t) \int_{\hat{c}}^{1 - \hat{c}} \alpha_c f(c) \, dc
\] (2.42)

where \(\hat{c}\) denotes a small value away from \(c = 0\). However, as \(\gamma << 1\), has been neglected, alternative methods are needed to estimate this term. One method is to treat \(c\) as a telegraphic signal [21, 90], and an alternative method is to presume that the turbulent flame front structure is represented by an unstrained laminar planar flame [19]. The later approach gives:
\begin{equation}
\dot{\omega}_c = \frac{\rho_u s_L^0 \varepsilon \tilde{c}(1 - \tilde{c})}{\delta_L^* (1 + \tau \tilde{c})} \quad (2.43)
\end{equation}

where $\delta_L^* = \int c(1 - c)/(1 + \tau c) \, dn$ is the laminar flame thickness, and $n$ is the distance along the flame normal. The parameter $\varepsilon = 1 - \tilde{c}\partial \tilde{c}^2/\partial (1 - \tilde{c})$ is related to $\gamma$ [19]. Hence, the above reaction rate closure can be used if one solves the transport equation for $\tilde{c}$, given in Eq. (2.30). In the limit of $\gamma \rightarrow 0$, it was shown [18] that the reaction rate closure becomes:

\begin{equation}
\dot{\omega} = \frac{2}{2C_m - 1} \bar{\rho} \bar{\varepsilon}, \quad (2.44)
\end{equation}

with $C_m \approx 0.7$ and $\bar{\rho} \bar{\varepsilon} = \bar{\rho} D (\nabla \tilde{c}'' \nabla \tilde{c}'')$ is the scalar dissipation rate. This closure shows a direct link between the reaction rate, and scalar dissipation rate $\bar{\varepsilon}$. Physically correct modelling of $\bar{\varepsilon}$ will allow one to determine the reaction rate. The closure for the mean scalar dissipation rate is challenging for premixed flames [100]. Using the classical models developed for passive scalar in non-reacting turbulence which gives $\bar{\rho} \bar{\varepsilon} = \bar{\rho} \partial \varepsilon^2 / \varepsilon \approx \bar{\rho} \bar{c}(1 - \tilde{c})\tilde{k} / \varepsilon$ in Eq. (2.44) and recovers the EBU mode Eq. (2.36).

### 2.5.3 Flame surface density model

In this widely used flamelet model [128], the mean reaction rate is described in term of the product of reaction rate per unit flame surface area, $\rho_u s_L$, and the flame surface area per unit volume, $\Sigma$, known as the flame surface density. In this method, the mean reaction rate is written as

\begin{equation}
\bar{\omega}_c = \rho_u \langle S_c \rangle \Sigma, \quad (2.45)
\end{equation}

where $\langle \rangle_s$ denotes averaging over the flame surface, and $S_c$ is the consumption speed. This method has the advantage of separating complex chemistry, incorporated into the consumption calculation, speed $\langle S_c \rangle_s$, from the turbulence-chemistry interaction through the FSD, $\Sigma$. There are two methods to provide a model for the flame surface density. One is using an algebraic model [23, 90], or solving a balance equation [24, 153]. A simple algebraic model is given as [23]:
2.5 Modelling of turbulent premixed combustion

\[ \Sigma \delta_L^0 = \frac{2C_D}{(2C_m - 1)} \bar{\rho} \left( 1 + \frac{2}{3} C_{e/s} \frac{1}{\sqrt{k}} \right) \left( 1 + \frac{C_D \bar{\varepsilon}}{C_{D_s} k s_0} \right) c' \]  

(2.46)

where the model parameters are of order unity. The unclosed transport equation for \( \Sigma \) is written as [24, 153]:

\[
\frac{\partial \Sigma}{\partial t} + \frac{\partial \bar{u}_i \Sigma}{\partial x_i} = -\frac{\partial \langle u'' \rangle_s \Sigma}{\partial x_i} + \langle a_T \rangle_s \Sigma + \langle a''_T \rangle_s \Sigma - \frac{\partial \langle s_d N_i \rangle_s \Sigma}{\partial x_i} + \langle s_d \frac{\partial N_i}{\partial x_i} \rangle_s \Sigma
\]  

(2.47)

where \( a_T \) is the flame strain rate and \( s_d \) is the relative flame propagation speed to the reactants with \( N_i \) being the normal vector to the flame surface towards the unburnt gases. The balance equation for the flame surface density is not closed and various terms require modelling. Such modelling has been studied widely and can be found in [190]. Developing such models has been the subject of many studies [30, 143, 144]. The FSD method has also been developed for LES of turbulent premixed flames and these works are summarised in [103] and [25]. The SGS flame stretch can become negative and new models for this are yet to be developed. The modelled FSD transport equation is available in commercial CFD packages and care must be taken in using them correctly and selecting model parameters as this approach involves many assumptions and approximations which may be valid under some conditions.

2.5.4 G-equation approach

The G-equation model, also called as level-set approach, is based on a non-reacting scalar \( G \) rather than a progress variable, \( c \). The flame thickness is zero and the flame front is described as a propagating surface tracked using a field variable \( \widetilde{G} \). The original form of the G-equation model was introduced by Williams [198]. Peters [142, 143] developed this method for the corrugated flamelets and thin reaction zones regimes for turbulent premixed flames. The flame is considered as an interface between burnt gas and unburnt mixture, and this surface is defined as an iso-surface of \( G(x, t) = G_0 \). The \( G \) equation is written as:

\[
\frac{\partial G}{\partial t} + u_j \frac{\partial G}{\partial x_j} = s_G \left( \frac{\partial G}{\partial x_i} \frac{\partial G}{\partial x_j} \right)^{1/2}
\]  

(2.48)

where \( s_G \) is the propagation speed of the flame relative to the unburnt mixture. This propagation speed may be expressed in terms of \( S_L \) corrected for stretch effects using Markstein num-
ber, which is a measure of the sensitivity of the laminar flame speed to the flame stretch [53]. Transport equations of $\tilde{G}$ and $\tilde{G}^{'2}$ have been developed for RANS approach [141, 142], using the above equation. This method for LES has been reviewed in [146]. However, it has been noted by Williams [199] that this approach is strictly valid for wrinkled flamelets and fuel lean combustion is less likely to be in this regime. Furthermore, $G$ equation is inherently unstable and some special numerical treatment is needed during the simulation to stabilise the calculation.

2.5.5 Artificially thickened flames

This model proposed by Colin et al. [37] approaches the problem by artificially thickening the flame front. The real flame thickness is scaled by the Arrhenius Pre-exponential constant, $A$, as $\delta \sim (\lambda/A)^{1/2}$. If, $A$, is scaled by a factor $F$, $\delta$, is increased. In order to keep the value of, $S_L$, the unchanged thermal diffusivity, $\lambda$, is also multiplied by, $F$, as it, scales as $\lambda = S_L \delta$. Hence the reaction layer thickness can be thickened and resolved on a computational mesh for LES. Since by increasing the thickness, the interaction between turbulence and chemistry is modified, the Damköhler number, $Da$, is decreased of a factor $F$. This model is mainly developed and categorized under LES simulation. [149, 190].

2.5.6 Conditional moment closure (CMC)

In comparison to non-premixed combustion, the conditional moment closure (CMC) for premixed and partially premixed combustion has not been advanced until recently [94]. Klimenko [93] and Bilger [9], independently derived a model for non-premixed turbulent combustion, where the averages of the reactive scalars are conditioned on the mixture fraction. This model is based on the hypothesis that in turbulent flames the fluctuations of all thermochemical quantities are correlated with the fluctuations of just one scalar. Klimenko and Bilger [94] later proposed an extension of this conditional moment closure (CMC) method to premixed combustion, where conditioning is with the progress variable, $c$. The main hurdle for premixed CMC is related to the closure for the conditional scalar dissipation rate of $c$. Some advances are made recently on this front and the CMC results for premixed flames are similar to those obtained using presumed PDF approach [6, 7], applied the CMC method to premixed combustion of a pilot stabilised Bunsen flame. For premixed flames, the transport equation for the conditional mean of species is written as [94]:

\[
\]

\[
\]
\[ (\rho|\varsigma) \frac{\partial Q_\alpha}{\partial t} + (\rho u_i|\varsigma) \frac{\partial Q_\alpha}{\partial x_i} = (\rho|\varsigma)(N_c|\varsigma) \frac{\partial^2 Q_\alpha}{\partial \varsigma^2} - (\omega|\varsigma) \frac{\partial Q_\alpha}{\partial \varsigma} + e_{Q_\alpha} + e_{y_\alpha} \]

(2.49)

where the reaction rates term, \( \omega_\alpha \) and \( \omega \), are given by Eqs. (2.4) and (2.30) respectively and the instantaneous scalar dissipation rate of species \( c \) is defined as \( N_c = D(\nabla c \cdot \nabla c) \). The symbols \( e_{Q_\alpha} \) is defined as [176].

\[ e_{Q_\alpha} \equiv \frac{\partial}{\partial x_i} \left( \frac{\partial Q_\alpha}{\partial x_i} \right) + \left[ 1 - Le_\alpha \right] D_\alpha \frac{\partial c}{\partial x_i} + \rho D_\alpha \frac{\partial c}{\partial x_i} \frac{\partial}{\partial x_i} \left( \frac{\partial Q_\alpha}{\partial \varsigma} \right) |\varsigma| \]

(2.50)

and represents the contribution of the molecular diffusion which is negligible when \( \text{Re} \) is large. The Lewis number for species \( \alpha \) is \( Le_\alpha \). The last term in equation 2.49 is:

\[ e_{y_\alpha} \equiv \left( \rho \frac{\partial y_\alpha}{\partial t} + \rho u_i \frac{\partial y_\alpha}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \rho D_\alpha \frac{\partial y_\alpha}{\partial x_i} \right) \right) |\varsigma| \]

(2.51)

The various terms in Eq.2.49, \( (\rho u_i|\varsigma) \), \( (N_c|\varsigma) \) and \( (\omega_\alpha|\varsigma) \) need to be modelled and various closure models have been discussed by[94] and [177]. The closure of the conditional mean scalar dissipation rate, \( (N_c|\varsigma) \), is linked to the unconditional mean scalar dissipation rate, \( \bar{\varepsilon}_c \) [6, 7]. Modelling of this mean scalar dissipation rate is discussed in section 2.5.8. CMC is more expensive than the flamelet methods described earlier, the number of transport equations that need to be solved for the thermochemistry is equal to \( (N+1) \) times the number of points in the conditioning variable space. However, in comparison with closure models, which are based on physical or phenomenological arguments, the mathematical framework of CMC is likely to provide better predictions of pollutants and their formation rates. In addition, CMC may be valid for all regimes of premixed combustion since no explicit approximations are made on the influence of turbulent eddies on the flame structure [7]. For partially premixed combustion, double conditioning is required, and this method is currently being studied [170].

### 2.5.7 Transported pdf approach

In this model, turbulent reacting flows are calculated using statistical methods based on the stochastic nature of turbulence. A complete statistical description of a turbulent reacting flow can be obtained by defining the joint pdf for the velocity components and the thermochemical
variables [152]. A transport equation for the joint PDF of scalar concentrations is solved along with equations for turbulence quantities [79, 152]. If the pdfs of the thermochemical variable are known, the mean reaction rate can be obtained from:

$$\dot{\bar{\omega}} = \int_{\psi} \dot{\bar{\omega}} P(\psi; x, t) d\psi$$

(2.52)

where $\psi = (Y_1, Y_2, ..., Y_N, T)$ is the scalar field vector that represents the species mass fractions of $N$ species in addition to temperature. This statistical description of the stochastic flow field is applicable to premixed, non-premixed and partially premixed combustion [11]. An evolution equation for the mass–weighted joint pdf $\tilde{P}(\psi)$, is [138, 152]:

$$\frac{\partial \bar{\rho} \tilde{P}(\psi)}{\partial t} + \frac{\partial}{\partial x_i} [\bar{\rho} \tilde{u}_i \tilde{P}(\psi)] + \sum_{\alpha=1}^{N} \frac{\partial}{\partial \psi_{\alpha}} \left[ \frac{1}{\rho} \tilde{\omega}_{\alpha}(\psi) \bar{\rho} \tilde{P}(\psi) \right] =$$

$$-\frac{\partial}{\partial x_i} \left[ \langle u''_i \psi \rangle \bar{\rho} \tilde{P}(\psi) \right] + \sum_{\alpha=1}^{N} \left( \frac{1}{\rho} \frac{\partial J_{i,\alpha}}{\partial x_i} \psi \right) \bar{\rho} \tilde{P}(\psi)$$

(2.53)

where $J_{i,\alpha} = V_{i,\alpha} Y_{\alpha}$ represents the molecular diffusion flux. The three terms on the LHS, are closed. The first term on the RHS is the turbulent flux term which is usually modelled using the gradient transport hypothesis. The second term on the RHS denotes the micro mixing and and poses the main modelling challenge for this approach [154]. However, the need to model this term, as well as the unclosed terms in the momentum equation, can be avoided if the evolution of the joint velocity–composition pdf is solved. The joint PDF equation is of $(N + 4)$ dimensions for unsteady reacting flows in three spatial dimensions involving $(N - 1)$ reactive scalars and temperature, and the molecular flux term will have a negative sign which requires the use of standard numerical approaches such as the finite difference or the finite volume methods, and the Monte-Carlo method [152] is generally used to solve the PDF transport equation. This high dimensionality poses difficulties for numerical solution [154]. This method is shown to give good solution for non-premixed combustion compared to flamelet based methods. However, for premixed flames the accuracy of this method is comparable to the flamelet based presumed pdf method and some examples of this are discussed in [120].
2.5.8 Presumed pdf approach

In this approach, shape of the pdf in (2.52) is presumed using moments, which are obtained from their balance equations [13]. It is important to note that this approach is only applicable to cases where the scalar fluctuations are small, hence, its applicability is limited to premixed combustion or non-premixed flames with fast chemical reactions [13]. The BML model and the $G$–equation approach described earlier in section 2.5.2 and 2.5.4 respectively, are examples of this where the progress variable and the scalar $G$, determine the thermochemical state. The number of scalar moments required for the tabulation is determined by the presumed pdf shape. The BML pdf requires only the first moments, $\tilde{c}$, while the widely employed beta–pdf [17, 149], requires the first two moments: $\tilde{c}$, and $c''$, which are obtained from their respective transport equations. Depending on the number or the definition of the representative scalars employed, differences between various presumed pdf approaches arise.

In the laminar flamelet models, the relationship is constructed from canonical laminar flame calculations and the reaction rate can be obtained using:

$$\tilde{\omega} = \int \tilde{\omega} P(\zeta) \, d\zeta$$  \hspace{1cm} (2.54)

where the flamelet reaction rate $\tilde{\omega}$, is taken from freely propagating laminar flame calculations having the same thermochemical attributes as that of the turbulent flame. This is the basis of the laminar flamelet approaches proposed by [15, 62].

It is worthwhile to examine the balance equation for the scalar variance, $c''$ as it is required for the presumed pdf approach. This equation is written as [149]:

$$\begin{align*}
\frac{\partial \tilde{p} c''}{\partial t} + \frac{\partial \tilde{p} \tilde{u}_i c''}{\partial x_i} + \frac{\partial \tilde{p} \tilde{u}_i c''}{\partial x_j} & = \frac{\partial}{\partial x_j} \left( \rho D_c \frac{\partial c''}{\partial x_j} \right) \\
& - 2\rho u_i'' \frac{\partial c}{\partial x_j} + 2\tilde{\omega} c'' \quad \text{reaction} \\
& - 2\rho D_c \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_i} \quad \text{dissipation}
\end{align*}$$  \hspace{1cm} (2.55)

The three terms in the LHS are the unsteady, mean convection and the turbulent transport terms respectively. The first two terms in the RHS denote the influence of molecular transport, and are negligible for large Reynolds numbers. The last term in the RHS is unclosed. It is known as the mean scalar dissipation rate $\tilde{\epsilon}_c$. It is written as:
\[
\bar{\rho} \tilde{\varepsilon}_c = \rho D_c \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_i}
\]  
(2.56)

where \( D_c \) is the diffusivity of the progress variable. This quantity denotes the rate of mixing between hot and cold fluid on the flame surface required to sustain combustion. Also, scalar dissipation rate is the decay rate of scalar fluctuations by turbulent micro mixing. This quantity needs to be modelled for RANS as well as for LES. For large eddy simulation, the SGS dissipation rate is detailed as \( \bar{\rho} \tilde{\varepsilon} = \bar{\rho} N_c - \bar{\rho} D_c \), where \( N_c = D_c (\nabla c \cdot \nabla c) \) is the instantaneous dissipation rate.

Modelling of \( \tilde{\varepsilon}_c \) is challenging [126, 127], as it should take into account turbulent mixing, chemical reaction, molecular diffusion, and their interactions as these processes are strongly coupled with one another in premixed flames [178]. One such model was developed in [98] by balancing the leading order terms of a transport equation for \( \tilde{\varepsilon}_c \) derived in [178]. This model is written as:

\[
\tilde{\varepsilon}_c \approx \frac{1}{\beta_c} \left[ (2K_c^* - \tau C_4) \frac{s_L}{\delta L} + C_3 \frac{\tilde{\varepsilon}}{k} \right] c''^2
\]  
(2.57)

This model accounts for turbulent as well as chemical time scales, and retains the coupling between chemical and diffusive effects. The heat release parameter, \( \tau \), is defined as \( \tau = (T_b - T_u) / T_u \), with subscripts \( b \) and \( u \) respectively denote burnt and un-burnt mixtures. The various model parameters are: \( \beta_c = 6.7 \), \( K_c^* = 0.85 \tau \) (for hydrocarbon mixtures), \( C_3 = 1.5 \sqrt{K_a} / (1 + \sqrt{K_a}) \) and \( C_4 = 1.1 / (1 + Ka)^{0.4} \). The parameter, \( K_c^* \) is related to flamelet dilation, while \( C_3 \) and \( C_4 \) represent the interaction between turbulent strain and scalar gradient [98]. Values of \( K_c^* \) for hydrocarbon and hydrogen-air flames at different equivalence ratios have been calculated in [159]. The flamelet curvature effects are represented by \( \beta_c \). The Karlovitz number is defined as \( Ka \equiv \sqrt{(u'/\delta^3) \Lambda} \), where \( \delta = \delta_L / \left[ 2(1+\tau)^{0.7} \right] \), \( u' = \sqrt{2k/3} \) is the turbulent r.m.s velocity and \( \Lambda \) is the integral length scale. These parameters cannot be changed arbitrarily and they are specified to satisfy aspects of turbulence-flame interaction [98, 101].

For SGS dissipation rate required for LES, the same equation with same \( K_c^* \) is used. The parameters \( C_3 \) and \( C_4 \) are defined using the subgrid velocity scale, \( u'_\Delta \), and filter width \( \Delta \) but using the same functional form discussed above. The parameter \( \beta_c \) can take a value different from 6.7 [36, 107, 110]. The variance involved in Eq. (2.55) should be taken as SGS variance. Elaborate discussion on SGS dissipation closure is given in section 5.2.
The third term in the right hand side of Eq. (2.55) denotes the contributions from reaction rate and is unclosed. An unstrained flamelet model, where the reaction rate closure is given by Eq. (2.54) is used which is given as:

\[
\overline{\omega} = \int_0^1 \phi(\zeta) P(\zeta; \tilde{c}, \tilde{c}^{\eta/2}) \, d\zeta
\]

(2.58)

where \(\zeta\) and \(P(\zeta)\) are the sample space variable and the marginal pdf of \(c\). The pdf, in this equation is presumed to be a Beta-function, and is determined using both \(\tilde{c}\) and \(c^{\eta/2}\). The required \(\tilde{c}\) and \(c^{\eta/2}\) are obtained from their respective transport equations described in Eq. (2.30) and (2.55), respectively. For the SGS variance equation, the above closure can be used but pdf should be the subgrid pdf (see section 5.2).

The models in Eq. (2.57) and (2.58) ensure that influence of chemistry on the evolution of \(\tilde{c}\) and \(c^{\eta/2}\) are included in a consistent manner. More specifically, the dissipation rate model in Eq. (2.57) includes the complex effects of turbulence and chemical reactions in generating gradients of \(c\). Capturing these subtleties are important to keep the modelling framework robust and accurate. Since the consistancies among the physical processes are maintained in the presumed pdf approach described above, it is called as FlaRe (Flamelets revised for physical consistencies) approach. Elaborate detail on this is given in [33, 105, 108, 110].

### 2.6 Engine simulations

In this section, a brief overview of the past combustion sub-models commonly used for multi dimensional CFD simulations of IC engines is given. Unsteady RANS simulations are used extensively as it is less demanding in terms of resources. RANS simulations typically employing variants of the two-equation model [119], have provided very useful contributions towards understanding of ICE flows, however it has also showed difficulties in predicting the operating conditions [28]. Typical combustion closures used in the past studies for IC engine simulations are reviewed and discussed in [77]. The widely used eddy break-up model [173] discussed in section. 2.5.1, predicted unphysical reaction rate near the wall [1]. The necessity of adjusting the empirical model coefficients was noted [1]. When the BML model, discussed in section 2.5.2 was employed in research engine problem, flame acceleration close to the wall was not observed. Drake et al. [42], employed a modified version of BML model for stratified combustion in a spray-guided direct-injection spark-ignition (DISI) engine. The flame wrinkling model was introduce by [193], where a wrinkling factor was introduced in the transport equation of a regress variable (one minus the progress variable). Using a
spectral or a semi empirical model for the local wrinkling factor, this model is expected to capture the evolution of an initial laminar flame kernel into a fully turbulent flame. Weller et al. [193] simulated a research engine and the pressure histories obtained had a good match compared to the experiments. Heel et al [80], studied the same research engine with the same model, for various operating conditions, and observed good agreement. They ascribed the discrepancies in the results, for some operating conditions, to the short comings of the combustion model used. The wrinkling model was extended by [91] for a DISI engine, where they used the model for stratified combustion. The coherent flame model (CFM) was used to simulate SI engine in [204]. In this study, the surface production term in the model to be calibrated for each engine.

The CFM flame wrinkling model is related to the flame surface density model discussed in section 2.5.3. Elaborate discussion on these can be read in [149]. Baritaud et al. [14] extended the original form of the CFM model to study the homogenous and stratified combustion. Dulcos and Zolver [43] used the extended coherent flame model (ECFM) in DISI engine at both homogeneous and stratified conditions. They showed good agreement with the experimental pressure measurements, however the model coefficient has to be calibrated based on previous engine data. ECFM with the same model constants was used by [81] in a different DISI engine. This model has been adopted by [95] for hydrogen combustion. It was validated for both DISI engines and port fuel injection (PFI). Galloni et al. [54] used the ECFM for simulation of a downsized SI engine. Similar to the previous studies, the model constants were tuned depending on the engine configuration. G-equation approach was validated by [50] for a homogenous charge SI engine. Tan et al. [181] used this model to simulate combustion in SI engine with exhaust gas recirculation (EGR). Dekena et al. [40] used the G-equation model for a DISI engine and Liang et al. [116] validated it for both SI and stratified DISI engines.

The transported PDF method has also been used for IC engine simulation in the past. Taut et al. [184] used the PDF method for simulation of a two-stroke SI engine. In this study pressure history comparison was not shown, only qualitative agreement with experimental measurements for the flame speed was shown. As noted by Haworth [78], these calculations show the feasibility of the transported PDF method in simulating complex three-dimensional combustion processes. All the above studies considered URANS approach, which is adequate if one is interested in obtaining the statistics of heat release rate, in-cylinder pressure rise, temperature, and other quantities of interest. Additionally, since RANS simulations capture time or ensemble averages other phenomena such as misfire or knock, which limit performance and efficiency, cannot be captured. In order to overcome these short comings, recently Large Eddy Simulations (LES) are adapted for engine flows with intricate geometry. This
is becoming possible because of the increase in the computational power and this approach also allows one to study cycle-to-cycle variations. The validity of these computational results depends on the closures used to describe turbulence, combustion and their interactions. In order to construct the statistics, LES must be run for at least few tens of cycles to have meaningful comparison with experiments since the relationship between the resolved field and the underlying turbulent field is a statistical one [77]. According to Granet et al. [68] and Goryntsev et al. [64], up to 25 cycles are required for the mean flow and 50 cycles for the cyclic fluctuations in order to get meaningful statistical results. Consequently, LES calculation for IC engine for many cycles will incur high computational cost. A review paper by Celik et al. [28] addressed the opportunities of LES in analysing in-cylinder flows.

The feasibility of LES techniques for IC engine simulations was discussed and some crucial issues such as computational cost and the need for better subgrid models in order to improve the quality of predictions was identified. In another recent review by Rutland [162], various combustion submodels suitable for IC engine simulations were discussed, and the considerable potentials for the improved LES submodels which could allow the use of RANS like mesh was pointed out. One of the first LES simulation in IC engines was performed by Haworth [122], who used an in-house code to perform LES simulation of a piston-cylinder assembly experimentally studied in [135]. Results showed good agreement for two of the three experimentally investigated piston positions, but better agreement in terms of mean and RMS velocities compared to RANS simulations was observed. Enaux et al. [48] simulated cold-flow LES of a real ICE setup and compared the prediction with experimental PIV measurements. Good agreement for the mean flow field and cyclic variation was observed. Goryntsev et al. [65] investigated the cold flow and hollow-cone gasoline spray injection. Results showed that the cyclic fluctuations were mainly attributed to the intake flow attributes rather than the influence of the fuel injection.

One of the first attempts in simulating the combustion process in an IC-engine using LES is reported in [185]. They adapted a CFD code AUBP, developed for aeronautical. The code is known as AVBP. The premixed combustion was modelled using the thickened flame LES model (TFLES), where the reaction zone is artificially thickened by modifying turbulent transport coefficient, and also the chemical source term. The model was adapted in order to account for high pressures and temperatures in the IC engines. This has been taken into account by using a reduced chemical scheme in order to calculate the adiabatic flame temperature and laminar flame speed for a range of high pressures and temperatures seen during the combustion stroke. Only 4 cycles were simulated in this study, however cyclic variation of the pressure trace due to combustion was reported. Enaux et al. [47] employed the TFLES model in combination with a simple energy deposition model (ED) for ignition of the
premixed gas, in an SI engine. The cycle-to-cycle variation (CCV) was studied by computing 26 consecutive cycles. In both the experiment and the simulations, the peak in-cylinder pressure for the individual cycles, were found to be independent of their preceding cycle. Using the same modelling approach, Granet et al. [68] compared 25 and 50 cycles for stable and unstable operating points, respectively, to the experimental measurements.

The importance of the early flame propagation was emphasised, while CCV for both operating points showed good agreement with the experiments. [188] simulated a SI engine using ECFM for LES and the tumble motion generated during the intake and its breakdown influencing the turbulence intensity at ignition was identified as the root cause for the observed CCV simulated using the 10 cycles. Fontanesi et al. [52] simulated a DISI engine and, they compared an Eulerian arc and kernel tracking ignition model (ATKIM) on a normal and a locally refined meshes by tracking the kernel growth using the ECFM model. The ATKIM model over predicted the ignition and the no ignition model approach showed better agreement with the measured pressure traces. Pitsch [146] presented a filtered equation for the \( G \)-equation in the LES context. The G-Equation in the LES for IC engine have been reported by Schmitt et al [165]. In their study, the flow field evolution, mixture formation and combustion process in an engine with methane direct injection was reported. The average in-cylinder pressure traces as well as the cyclic variability were compared to experimental data and very good agreement was found. Koch et al. [97] conducted LES calculations of a port-injected 4-valve SI engine. In their work combustion is simulated using \( G \)-equation. Up to 40 consecutive simulation cycles have been performed in order to analyse the CCV behaviour in a perfectly premixed SI engine. Local dependencies around the spark plug region, which influence the early combustion stage and hence the CCV have been evaluated.

The choice between the URANS and LES for in-cylinder reacting flow calculation strongly depends on the objectives of the investigation. If one is interested in the cycle- to-cycle variation, LES is the only choice but if the interest is only on the statistics, URANS is adequate. Also, all of the above studies and [44] showed that the parameters of these models had to be calibrated carefully using engine data to observe a good agreement with measurements. Furthermore, it has been suggested in [199] that the above approaches, \( G \)-equation and FSD are valid typically for turbulent combustion in wrinkled flamelets regime but the engine combustion is expected to range from corrugated flamelet to distributed reaction zones regime including thin reaction zones [137]. Hence, transported PDF approach has also been used in past studies [78, 184]. All of these approaches used some form of model tuning. If the model parameters are connected closely to the fundamental physics of the problem, then one could minimise, if not fully eliminate, the tuning. Such a model has been developed using flamelet concept and tested for a number of flame configurations.
including labscale [4, 5, 34, 35, 39, 100, 179] and practical [160, 163] burners. Its subgrid scale version for LES has also been developed and tested for premixed [107, 108, 110] and partially premixed [36] combustion. The model used in this work, called as Flamelets Revised for physical consistencies (FlaRe), explained in section 2.5.8 is based on tabulated chemistry approach and it maintains physical consistencies among various processes in turbulent combustion. This approach relates the combustion model parameters directly to fundamental physics allowing their estimates based on the local turbulence and thermo-chemical conditions and thus they are not tuneable. Hence, they evolve in the simulation for both URANS and LES approaches. The two key engine parameters load and speed influence the flow and thermo-chemical conditions inside the cylinder and thereby affect the turbulence-combustion interaction (TCI) which controls the values for the combustion model parameters.

The studies cited above for FlaRe identified that there is only one adjustable parameter, $\beta_c$, see in Eq. (2.57), which is related to the flame curvature and its influence on the fuel burn-rate. The flame curvature results from the competing effects of turbulence, thermo-chemistry and TCI. Since the in-cylinder flow and thermodynamic conditions vary strongly with engine speed and load, the fuel burn-rate or reaction rate is likely to have some sensitivity to $\beta_c$ although previous studies cited above showed this sensitivity to be weak in continuous combustion systems. Hence, the specific aim of this study is to investigate the sensitivity of engine combustion to $\beta_c$ by simulating in-cylinder reacting flows in a premixed charge SI engine operating at different loads and speeds and by comparing numerical results to measurements in [175]. URANS is chosen as a first step before embarking on LES. It is also well accepted that the laminar burning velocity, $S_L$ is a central quantity for many combustion models and thus it is important to understand its behaviour at conditions relevant for next generation of internal combustion engines. This is studied in Chapter 3, first.
Chapter 3

Gasoline laminar flame behaviour at elevated temperature and pressure

In this chapter laminar flame computations at thermo-chemical conditions expected in future engines, have been performed, using state-of-the art comprehensive chemical mechanisms, validated well in previous studies, for the reactant mixtures of Gasoline-air and Iso-octane-air. Since, $S_L$ is a central quantity for many combustion models and thus it is important to understand its behaviour at conditions relevant for next generation of internal combustion engines. The detail on the laminar flame calculations and the chemical kinetics mechanisms used are discussed in section 3.2. Results are presented in section 3.4 and conclusions are summarised in the final section.

3.1 Introduction

The emission legislation for automobile engines are becoming increasingly stringent to curtail environmental impact of fossil fuel combustion in these engines. This drives a search for finding new combustion technologies that would offer cleaner and efficient combustion with high thermal efficiency and very low emissions of NO$_x$, soot and other pollutants. Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) technology with low NO$_x$ emission and about 10 to 15% improvement in fuel efficiency are promising alternatives to current IC engine combustion technologies [85]. However, maintaining this performance over a broad range of operating conditions (or loads) can be challenging. This is because the expected pressure and temperature conditions required for these combustion concepts can be larger than those in the conventional engines. For example, the in-cylinder pressure peak can reach up to 11.5 MPa with engine boost
system [85] for the above alternative combustion concepts. The combustion characteristics and its interaction with turbulence at such high pressure condition can be quite different from those in conventional conditions and are yet to be investigated in detail.

The recent advances in computational hardware, methodologies, and mathematical modelling techniques for turbulent combustion are lending computational fluid dynamics (CFD) as an important tool for developing modern engines. Thus, the CFD simulations and analysis of turbulent reacting flows are embraced by OEMs as an integral part of their engine design processes. The state-of-the-art of turbulent combustion modellings for multi-dimensional in-cylinder flow analysis were reviewed in earlier studies remarking that the mathematical models will have adequate fidelity if their parameters were closely tied to the physics of the problem [41, 77]. Such models are needed to investigate new combustion concepts involving fuel-lean homogeneous and stratified charge mixtures. This is because the in-cylinder combustion of these mixtures can include strong spatio-temporal variations of turbulence-chemistry interaction and competing effects of flow and thermo-chemistry. Hence, the models should be able to adopt to these changes inherently. This is possible only if the model parameters are related closely to the background physics.

It is well accepted that the laminar burning velocity, $S_L$, is an essential parameter to determine the fuel burn rate [121] and consequently the power output and efficiency. Also, it is involved in almost all of the sophisticated turbulent combustion models for premixed and partially premixed charges [137]. This fundamental quantity varies with pressure, $p$, temperature, $T$, and equivalence ratio of the fuel-air mixture. The pressure and temperature dependence of $S_L$ is typically represented using a power law expression:

$$
\frac{S_L}{S_{L,0}} = \left( \frac{T}{T_0} \right)^\alpha \left( \frac{p}{p_0} \right)^\beta,
$$

where $S_{L,0}$ is the laminar burning velocity at $p_0$ and $T_0$ for a given equivalence ratio, $\phi$. The exponents $\alpha$ and $\beta$ can vary with $\phi$ [121, 131] and are obtained using extensive measurements. The laminar burning velocity at $p_0 = 1$ bar and $T_0 = 298$ K is well investigated for simple hydrocarbons and hydrogen fuels [113]. The variation of laminar burning velocities for fuel-air mixtures of iso-octane, n-heptane, primary reference fuels (PRF) and gasoline with equivalence ratio at elevated mixture temperature and pressure was also investigated in the past [55, 87, 125]. The maximum pressure and temperature of the fuel-air mixture were limited to (1 MPa, 473 K) in [55], (2.5, 373) in [87] and (0.6, 358) in [125]. All of these studies showed that $\beta$ in Eq. (3.1) takes a negative value implying that $S_L$ decreases with increase in $p$ for a given mixture temperature and equivalence ratio.
3.2 Computational detail

The classical theory of premixed flames suggests that the mass burning rate per unit area \( \dot{M} = \rho_u S_L \), where \( \rho_u \) is the reactant density, varies as the square root of fuel consumption rate [202], which was originally identified by Zeldovich and Frank-Kamenetski [203]. This theory suggests that \( \beta = (n - 2)/2 \), where \( n \) is the overall order for the global combustion reaction. For most hydrocarbon stoichiometric and fuel-lean combustion in air \( n \) is typically smaller than 1.2 [114] and thus \( \beta \) is smaller than \(-0.4\), while the experimental measurements suggest that \( \beta \sim -0.5 \) [186]. For the PRFs-air mixtures, this exponent was shown to be about \(-0.3\) over the pressure varying from 1 to 10 bar with mixture temperature ranging between 358 to 450 K [16, 87, 156]. The pressure dependence of \( S_L \) arise because of the fundamental importance of the pressure-sensitive chain reactions involved in the combustion chemistry - the relative importance between the chain branching and termination reactions changes with pressure [114]. These kind of analyses are typically done using lower hydrocarbon such as methane for example and thus, one can ask if these findings would hold or not for higher hydrocarbons specifically for iso-octane or gasoline combustion.

Iso-octane is one of the PRFs and thus it is important to know the pressure dependence of its laminar burning velocity at thermo-chemical conditions expected in future engines. The reactant mixture temperature ranging from 850 to 950 K and pressures ranging from 3 to 4 MPa are of interest here because the low-temperature and high-temperature oxidations of fuel were observed to occur at these conditions in a dual-fuel stratified PCCI engines [85]. Thus, the laminar flame behaviour for stoichiometric mixtures of gasoline surrogate and iso-octane with air at the above conditions are of interest. Specifically, the objective in this work is to find an answer to the question: is there a monotonic decrease of \( S_L \) with \( p \) as noted above or something else for these mixtures at thermo-chemical conditions of interest. As discussed earlier \( S_L \) is a central quantity for many combustion models and thus it is important to understand its behaviour at conditions relevant for next generation of internal combustion engines.

This objective is addressed by performing laminar flame computations using the state-of-the-art comprehensive chemical mechanisms, validated well in previous studies, for the reactant mixtures of interest here.

3.2 Computational detail

The conservation equations for mass, momentum, energy and various chemical species mass fractions involved in the combustion chemistry are solved for a freely propagating one-dimensional laminar premixed flame. The specific forms of these equations and the associated boundary conditions are well known and they can be found, for example in [171]. The
laminar mass burning flux, $\dot{M}$ and hence $S_L$, appears as the eigenvalue of the system of above equations and thus the laminar burning velocity is computed as a part of the solution. The coupled algebraic equations resulting from the discretisation of these conservation equations are solved using an adaptive gridding technique in PREMIX code of the CHEMKIN-Pro software and the accuracy of the solution is controlled by limiting the parameters for gradient and curvature of the spatial variations of temperature and various species mass fractions to be lower than set limits. These parameters were specified to be about 0.01 for both (gradient and curvature) parameters. The molecular transport is modelled using mixture-averaged formulation available in the software to save computational efforts since the difference in the results with this and multi-component diffusion velocity formulations were observed to be very small for the conditions investigated in this study. As noted before, behaviours of laminar premixed flames at relatively high temperature and pressure are of interest and thus the reactant temperatures range from 850 to 950 K for pressures varying from 30 to 40 bar. These conditions are chosen based on the expected in-cylinder pressure and temperature of mixture for the next generation of internal combustion engines [83, 104]. The combustion chemistry is modelled using three different mechanisms of varied complexity described next.

### 3.3 Chemical mechanisms

One of the earlier detailed iso-octane mechanisms was developed by Warnatz [192], which was upgraded subsequently by Westbrook et al. [194] to investigate engine knock. This mechanism contained 765 reversible reactions involving 212 species. Curran et al. [38] developed a comprehensive mechanism involving about 860 species and 3600 reactions for combustion of iso-octane-air mixtures for reactant temperature up to 1700 K and pressure ranging from 0.1 to 4.5 MPa. Other mechanisms developed in the past to study laminar flame speeds of iso-octane and other hydrocarbons were reviewed by Ranzi et al. [156].

Mehl et al. [130] developed a comprehensive mechanism involving 6000 reactions and 1550 species for combustion of gasoline surrogate mixtures by merging n-heptane, iso-octane and toluene mechanisms. This comprehensive mechanism was validated for reactant temperature as high as 1200 K and pressure of 5 MPa and thus it is useful to investigate combustion phenomena at engine relevant conditions. This mechanism can also be used to investigate combustion of pure iso-octane (without species like n-heptane or toluene and other trace species) systematically at conditions of interest for this study - reactant temperature varying between 850 to 950 K and pressure up to 4 MPa. The mechanism of Curran et al. [38] is a sub-mechanism of the comprehensive set of Mehl et al. [130]. For comparison purposes, two skeletal mechanisms for combustion of iso-octane in air are used. A skeletal mechanism
involves 49 reactions and 29 species was proposed by Hasse et al. [75] and is referred as Mech-1 in the discussion below. The second skeletal mechanism by Pepiot-Desjardins and Pitsch [139], referred to as Mech-2 below, is considerably larger as it has 109 species and 393 reactions. The comprehensive mechanism of Mehl et al. [130] is referred as Mech-3 in the discussion below. Details of these mechanisms, such as rate parameters, third body collision efficiency factors, etc., are available in the respective studies cited above. These three mechanisms are used to investigate the behaviour of $S_L$ at thermo-chemical conditions of interest here.

Stanglmaier et al. [174] reported that the laminar burning velocity of gasoline was considerably different from that of iso-octane at higher pressure and temperature based on their experiments. Thus, gasoline surrogate, in addition to iso-octane, mixture is also considered for this study. The gasoline surrogate used here has a RON (Research Octane number) of about 91 and is a mixture of iso-octane (57% by volume), n-heptane (16%), toluene (23%) and 1-pentene (4%), which is taken from the study of Kukkadapu et al. [102].

### 3.4 Results and discussion

#### 3.4.1 Validation cases

Experimental data for $S_L$ of stoichiometric iso-octane-air mixture at high temperature and pressure (about 900 K and 3 to 4 MPa) are not available in the literature and thus a direct comparison of the values computed in this study cannot be made. However, the available flame speed measurements are carefully selected to validate the chemical mechanisms and the approach used for this study. Since the interest is on $S_L$ at elevated temperature and pressure, the experimental data are chosen systematically for validation and the results are shown in Fig. 3.1. The measurements were taken by Bradley et al. [16], Lawes et al. [115], Mandilas et al. [124], Jerzembeck et al. [87], Kelley et al. [92], and Galmiche et al. [55]. The maximum pressure and temperature explored in these studies are 2.5 MPa and 473 K respectively. These values are nearly 50% of the maximum values of interest for this study.

Galmiche et al. [55] showed that there are significant discrepancies between the measured and computed laminar burning velocity of iso-octane-air mixtures. They used the Mech-1 mechanism of Hasse et al. [75] and another mechanism from Jerzembeck et al. [87]. This second mechanism is similar to the Mech-2 mechanism used here. It is also important to note that there are significant discrepancies in the experimental data shown in Fig. 3.1, specifically for $T_u = 373$ K. This is due to the uncertainties associated with the difference in the experimental setup and methodologies employed [55, 169]. The results shown in Fig. 3.1 are
Fig. 3.1 Comparison of measured and computed $S_L$ for stoichiometric iso-octane-air mixtures at various reactant temperature, $T_u$, and pressure. Results are shown for three mechanisms along with commonly used flame speed correlations: Cor1 is from [70], Cor2 is from [131].
in agreement with measurements reported in past studies and also this comparison improves for the comprehensive mechanism of Mehl et al. [130], Mech-3, in general. This echoes the conclusion of Galniche et al. [55] that elaborate and accurate mechanisms are required for iso-octane combustion. It is quite likely that this observation also applies to gasoline surrogate and PRF mixtures and the published $S_L$ measurements for these mixtures are typically available for temperatures ranging from 298 to 400 K at atmospheric pressure [117]. Thus, further measurements at elevated pressures of interest for future engines are required.

Two commonly used flame speed correlations are also shown in Fig. 3.1 for comparison purpose. The flame speeds at atmospheric pressure are predicted quite well by these correlations. Also, they seem to capture the flame speed variations with $p$ for various $T_u$ up to 10 bar and they severely overestimate $S_L$ for higher pressures. The values of flame speed computed using Mech-2 are close to those obtained for Mech-3 up to a pressure of 10 bar for all $T_u$ shown in Fig. 3.1. However, $S_L$ values from the Mech-2 become gradually smaller than those from the Mech-3 as $p$ increases beyond 10 bar. More experimental measurements of the laminar flame speeds for higher pressures are required for full assessment of these mechanisms. However, one must note that the pressure dependent elementary reactions can become important at elevated pressures and these reactions are present only in comprehensive mechanisms. Their influences on autoignition delay times were noted in previous studies [102] and we shall explore their role on flame propagation at the conditions considered for this study.

### 3.4.2 Flame speed and structure at elevated temperature and pressure

If the autoignition is likely to occur for a given $T_u$ and $p$ then a flame solution ceases to exist leading to numerical divergence while solving the required conservation equations with convection, diffusion and reaction balance for flame propagation. This is because the ignition delay time is of the same order as the characteristic flame time when the autoignition is likely to occur [129]. The conditions, $T_u$ and $p$, at which the numerical divergence occurs are plotted in Fig. 3.2 for the two mechanisms, Mech-2 and Mech-3. The region below each curve allows a flame solution and the region above is for autoignition (marked as “No Flame” in the figure). The results are shown for stoichiometric iso-octane and air mixture using both the Mech-2 and Mech-3 mechanisms. The gasoline surrogate mixture requires a comprehensive mechanism and thus the results obtained using the Mech-3 are shown for this mixture. The adiabatic compression curve is also shown for reference and this curve is obtained using $\gamma = 1.3$ which is an average value of $\gamma$ over the temperature range of $298 \leq T \leq 1500$ K [29]. The onset of the autoignition is sensitive to the detail in the chemical kinetics mechanism used. The skeletal mechanism, Mech-2, suggests autoignition to occur
Fig. 3.2 Flame and autoignition regions in $T$-$P$ space predicted using Mech-2 ($\times$) and Mech-3 (circles) mechanisms for stoichiometric iso-octane and air mixture. The results are also shown for the gasoline surrogate mixture (open circles). Light blue rectangular region shows the mixture conditions explored.
3.4 Results and discussion

above 45 bar for $T \geq 800$ K whereas the comprehensive mechanism, Mech-3, allows flame solution as seen in Fig. 3.2. The rectangular region marked shows the mixture conditions explored to investigate the flame structure and speed at elevated temperature and pressure. Some of these conditions are suggested to be autoignition by the skeletal mechanism but the comprehensive mechanism suggests flame propagation. The chemical kinetic description of iso-octane combustion requires an elaborate mechanism as concluded by Galmiche et al. [55] and thus further results discussed below are for the Mech-3, the comprehensive mechanism of Mehl et al. [130]. Figure 3.3 shows the spatial variations of temperature and few major and minor species across the computed flames for 40 bar pressure and two reactant temperatures, 900 and 950 K. The distance through the flame is normalised using the respective thermal thickness, $\delta_{th}$, as $x = (\hat{x} - \hat{x}_0) / \delta_{th}$, where $\hat{x}$ is the dimensional distance through the flame and $\hat{x}_0$ corresponds to the location for $c = (T - T_u) / (T_b - T_u) = 0.5$. The thermal thickness is defined as $\delta_{th} = (T_b - T_u) / |dT / dx|_{max}$ and the product temperature is denoted using $T_b$. These profiles are typical of freely propagating laminar premixed flames with its maximum heat release occurring at about $x = 0$ and only a small part of the domain is shown in this figure. The burning rate mass flux $\dot{M} = \rho_u S_L$ is directly related to the fuel consumption rate per unit volume, $\dot{\omega}_f$, integrated across the flame, ie., $\dot{M} = \int \dot{\omega}_f \ dx / Y_{f,u}$. It is quite easy to verify this by integrating the fuel mass fraction transport equation across the steady laminar flame and applying the boundary conditions. The variation of $\dot{M}$ normalised by its value at $p_0 = 1$ bar is plotted against $(p/p_0)$ in Fig. 3.4. Logarithmic scales are used to emphasis a power-law behaviour, ie., $\dot{M} \sim p^m$, which implies that $\beta = (m - 1)$ (see Eq. 3.1). This gives $m = n/2$, where $n$ is the overall order of the global combustion reaction. The generally accepted value of $\beta \simeq -0.5$ for most of the hydrocarbons suggests that $m = 0.5$, which is different from $m \simeq 0.75$ deduced from the results in Fig. 3.4 for $p \leq 10$ bar. However, this computationally deduced value of 0.75 is close to the experimental value of $m \simeq 0.78$ reported in [70] for iso-octane combustion with air. A close scrutiny of the results in the figure suggests that the value of $m$ is smaller for $p$ larger than 10 bar but it starts to increase beyond about 33 bar. This increase is observed to be negligible for 850 and 900 K iso-octane mixture but it is appreciable for iso-octane at 950 K and also for the gasoline surrogate mixtures shown in the figure. This behaviour clearly suggests that $m$, thus the overall order of the combustion reaction, varies with pressure. It is also worth to note that these changes are observed for pressures well within the range of validity (up to 50 bar) for the chemical mechanism, Mech-3.

One can deduce the flame speed, $S_L$, variations with $p$ using the mass burning rate results discussed above. If one needs to have a negative pressure dependence (ie., $\beta < 0$ for Eq. 3.1) then $m$ must be less than 1 (see above) but the sharp increase in the slope of the curves shown
Fig. 3.3 Spatial variation of $T$ and few selected species mole fractions across the flame for $T_u = 900$ K (top row) and 950 K (bottom) at 40 bar for Mech-3.
Fig. 3.4 Variation of normalised burning rate mass flux with pressure for iso-octane and gasoline surrogate mixtures at three different temperatures.
in Fig. 3.4 suggests that $\beta > 0$. Indeed, this is observed in Fig. 3.5 showing the normalised flame speed variation with normalised pressure for both iso-octane and gasoline mixtures. The upward turn around 36 bar for the iso-octane mixture at 950 K shows that $\beta > 0$. Such a behaviour is seen for the gasoline surrogate mixtures also. The insets in Fig. 3.5 depict the variation of $\beta$ with $\ln(p/p_0)$ showing that the laminar flame speed increases with pressure beyond about 33 bar for the conditions considered in this study, which are of interest for alternative engine combustion technologies. This behaviour of $S_L$ increasing with $p$ is in contrast to the behaviour at relatively lower pressures and this is because of the change in the behaviour of pressure dependent reaction producing OH as discussed in the next section. The increase in $S_L$ with $p$ was also reported in the past for stoichiometric methane-air mixture at $T_u = 1450$ K and this behaviour was suggested to come from autoignition events [73], for which $S_L$ definition is quite ambiguous. The current observation is for premixed flames and is because of the change in the role of pressure dependent reaction involving OH.

### 3.5 Sensitivity analysis

The fuel, for example iso-octane, is consumed by a number of elementary reactions involving radicals and intermediate species and fuel pyrolysis. Thus, the fuel consumption rate is the sum of net rates of these elementary reactions, ie., $\dot{\omega}_f = W_f \sum \dot{\omega}_i$, where $W_f$ is the molecular mass of the fuel species. Analysing these reactions by rank ordering them according to
their contribution to the total fuel consumption rate allows us to identify the first 15 most important reactions involving iC$_8$H$_{18}$ and these reactions are listed in Table 3.1. The reaction numbers listed in the table are those in the chemical mechanism [130]. The first 4 are fuel pyrolysis and the other reactions represent the fuel-attack by radicals and an intermediate, CH$_3$. The net rates of these reactions integrated across the flame are shown in Fig. 3.6 for both iC$_8$H$_{18}$ and gasoline surrogate mixtures at four different pressures, 35, 40, 45 and 50 bar, and two reactant temperatures, 850 and 900 K. It is apparent that the relative contributions of these reactions to the fuel consumption rate remain almost the same for both iso-octane and gasoline mixtures for both temperatures. Generally, the rates of these reactions increase with reactant temperature as one would expect. The rates of reactions 3214 to 3224 and 3230 either decrease or remain more or less constant with pressure and thus they are not responsible for the increase in $S_L$ (or fuel consumption rate) with $p$.

The rates of reactions involving OH, numbered 3226 to 3229 in Table 3.1, standout for all the cases shown in Fig. 3.6 and also their relative contributions increase with $p$, implying that these reactions are responsible for the sharp increase in $S_L$ and $\dot{M}$ with $p$. All of these elementary reactions listed in Table 3.1 are bimolecular and so their rates do not

### Table 3.1 First 15 most important reactions involving iC$_8$H$_{18}$

<table>
<thead>
<tr>
<th>Number</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>3214</td>
<td>iC$<em>8$H$</em>{18}$ = YC$<em>7$H$</em>{15}$ + CH$_3$</td>
</tr>
<tr>
<td>3215</td>
<td>iC$<em>8$H$</em>{18}$ = PC$<em>7$H$</em>{15}$ + CH$_3$</td>
</tr>
<tr>
<td>3216</td>
<td>iC$<em>8$H$</em>{18}$ = TC$_4$H$_9$ + IC$_4$H$_9$</td>
</tr>
<tr>
<td>3217</td>
<td>iC$<em>8$H$</em>{18}$ = NEOC$<em>3$H$</em>{11}$ + IC$_3$H$_7$</td>
</tr>
<tr>
<td>3218</td>
<td>iC$<em>8$H$</em>{18}$ + H = AC$<em>8$H$</em>{17}$ + H$_2$</td>
</tr>
<tr>
<td>3219</td>
<td>iC$<em>8$H$</em>{18}$ + H = BC$<em>8$H$</em>{17}$ + H$_2$</td>
</tr>
<tr>
<td>3220</td>
<td>iC$<em>8$H$</em>{18}$ + H = CC$<em>8$H$</em>{17}$ + H$_2$</td>
</tr>
<tr>
<td>3221</td>
<td>iC$<em>8$H$</em>{18}$ + H = DC$<em>8$H$</em>{17}$ + H$_2$</td>
</tr>
<tr>
<td>3222</td>
<td>iC$<em>8$H$</em>{18}$ + O = AC$<em>8$H$</em>{17}$ + OH</td>
</tr>
<tr>
<td>3224</td>
<td>iC$<em>8$H$</em>{18}$ + O = CC$<em>8$H$</em>{17}$ + OH</td>
</tr>
<tr>
<td>3226</td>
<td>iC$<em>8$H$</em>{18}$ + OH = AC$<em>8$H$</em>{17}$ + H$_2$O</td>
</tr>
<tr>
<td>3227</td>
<td>iC$<em>8$H$</em>{18}$ + OH = BC$<em>8$H$</em>{17}$ + H$_2$O</td>
</tr>
<tr>
<td>3228</td>
<td>iC$<em>8$H$</em>{18}$ + OH = CC$<em>8$H$</em>{17}$ + H$_2$O</td>
</tr>
<tr>
<td>3229</td>
<td>iC$<em>8$H$</em>{18}$ + OH = DC$<em>8$H$</em>{17}$ + H$_2$O</td>
</tr>
<tr>
<td>3230</td>
<td>iC$<em>8$H$</em>{18}$ + CH$_3$ = AC$<em>8$H$</em>{17}$ + CH$_4$</td>
</tr>
</tbody>
</table>
Fig. 3.6 Net rate of elementary reaction involving iso-octane, see Table 3.1, integrated across the flame. The results are shown for both gasoline surrogate and iso-octane mixtures at 4 pressures, 35, 40, 45 and 50 bar, with $T_u = 850$ (left set of frames) and 900 K (right).
depend on pressure. Hence the increase in their net rates with \( p \) should come through the relative role of pressure dependent reactions involving OH. Typically, pressure dependent reactions are chain terminating reaction, i.e., they consume radicals like OH. A careful scrutiny of the chemical mechanism identifies a pressure dependent OH-producing reaction, \( \text{H}_2\text{O}_2(+\text{M}) \leftrightarrow \text{OH} + \text{OH}(+\text{M}) \), which is numbered as 16 in the mechanism [130].

Fig. 3.7 Variation of net reaction rate with pressure for reactions 3226 to 3229 and 16. The reaction rates are integrated across the flame for the gasoline surrogate mixture at 900 K. The reaction 16 is \( \text{H}_2\text{O}_2(+\text{M}) \leftrightarrow \text{OH} + \text{OH}(+\text{M}) \).

Figure 3.7 shows the variations of net rates with \( p \) for reactions 3226 to 3229 and 16. A positive value implies that net reaction is in the forward direction and a negative value implies the backward direction. The net rates of reactions 3226 to 3329 use the scale on the left side of the figure while reaction 16 uses the scale on the right. These reaction rates
are integrated across the flame and they are shown for the gasoline mixture at 900 K. These results are consistent with the results in the Figure 3.6. The sum of these net rates for reactions 3226 to 3329 is also shown in the Figure 3.7, marked as “Total”. It is quite clear that the consumption of iC\textsubscript{8}H\textsubscript{18} increases with \( p \) and this increase is due to the change in the role of reaction 16, which gradually shifts to the right as the pressure increases implying that this reaction changes from OH-consuming to OH-producing reaction, the net rate of this reaction changing from negative to positive values as in Figure 3.7. A similar behaviour is seen for other temperatures in the range, 850 to 950 K, considered for this study. Thus, the increase in \( S_L \) with \( p \) is because of the change in the role of reaction 16. Since this reaction is pressure dependent and the collision partner M includes all the species except H\textsubscript{2}O\textsubscript{2} in the mixture, the overall order of the combustion reaction also changes with \( p \).

### 3.6 Summary

Freely propagating laminar premixed flames of stoichiometric mixtures of gasoline surrogate and iso-octane with air are computed in the view to understand their structures and burning velocities at conditions which are of interest for future IC engine combustion technologies such as PCCI and HCCI. The reactant temperature and pressure of interest for this study are \( 850 \leq T_u \leq 950 \) K and 3 to 4 MPa. These flames are computed using CHEMKIN-PRO software and the combustion kinetics are modelled using three different mechanism of varied level of detail and complexity. These mechanisms are validated using carefully selected experimental data of burning velocity for iso-octane from several past studies. It is observed that elaborate and accurate mechanisms are required to capture iso-octane combustion and to predict its laminar burning velocity as noted by Galmiche et al. [55]. This observation also applies for gasoline surrogate mixtures.

The computations using a comprehensive mechanism [130], denoted here as Mech-3, suggest that propagating flames exists for the temperature (850 to 950 K) and pressure up to 80 bar whereas a skeletal mechanism [139], denoted as Mech-2, yield no flame for \( T = 900 \) K and \( p > 45 \) bar as shown in Fig. 3.2 suggesting possible autoignition. The results obtained using the comprehensive mechanism, which is valid up to 50 bar, are analysed in detail. The burning velocity of both stoichiometric iso-octane and gasoline surrogate mixtures decreased with pressure for the temperature range of interest \( (850 \leq T \leq 950 \) K) and these results, both flame structure and burning velocity, are consistent with the classical theory of premixed flames. The pressure exponent, \( m \simeq 0.75 \), for the mass burning rate flux calculated using the laminar flame results of iso-octane flames up to 30 bar is close to the experimental value of 0.78 [70]. However, this mass flux starts to increase quite significantly beyond
this pressure for the temperature range investigated and thus the laminar burning velocity increases with pressure. This behaviour is in contrast to that suggested by a commonly used correlation given in Eq. (3.1) and it ensues for the following reasons. The net rate of pressure dependent reaction $\text{H}_2\text{O}_2(\text{+M}) \leftrightarrow \text{OH} + \text{OH}(\text{+M})$ changes progressively from negative towards positive value as the pressure increases suggesting that this reaction changes from OH-consuming to OH-producing reaction. Thus, the rate of iso-octane consumption through reactions 3226 to 3229 in Table 3.1 involving OH increases with $p$ leading to the observed behaviour (increase) of $S_L$ with $p$. It is worth noting that this behaviour is for pressures well within the range of validity for the comprehensive chemical mechanism used in this study. It is imperative that chemical mechanisms validated carefully for pressures up to 100 bar and beyond are of interest in the view of future combustion technologies which may be friendlier to the environment.
Chapter 4

Spark-ignition engine simulation

Results in the previous chapter has shown the importance of using detailed chemical mechanism for IC engine related conditions involving elevated temperature and pressures. In this chapter, the sensitivities of unstrained flamlet (FlaRe) model used for engine combustion to the spark ignition treatment, chemical kinetics and flame curvature are investigated. The CFD software STAR-CD is used for the simulation in-cylinder reacting flows. In addition, the module es-ice, which handles the moving grid in IC engine applications, is also utilised in the simulations. This chapter is organised as follows. A description of the experimental engine setup is given next, followed by a discussion on the numerical model, methodology, and tools used for the engine simulation using FlaRe approach. Results are discussed in the subsequent section and concluding remarks are given in the final section.

4.1 Engine description

Experimental investigations were conducted on a 250 cc single cylinder, four-stroke SI engine in the past [175]. Fig 4.1 shows the computational domain considered for engine simulations along with boundary conditions, which are described in the next section. The various symbols used to denote the boundary conditions in Fig 4.1 are explained later in section 4.2.5. The engine parameters are listed in Table 4.1. The combustion chamber is fully symmetric with a pent roof cylinder head and, the intake and exhaust ports. A spark plug located between four valves and is slightly off-centered. The gasoline fuel is injected using a port injection system. This liquid fuel injection is not modelled and a homogeneous charge is taken to enter the cylinder through the intake port. The engine was run for a range of operating conditions and data were collected for 144 cycles for each operating point.

The in-cylinder pressure was measured with a temporal resolution of 0.2° CA using a piezo-electric pressure sensor and the absolute pressures inside the intake and exhaust
Fig. 4.1 A schematic of a part of the symmetric computational volume along with boundary conditions used in the simulations. The outlet boundary conditions are shown for a case without backflow. The colour represents the velocity magnitude when the piston is at (BDC). The outlet ducts were measured using pressure transducers. The engine was fuelled with homogenous gasoline-air mixture at stoichiometric conditions.

Table 4.1 Engine parameters[96].

<table>
<thead>
<tr>
<th>Engine configuration</th>
<th>4-stroke, single-cylinder, SI engine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displaced volume</td>
<td>250 cc</td>
</tr>
<tr>
<td>Bore/Stroke</td>
<td>75/56 mm</td>
</tr>
<tr>
<td>Number of valves</td>
<td>4</td>
</tr>
<tr>
<td>Fuel injection</td>
<td>PFI at 4 bar</td>
</tr>
<tr>
<td>Fuel</td>
<td>Standard gasoline (RON 95)</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>12.5:1</td>
</tr>
</tbody>
</table>

Five operating conditions are considered for this work and these conditions, the engine speed, torque and brake mean effective pressure (BMEP), are listed in Table 4.2. The operating point close to full load condition corresponds to Case 2 (3500 RPM, BMEP of 9.9 bar) and has a torque of 20 Nm. This condition is used as a reference condition here.
to investigate the sensitivity to, ignition treatment, chemical mechanism effects, unburnt temperature, and comparison with $G$-equation model, in sections 4.3.1, 4.3.2, 4.3.3, and 4.3.4, respectively. The ignition angles listed in the table are after the top dead centre (aTDC). All of these five conditions are operated with stoichiometric mixture, air-to-fuel ratio of $\lambda = 1$.

Table 4.2 Engine operating conditions

<table>
<thead>
<tr>
<th>Case</th>
<th>Load (mbar)</th>
<th>Speed (RPM)</th>
<th>Ignition angle (degree)</th>
<th>BMEP (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>950</td>
<td>4000</td>
<td>686.25</td>
<td>9.4</td>
</tr>
<tr>
<td>2</td>
<td>950</td>
<td>3500</td>
<td>689.6</td>
<td>9.9</td>
</tr>
<tr>
<td>3</td>
<td>925</td>
<td>3500</td>
<td>680.25</td>
<td>8.3</td>
</tr>
<tr>
<td>4</td>
<td>WOT</td>
<td>3500</td>
<td>694.5</td>
<td>11.0</td>
</tr>
<tr>
<td>5</td>
<td>WOT</td>
<td>3000</td>
<td>697.5</td>
<td>9.9</td>
</tr>
</tbody>
</table>

The following sections will discuss further details required to complete the CFD simulation and how they were handled.

4.2 Numerical setup

The URANS calculations of this work are performed using STAR-CD v4.22 [27] together with the module es-ice for handling the moving mesh. The combustion model, FlaRe approach, explained in section 2.5.8, is implemented in STAR-CD using user defined subroutines and scalars.

4.2.1 Model implementation

This implementation is shown schematically in Fig. 4.2 using a flow chart. The compressible Navier-Stokes equations for mass, momentum and energy (enthalpy) are solved using STAR-CD CFD code, which is indicated in the left hand column of the flow chart. The turbulence is modelled using $k-\varepsilon$ RNG model available in STAR-CD code. The combustion models available in the code are deactivated and thus temperature rise due to combustion is achieved by including a source term for the heat release rate per unit volume, $\bar{q}$, in the Favre-averaged sensible enthalpy, $\bar{h}$, equation written as:
\[
\frac{\partial \tilde{p} h}{\partial t} + \frac{\partial}{\partial x_j} \left( \tilde{p} \tilde{h} \tilde{u}_j \right) = \frac{\partial \tilde{p}}{\partial t} - \frac{\partial}{\partial x_j} \left( q_j + \tilde{p} \tilde{u}_j \tilde{u}'' h'' \right) + \frac{\partial}{\partial x_i} \tau_{ij} \tilde{u}_j \\
+ \tau_{ij} \frac{\partial u''}{\partial x_i} + \tilde{q}.
\]

(4.1)

using the standard notations. In the tabulated chemistry approach, the heat release rate, reaction rate, and other quantities related to thermo-chemical processes are precomputed and tabulated as a function of Favre-averaged reaction progress variable, \( \bar{c} \), and its variance, \( \bar{c}'\prime'' \). The progress variable is defined here using the mass fraction of water vapour, \( Y_{H_2O} \), as \( c = Y_{H_2O}/Y_{H_2O}^b \), where the superscript \( b \) denotes burnt mixture value, and it is a monotonic function taking a value of 0 in the fresh reactants and 1 in the fully burnt products. The two quantities, \( \bar{c} \) and \( \bar{c}'\prime'' \), required for the table look-up during the simulations need to be transported as explained in section 2.5.8 and their governing equations are Eq. (2.30) and (2.55). The transport equations for \( \bar{c} \) and \( \bar{c}'\prime'' \) are included using user defined scalars and subroutines and are solved along with the enthalpy equation as shown in the flow chart. Various sources and sinks, \( \bar{q}, \bar{\omega}, \bar{\omega}'\prime'' = \bar{\omega} c - \bar{\omega} \bar{c} \), and \( \bar{\epsilon}_c \) are modelled using the FlaRe approach, which is described next. The implementation of this approach in the code and its
interaction with STAR-CD is shown in the flow chart. The box highlighted using dashed lines is related to the FlaRe approach, which is described in section 2.5.8. The temperature, $\tilde{T}$, is obtained using the calculated $\tilde{h}$ and $\tilde{h} = \int_{T_0}^{T} \overline{C}_{p_{mix}} \, dT$, where $\overline{C}_{p_{mix}}$ is the specific heat capacity of the mixture. The mean reaction rate, $\overline{\dot{\omega}}$, and heat release rate, $\overline{\dot{q}}$ are modelled using Eq. (2.58) described in section 2.5.8, $\varepsilon_c$ is modelled using Eq. (2.57). Fluid mixture density is obtained using the state equation.

### 4.2.2 Flamelet library generation

For given values of $\overline{\tilde{c}}$ and normalised variance, $g \equiv \overline{c''^2} / \overline{c(1-\overline{c})}$, Eq. (2.58) and (2.55) can be used to build a library for $\overline{\dot{\omega}}$, $\overline{\dot{\omega} c}$ and other required quantities. The moving piston and the compression of the end gases lead to changes in the unburnt mixture temperature, $T_u$ and pressure, $p$. In order to account for this, the look-up table has to be four-dimensional, where the mean reaction rate and other required quantities are a function of $\overline{\tilde{c}}$, $c''^2$, $T_u$ and $p$. A number of freely propagating laminar flames at various $T_u$ and $p$ for a given equivalence ratio are computed for $300 \leq T_u \leq 1000$ K and $5 \leq p \leq 80$ bar, which are the expected range of operating conditions for the engine considered for this work. The look-up table is generated with a resolution of 0.01 in $\overline{\tilde{c}}$, 0.02 in $g$, 5 bar in pressure and 100 K in $T_u$. The laminar flame speed and its thermal thickness are also included.

### 4.2.3 Chemical mechanisms

Gasoline fuel used in the experimental engine is a complex mixture of several hydrocarbons, without a standard mixture composition [84] and currently it is not possible to describe gasoline combustion with detailed kinetics [148]. For the computations of this work, iso-octane is used as a surrogate, which is a widely accepted single component fuel for gasoline. A number of reduced, skeletal and detailed chemical mechanisms for iso-octane can be found in the literature. In this work two chemical kinetic mechanisms for iso-octane are considered. The first is the skeletal mechanism of Hasse et al. [75], which consists of 29 species and 49 reactions. The second is the detailed mechanism of Mehl et al. [130], which is significantly larger involving 1,500 species and 6,000 reactions.

### 4.2.4 Computational mesh

The engine geometry consists of the intake port (including the inlet valve), the combustion chamber (cylinder) and the exhaust port (including the exhaust valve). Only half of the geometry is used for meshing by considering the geometrical symmetry of the engine.
Computational mesh used in this work consists of hexagonal cells [96], with 103,000 cells at intake, 84,000 at exhaust runners and 135,000 in the chamber at BDC. This grid resolution was also used in [96] for LES of this engine at the same operating point and this grid was observed to be good for LES. Since the scales resolved in URANS are larger than the scales resolved in LES, it is deemed that this grid is adequate for the feasibility study explored here. This mesh is used here in the RANS context as a first step without further investigations into mesh refinement. Note that with this grid resolution and a constant time step of 0.1° CA, the mean Courant number is well below 0.3 throughout the high pressure cycle, while the maximum local value found in the domain peaks around 9.5 shortly after spark advance and decays below 2 during the combustion event.

4.2.5 Initial and boundary conditions

Simulations are started at about 30 CAD before the intake valve opening (IVO), which is at 300 CAD after the TDC. The exhaust valve is open at this (300) crank angle. The cylinder and exhaust ducts are initialised to have fully burnt products and the temperature of this mixture inside the cylinder is set to have 900 K based on preliminary simulations and past studies [96]. The sequence of engine events is shown in Fig 4.3, which is fed to the valve movements for the simulations. The wall function of Angelberger et al. [8] is chosen to specify the wall heat transfer by keeping the wall temperatures constant at the values listed in Table 4.3 along with no-slip condition for the velocities.

![Valve lift and crank angle diagram](image)

**Fig. 4.3 Events sequence in the engine, which shows the valve movement plotted against the crank angle for Case 2.**
4.2 Numerical setup

<table>
<thead>
<tr>
<th>Wall</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder</td>
<td>400</td>
</tr>
<tr>
<td>Piston crown</td>
<td>470</td>
</tr>
<tr>
<td>Combustion dome</td>
<td>470</td>
</tr>
</tbody>
</table>

The inlet and outlet are specified with pressure which varies with the CA as noted in Fig 4.1. The pressure values are obtained from the measured phase-locked mean pressures using the ensemble averaged value for the 144 cycles measured in the experiments [96]. Moreover, constant average temperatures are prescribed at the inlet and outlet, which defines the trapped mass in the cylinder. Dirichlet boundary conditions are used for the scalar variables ($e_c$ and $c''_2$) and turbulence quantities at the inlet. For the outlet, Neumann boundary conditions are applied, where the gradients of $h$, $k$, $\bar{e}$, $\bar{c}$ and $c''_2$ are set to be zero. In case of backflow, the quantities such as temperature and turbulence variables are also specified at the outlet.

4.2.6 Computational details

The governing equations and closure models discussed earlier in this section are solved using the finite-volume method. The pressure-velocity coupling is maintained using PISO algorithm [86]. The time-step is kept constant at 0.1 CAD. The transport equations are discretised in space using second-order MARS scheme. The temporal discretisation scheme is based on the fully-implicit Euler scheme and explicit deferred correctors. The accuracy of this approach available in STAR-CD is between first and second order.

4.2.7 Ignition treatment

Ignition is achieved in this study by a simple “energy deposition” approach and similar methods were used in previous studies [68, 97, 165]. In this approach, the amount of ignition energy can be altered by varying the volume and duration used for ignition. The limitation of such ignition treatments and the importance of early kernel growth was noted in [97]. Extensive ignition modelling is required for proper treatment of initial kernel growth. Since the focus here is on the feasibility of the combustion model described earlier for IC engine simulation, the ignition is taken to be a simple energy deposition.

Experimental data showed that $T_u = 642$ K and $p = 10.8$ bar at sparking CA. Fig 4.4 shows the mean combustion heat release rate per unit mass from the flamelet library using
Fig. 4.4 Variation of heat release rate with $c$ for $T_u = 650$ K and $p = 10$ bar.

Hasse et al. [75] mechanism at $T_u = 650$ K and $p = 10$ bar, which are the tabulated conditions closest to the experimental values at sparking.

Data in this figure is used to determine the maximum amount of energy that can be used for ignition at this temperature and pressure. It shows that the maximum heat release rate occurs at $\tilde{c} = 0.75$ at $g = 0.1$, which is used to estimate the input during spark timing. In this simple spark model, the power supplied is varied as $e^{-t/\tau}$, where $\tau$ is the spark duration in ms as shown in Fig. 4.5. Ignition is achieved by including source terms in Eqs. (4.1) and (2.55) for the spark duration.

Two ignition treatments are considered in this study; first case uses 2 cells with the ignition duration set to $4^\circ$ CA and second case uses 4 ignition cells with a duration of $2^\circ$ CA. Fig 4.5 shows the ignition power and energy used in these two ignition treatments. This figure shows that the total ignition energy used in these ignition treatments is roughly 30 mJ. This is close to the secondary energy values of 28 mJ reported by the manufacturer of the ignition coil used in the engine [LLP].
4.3 Results and discussion

4.3.1 Influence of ignition treatment

Pressure traces obtained from a sensitivity study to the ignition treatment are shown in Fig 4.6. In this figure, computed pressure traces are compared with experimental measurements, which are the mean of 144 cycles. Numerical results shown in this figure are obtained using the skeletal mechanism of Hasse et al. [75] and the flamelet library is generated with a resolution of 50 K in the unburnt temperature.

Results in Fig 4.6 show that using 2 cells with a duration of 4° CA predicts the early combustion phase accurately (up to 720° aTDC). However, the combustion is too fast from this point, which leads to a 20% overprediction of the peak pressure when compared with experimental data. On the other hand, using 4 ignition cells with a duration of 2° CA leads to slower combustion not long after ignition. For this case, the peak pressure is over predicted by 10%, with the peak occurring at a later stage. Fig 4.7 shows the heat release rate (HRR) and cumulative heat release for the same ignition treatments using Hasse et al. [75] mechanism. These figures show similar behaviour observed for the in-cylinder pressure, i.e. the agreement is good for the early combustion phase but both ignition treatments overpredict the amount of heat released during the later stages.
The pressure overestimate could be due to the mismatch in the burn rate which could arise from (1) chemical mechanism, (2) estimation of unburnt mixture temperature and (3) history from ignition treatment. The influence of chemical mechanism to be discussed below comes through the flamelet structure and flame speed. The accuracy of these mechanisms is important to obtain a good agreement with laminar flame speed measurements. As discussed in chapter 3, Fig 3.1 shows reasonable agreement for the flame speeds with available experimental data. However, these experimental data are for much lower temperatures and pressures than the ones observed near the engine TDC, where temperature is about 900 K with pressure up to 60 bar. Also, the progress variable threshold used to calculate the unburnt mixture temperature has an effect on the peak pressure (difference of about 5%) as discussed later.

The results presented in this section indicate the importance of choosing a correct ignition model, since the subsequent flame propagation depends on the initial flame kernel growth. The simple model used in this work gives reasonable pressure trace, however, it needs to be refined for improved treatment of the initial kernel growth and its interaction with local turbulence and thermochemical conditions.
4.3 Results and discussion

Fig. 4.7 (a) Heat release rate and (b) cumulative heat release for two different ignition treatments using the mechanism of Hasse et al. [75].

### 4.3.2 Chemical mechanism effect

The sparking sensitivity study carried out using Hasse et al. [75] mechanism showed that using 2 cells with an ignition duration of 4° CA gave a better agreement for the pressure evolution up to 720° CA, hence this ignition treatment is used here to compare the effect of the chemical mechanism.

Fig 4.8 compares pressure variations computed using these two chemical mechanisms. This figure shows that Mehl et al. [130] mechanism underpredicts early combustion soon after ignition. However, when compared to Hasse et al. [75] mechanism, the peak pressure prediction is improved (the peak pressure is underpredicted by 3%). These results can be explained by the differences in laminar flame speeds of these two mechanisms shown in Fig 3.1, which showed that for identical conditions, Mehl et al. [130] mechanism gives lower $S_L$ when compared with Hasse et al. [75]. This allows one to make comparative evaluations.

Contour plots of the heat release rate, $\dot{q}$, at different crank angles for both chemical mechanisms are shown in Fig 4.9. These figures can be used to visualise how combustion takes place inside the engine. For all the crank angles considered in this figure, $\dot{q}$ is higher for Hasse et al. [75] mechanism, yielding an over prediction of peak pressure as in Fig 4.8. This over prediction is consistent with generally larger values of the laminar flame speed for this mechanism as shown in Fig 3.1.
Fig. 4.8 Pressure trace comparisons using chemical mechanism of Hasse et al. [75] and Mehl et al. [130].

Fig. 4.9 Contours of heat release rate during combustion, $\dot{q}$, at different crank angles using mechanisms of (a) Hasse et al. [75] and (b) Mehl et al. [130].
4.3 Results and discussion

These results show the importance of choosing a mechanism that can correctly predict the laminar flame characteristics of the mixture. None of the mechanisms used in this study has been validated for the high temperature and pressure conditions experienced inside the cylinder. Thus it is imperative that one needs further measurements of laminar flame characteristics at unburnt mixture temperature and pressure expected in future engines.

Fig 4.10 shows the HRR and cumulative heat release for both chemical kinetic mechanisms. It can be seen that the mechanism of Hasse et al. [75] gives a good agreement for the HRR up to 720° CA but both mechanisms overpredict the peak HRR. This overprediction of HRR can explain the steeper gradients for the cumulative heat release of the simulation results. One reason for this overprediction could be the calculation of $T_u$, which is addressed in the next section.

4.3.3 Unburnt temperature calculation

Unburnt temperature, $T_u$, is one of four variables used to retrieve values from the flamelet library. Therefore, it is important to predict $T_u$ accurately. In this work, $T_u$ is calculated by averaging the temperature of cells below a certain threshold value of $\tilde{c}$. Fig 4.11 shows the calculated $T_u$ for three different $\tilde{c}$ thresholds. Plots in this figure are obtained using the mechanism of Mehl et al. [130], with increments of 50 K for $T_u$ in the flamelet library. This
figure shows that the difference in maximum $T_u$ is about 15 K for the three values considered here, i.e. a 2% difference between the results. This figure also shows that the results obtained using the three thresholds start to deviate around 715°CA. Beyond this crank angle, the number of cells available for volume averaging becomes small and explains the relatively high sensitivity to the threshold value at these crank angles.

![Graph showing sensitivity to threshold for $T_u$ calculation](image_path)

Fig. 4.11 Sensitivity to $\tilde{c}$ threshold used to calculate $T_u$: (a) calculated $T_u$ and (b) corresponding pressure traces. Mechanism of Mehl et al. [130] is used for the simulations.

A lower threshold value implies that it is further away from the flame, thereby, giving a lower $T_u$. This in turn gives slower combustion and lowers the peak pressures as shown in Fig 4.11b. The differences in peak pressures between the simulated and measured data are within 5%, indicating that using lower values of threshold will not significantly change the results.

The results presented so far were obtained using a resolution of 50 K for $T_u$ in the flamelet library. Sensitivity studies using $T_u$ resolutions of 25, 50 and 100 K did not show any difference in the peak pressures, which shows that a resolution of 100 K is sufficient.

### 4.3.4 Combustion model comparison

The flamelet model described in this work is compared with the widely used $G$-equation model [198] available in STAR-CD. The ignition treatment for $G$-equation is similar to the simple energy deposition approach described earlier for the flamelet model. The size of this kernel and the corresponding $G$ variance are chosen to match the measured pressure trace and the flamelet results for the first 10° CA from the spark advance so that the model comparison can be made in a meaningful manner. The transport equation for $\tilde{G}$ requires a model for the turbulent flame speed, $s_T$, which is usually of the general form [142]:

$$s_T = s_L^0 \left[ 1 + A \left( u'/\delta_L^0 \right)^n \right],$$

where $n$ is around 0.7 [197] and, for $s_L$, one of the correlations or
the CHEMKIN result shown in Fig 3.1 can be employed. Following the common practice, the correlation of Gülder [71] is used for the $G$-equation results reported here.

![Graph showing pressure trace comparisons](image)

**Fig. 4.12** Pressure trace comparisons using the flamelet based combustion model (Hasse et al. [75] mechanism using 2 cells for ignition at a duration of 4° CA) and $G$-equation with different values for the flame speed coefficient, $A$.

Fig 4.12 shows the results obtained using the flamelet (with the mechanism of Hasse et al. [75]) and $G$-equation models. The results from $G$-equation are highly sensitive to the flame speed coefficient, $A$, that appears in the $s_T$ model. This parameter has to be chosen carefully to get a good agreement with measurements and a close agreement for the operating condition considered here is obtained for $A = 3.3$. Although this carefully selected $s_T$ model improves the peak pressure significantly compared with the flamelet model, the early combustion phase is not represented accurately by this model. This figure also shows that the results using $G$-equation start to deviate soon after ignition (around 700° CA) even for low values of $A$, while the flamelet model shows considerably better agreement up to 720° CA, which is significant.

It is important to note that the current implementation of $G$-equation in STAR-CD requires some adjustments for both the ignition and the turbulent flame speed (through the parameter $A$) to obtain a good agreement with measurements. Furthermore, $S_L$, used in the $s_T$ model, is obtained using the correlation of Gülder [71], which was shown above to overpredict the $S_L$. However, in the flamelet model discussed in this work, apart from the sensitivity to ignition, there are no adjustable parameters. The combustion model
parameters used in this work are identical to the ones used in previous studies on a range of applications [2, 5, 35, 160, 161, 164, 179].

4.3.5 Flame curvature induced effects

Before presenting engine simulation results, the behaviour reaction rate and other quantities involved in $\beta_c$ are analysed using the flamelets. This is done specifically to understand the behaviour of $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$ at high pressure and temperature relevant for engine conditions. This discussion is followed by a sensitivity analysis for the reference engine condition (Case 2 in Table 4.2), which is followed by a discussion on the performance of this model for different engine speed and load.

The parameter $\beta_c$ in Eq. (2.57) is related to the behaviour of $(T_4 - D_2)$ [31], where

$$T_4 = 2D_c \left( \frac{\partial c}{\partial x_i} \frac{\partial \dot{\omega}}{\partial x_i} \right)$$
and

$$D_2 = 2 \rho D_c^2 \left( \frac{\partial^2 c}{\partial x_j \partial x_i} \right) \left( \frac{\partial^2 c}{\partial x_j \partial x_i} \right)$$

Indeed, the quantities involved in the above two equations are Favre fluctuations, which are unavailable in URANS framework and one needs DNS data, see chapter 5 for the analysis using DNS data. Here flamelet quantities are used because combustion time-scale is typically smaller compared to flow and piston motion time-scales. The second derivative involved in $D_2$ is related to the flamelet curvature, which will be influenced by the molecular diffusivity and the spatial variation of flamelet propagation which is related to $\nabla \dot{\omega}$. Thus, one sees clearly that $\beta_c$ behaviour is strongly correlated with $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$, which are scale dependent quantities. Thus, one needs to be cautious in selecting a value for this parameter. Pervious RANS and URANS studies [4, 5, 34, 35, 100, 160, 164, 179] showed that a value of $\beta_c = 6$ to 7 works quite well for wide range of flame and flow conditions for continuous combustion systems having a constant $T_u$ and $p$. In IC engines, the unburnt mixture temperature and pressure will vary with load and speed further to their variation with time because of piston movement. Thus, it is imperative to study the behaviour of fundamental quantities related to $\beta_c$ which is done here using flamelet quantities. Analysis using direct numerical simulation data has been reported elsewhere [31] and detail can be found there.

Fig 4.13 shows the variations of temperature and reaction rate for three different values of $T_u$ and $p$ observed in IC engine simulations. It is well known and also seen in Fig 4.13 that increasing $T_u$ and $p$ results in thinner flame and higher reaction rate. The blue line corresponds to the flamelet having $T_u = 900$ K and it has the thinnest reaction zone. As the temperature and pressure decreases to $(800, 30)$ and $(600, 10)$ the reaction zone becomes
thicker. This will influence the gradients related to $\beta_c$, which are shown in Fig 4.14. The behaviour of these gradients are as expected and consistent with the variation of $\dot{\omega}$ shown in Fig. 4.13. The variation of $c$ with distance through the flamelet would be similar to the temperature variation shown in Fig. 4.13. The results in Fig 4.14 illustrates the increase of $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$ with pressure and temperature.

It is quite clear that the changes in $T_u$ and $p$ influence these gradients strongly and thus one can expect that $\beta_c$ is also likely to change with CAD even in a single operating condition. This change can only be captured using dynamic approach for LES. Since, the statistics are of interest with URANS, one can hope to have a single value of $\beta_c$, which was indeed tested for the reference case, Case 2 in Table 4.2, in an earlier study [3] using a value of 6.8 for this parameter. This value may also change with operating conditions. This is assessed systematically in the followings. First, the sensitivities of in-cylinder pressure rise and cumulative heat release rate to $\beta_c$ are explored for the reference condition, Case 2. Then, the value of this parameter is used to assess the performance of this model for other engine operating conditions.
Fig. 4.14 Variations of $\nabla \dot{\omega}$, $\nabla^2 c$, $\nabla c$ through the flamelets.
Fig. 4.15 Variation of in-cylinder pressure and cumulative heat release rate with CAD for various $\beta_c$. The variation of percentage change in the peak pressure with $\beta_c$ is shown in (c).
4.3.6 Effect of $\beta_c$

Ten different values of $\beta_c$ ranging from 4 to 14 are tested for the reference case (Case 2 in Table 4.2). This operating condition has an engine speed of 3500 RPM and is close to the full load with a BMEP of 10 bar.

Fig 4.15a, and 4.15b compare the variations of computed in-cylinder pressure and cumulative heat release rate with CAD to the respective measurements. The percentage change in the peak pressure with $\beta_c$ is shown in 4.15c. For the lowest, $\beta_c = 4$, and highest, 14, values considered here, the combustion process is observed to be very fast, which is shown by the sharp raise in the cylinder pressure and cumulative heat release rate. There is an over prediction of about 27% and 50% in the peak pressures for these model parameter values as seen in Fig. 4.15c. However, as the $\beta_c$ values increase from 4 the peak pressure prediction is improved as seen in Fig 4.15. The variation of percentage difference in the computed peak pressure, in comparison to the measured value, with $\beta_c$ is shown in Fig 4.15c. For the calculations using $\beta_c$ between 6 to 12 the computed peak pressures are about 15% larger than the measured value.

The influence of $\beta_c$ on the burning rate is as follows. If this parameter value increases then the dissipation rate in Eq. (2.57) decreases, which in turn increases the variance $\tilde{\epsilon}^2$. This increase in variance for a given $\tilde{c}$ yields a lower reaction rate locally, but the increase in $T_u$ and $p$ arising from the compression of in-cylinder mixture increases the reaction rate. The resultant behaviour depends on these two effects, which is quite non-linear. This gives a non-monotonic variation of the burning rate with respect to $\beta_c$, which can also be seen in Fig 4.15a and 4.15b. It is quite clear that there is some sensitivity to $\beta_c$ and this varies with the value of $\beta_c$ itself as seen in Fig 4.15c. Based on this analysis, a value of $\beta_c = 9$ is selected for simulating other operating conditions noted in Table 4.2. Temporal evolution of $\tilde{c} = 0.1$ iso-surface, coloured by temperature, is shown in Fig 4.16, starting from an instant just after sparking to 769.98 CAD. These pictures are shown for CAD 697.21, 700.05, 714.96, 739.95, 755.07, and 769.98. These figures can be used to visualise the flame evolution inside the cylinder.

4.3.7 Change of speed and load

Measured and predicted cylinder pressure histories for five operating conditions considered for this study are compared in Fig 4.17. As noted earlier, a value of $\beta_c = 9$ is used for all these cases. Just to remind ourselves, Case 2 is the reference case used for the results reported in Fig 4.15. The engine speed decreases when one moves from Case 1 to Case 5 horizontally in the Fig 4.17 and if one move vertically then the engine load increases. The yellow point on
the pressure curve corresponds to the ignition crank angle. The ignition timing varies for each operating condition (see Table 4.2). As shown in this figure, the computed cylinder pressure histories are close to the experimental results for the 5 operating conditions investigated. Case 2 shows a fair agreement between the computed and experimental result with a slight over prediction. Rate of pressure rise and the peak pressure are fairly well predicted for almost all cases suggesting that the modelling approach used here is promising and the sensitivity of the results to $\beta_c$ is weak for the conditions investigated here.

### 4.4 Summary

RANS simulations of a small 250 cc single-cylinder gasoline full-metal engine has been conducted for five operating conditions using a flamelet based combustion model (FlaRe). In this approach, the progress variable and its variance equations are solved with physically
consistent closures along with other conservation equations. The various sources and sinks in the progress variable, its variance and sensible enthalpy equations are obtained using a look-up table approach. This modelling was successfully used for continuous combustion in gas turbines, lab-scale flames in many past studies. All of these studies demonstrated that the FlaRe model worked well and gave flame and flow statistics quite close to measured values. Also, those studies identified that there is one model parameter, $\beta_c$, related to flame curvature which is influenced by the spatial gradients of reaction rate and progress variable. Thus, it may vary spatially and temporally, and it is also scale dependent. Thus, it is well suited for dynamic evaluation in LES, but for URANS calculations this is not possible.

The simulation of reference condition at 3,500 RPM close to full load (Case2), showed high sensitivity to the ignition treatment for which a simple energy deposition approach has been adopted as a first step. The sensitivity of the model was further assessed with respect to the chemical kinetics used for the flamelet library generation, for which a skeletal and a detailed iso-octane mechanism have been used.

The results show large discrepancies in the laminar flame speeds between the two kinetics – and also when compared to experimental data – which manifest themselves in significant differences in the pressure evolutions. Furthermore, calculation of the unburnt temperature was found to give differences of 5% when compared with measurements, while the temperature increment used for the tabulation of the library showed little sensitivity between 100 K, 50 K and 25 K.

The model has been compared to the widely used level-set approach ($G$-equation combustion model), for which substantial sensitivity to the turbulent flame speed parameter is evident. While better agreement for the peak pressure could be achieved using $G$-equation with a calibrated flame speed parameter compared to the flamelet model with unchanged parameters, the pressure rise between spark advance and 720° CA shows better agreement for the flamelet model.

The sensitivity of engine simulations to $\beta_c$ parameter was considered for this study, first considering the reference engine operating condition and then a range of operating conditions by varying speed and load. The simulation of reference condition showed that there is sensitivity of different level depending on the value of $\beta_c$. However, it is observed that there is a range with reduced sensitivity and a representative value of $\beta_c = 9$ is chosen for subsequent simulations of other operating conditions. The results show that this value works quite well for the speed and load conditions considered here and the agreement with measurements is found to be good.

Further efforts required have been highlighted including in particular the ignition treatment, the unburnt mixture temperature estimate and the chemical kinetics used for flamelet
library generation. Also, these results suggest that the FlaRe modelling framework is promising for IC engine simulations. However, dynamic evaluation of $\beta_c$ is more appropriate for simulations of in-cylinder flow and combustion in modern environmentally friendlier engines to investigate cycle-to-cycle variations and pollutants production using LES paradigm.
Chapter 5

Model assessment using DNS data

Following the observations from the previous chapters and the need for dynamic evaluation of $\beta_c$, the DNS data of isochoric combustion [200, 201] is used here to investigate (i) the unstrained flamelet closure for the SGS reaction, (ii) the behavior of $\beta_c$ and (iii) its dynamic evaluation for LES. This chapter is organised as follows. The SGS combustion modeling is discussed briefly in section 5.2. The detail of DNS data and its processing are explained in section 5.3. The results are discussed in section 5.5 and the conclusions are summarised in the final section.

5.1 Introduction

The performance and characteristics of Internal Combustion (IC) engines can be improved using various concepts such as Homogeneous Charge Compression Ignition (HCCI), Port fuel injection (PFI), and Direct Injection (DI). These have the potential to reduce in-cylinder pollutant formation and increase the overall efficiency. However, achieving these goals is challenging and an improved understanding of the underlying physics of turbulent combustion in IC engines operating with the above concepts is necessary. Hydrogen is recognised as an attractive and a promising fuel for future main stream IC engines and gas turbines. If it is used with optimised engine operating conditions, there are emission benefits, including elimination of soot, unburned hydrocarbons, and greenhouse gases. Aside from pollutant reductions, hydrogen is also recognised as an important fuel because it can be derived from various renewable sources. Thus, understanding turbulent combustion of hydrogen and its modelling, in general, is important.

The advent of computational hardware, methodologies and modelling approaches in recent times make computational fluid dynamics (CFD) an important and cost-effective tool to gather required insights on the in-cylinder flow, combustion and their interactions. Direct
Numerical Simulation (DNS) resolves all the relevant length and time scales involved in turbulent reacting flows without any modelling assumptions. Thus, DNS can be considered as numerical experiments helping us to gather fundamental insights and thereby provide unique opportunities to test and validate modelling hypotheses for turbulence-chemistry interactions. This is because all the information required for these kinds of analysis can readily be deduced from DNS data. However, the computational burden of including complex engine geometries and flow paths preclude the DNS for engine flows. Many DNS studies have been conducted in the past to investigate hydrogen-air turbulent premixed flames in a variety of flame and flow configurations, such as planar [150, 166, 167, 182] and oblique ("Vee") [69, 133] flames propagating in homogeneous turbulence, swirling flames [132, 183, 191] and jet flames [88, 168]. Many useful insights are deduced from these studies for isobaric combustion. In IC engines, combustion occurs at constant volume under pressure rising conditions and thus, the reactant temperature and pressure change with time over wide ranges, which can be mimicked by simulating turbulent combustion inside a vessel of fixed volume.

Yenerdag et al. [200, 201] conducted such a simulation and considered hydrogen-air premixed flame initiated using an initial spherical kernel and propagating in a turbulent flow to mimic the combustion processes observed in an IC engine with its piston at the top dead centre (TDC). However, the pressure rise during the combustion in the DNS was not as big as in an IC engine but sufficient to address the objectives of this investigation, which are elaborated later in this section.

Unsteady Reynolds averaged Navier-Stokes (URANS) simulations are used extensively to simulate in-cylinder turbulent reacting flows in industries because of its computational cost. Large Eddy Simulations (LES) are, however, becoming feasible for engine combusting flows with intricate geometry because of the recent advances in computational capabilities. This allows us to study cycle-to-cycle variations. The validity of these simulations depends on the closures used to describe turbulence, combustion and their interactions. The combustion modelling, its accuracy and robustness play a vital role in this.

The currently emerging Large Eddy Simulation (LES) models for engine flow exhibit large uncertainties with respect to the subgrid scale (SGS) models [162] and combustion is a SGS phenomenon. Various combustion closures developed in the past to tackle turbulent premixed combustion are reviewed and discussed in [137, 143, 149]. Out of these many modelling methods, flamelet based methods are quite attractive for engine application as they are relatively simple and computationally less expensive. As discussed more in details in section 2.6, the progress and application of LES for engine flows has been reviewed in [41, 76, 77, 162] noting that (i) LES requires a low level of empiricism, (ii) advanced
subgrid turbulence model can ease computational grid requirement [162] but will increase computational cost and (iii) the SGS combustion models will have adequate fidelity if their parameters were closely tied to the physics of the problem [41, 77]. One such combustion closure, *FlaRe* (Flamelets revised for physical consistencies) is developed at Cambridge University, discussed in section 2.5.8 using flamelets and this method is of interest for this chapter.

The *FlaRe* approach discussed briefly in section 2.5.8 is based on unstrained flamelets and is investigated here using DNS data of turbulent combustion of hydrogen-air mixture in pressure rising condition. This model is based on tabulated chemistry approach and maintains physical consistencies among various SGS processes in turbulent combustion (see section 5.2) since the model parameters are linked directly to these (flow and thermo-chemical) processes. Thus, these parameters can be estimated based on the local turbulence and thermo-chemical information available within the simulation paradigm (URANS or LES). This model has been tested for laboratory scale flames [4, 5, 39, 100, 179] and practical burners [160, 164] including engine relevant flow and flame conditions [2]. Its capability for IC engine simulation has also been tested in [3, 60] using URANS approach.

Its subgrid scale version has been developed and tested for premixed [107, 110] and partially premixed [36] flames. This approach has a scale dependent parameter, $\beta_c$, to include effects arising from flame curvature related phenomena, which are strongly related to the SGS thermo-chemical processes. Since the in-cylinder reactant temperature and pressure vary with time, the mutual influence of flame curvature and thermo-chemical activities may be stronger compared to those in isobaric combustion and thus the $\beta_c$ value is likely to change with time.

A dynamic procedure for $\beta_c$ was developed and tested using DNS data [57, 108] and its behaviour in LES was also assessed by comparing LES statistics [108] with measurements in turbulent Bunsen flames. Langella et al. [108] found small difference in the Bunsen flames statistics obtained using an empirically determined (static) $\beta_c$ value and the dynamic procedure. This could be because (i) the empirical value was chosen carefully and (ii) combustion in the Bunsen flames occurs at constant pressure with no changes in the temperature and pressure of the incoming reactant. As noted earlier, the thermodynamic conditions of the reactant mixture change with time in isochoric combustion because of the compression caused by the expanding gases. This is similar to that occurring inside an IC engine. Thus, the objectives of this study are (i) to test the unstrained flamelet closure for the SGS reaction rate and (ii) to investigate the behaviour of $\beta_c$ and its dynamic evaluation for constant volume turbulent combustion of hydrogen-air mixture. These objectives are achieved by analysing the DNS data of isochoric combustion [200, 201].
5.2 SGS combustion modelling investigated

In this section, some equation from the background and specifically, section 2.5.8, have been repeated for easy reference and clarity of the discussion in this chapter.

A reaction progress variable is typically used to track the progress of premixed combustion and this variable is defined using either temperature or scalar mass fractions. Here, it is defined using water mass fraction, $Y_{H_2O}$,

$$
c = \frac{Y_{H_2O}}{Y_{H_2O}^b} \tag{5.1}
$$

where the superscript $b$ indicates the burnt mixture. Thus, $c$ varies from 0 in the reactant mixture to 1 in the products. The transport equation for its Favre-filtered value, $\overline{c}$, is

$$
\overline{p} \frac{D\overline{c}}{Dt} = \frac{\partial}{\partial x_i} \left( \overline{p} \frac{\partial \overline{c}}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \overline{p} \overline{u_i c} - \overline{p} \overline{u_i \overline{c}} \right) + \overline{\omega_c} \tag{5.2}
$$

using standard notations with $\otimes$ as the molecular diffusivity of $c$ and $D/Dt$ is the substantial derivative. The filtered reaction rate, $\overline{\omega_c}$, is modelled using

$$
\overline{\omega_c} = \overline{p} \int_0^1 \frac{\dot{\omega}_c(\zeta)}{\rho} \tilde{p}(\zeta; \overline{c}, \overline{c^{\prime 2}_{sgs}}) \, d\zeta \tag{5.3}
$$

where $\zeta$ is the sample-space variable for $c$. The SGS Favre probability density function (pdf) of $c$ is denoted as $\tilde{p}(\zeta)$ and is modelled using a Beta function for given values of $\overline{c}$ and SGS variance, $c^{\prime 2}_{sgs}$. The flamelet reaction rate, $\dot{\omega}_c(\zeta)$, is obtained using unstrained laminar flame computed for a given reactant temperature, $T_u$ and pressure, $P_u$. The combustion kinetics can be represented using a complex chemical mechanism and the same mechanism employed in the DNS is used for this study. The SGS variance, $c^{\prime 2}_{sgs} = \overline{c^2} - \overline{c}^2$, is obtained in LES through its modelled transport equation, which is

$$
\overline{p} \frac{D\overline{c^{\prime 2}_{sgs}}}{Dt} \approx \frac{\partial}{\partial x_i} \left[ (\otimes + \mathcal{D}_T) \frac{\partial \overline{c^{\prime 2}_{sgs}}}{\partial x_i} \right] - 2\overline{p} \tilde{c} + 2 \left( \overline{\omega_c c} - \overline{\omega_c \overline{c}} \right) + 2\mathcal{D}_T \left| \frac{\partial \overline{c}}{\partial x_i} \right|^2, \tag{5.4}
$$

where $\mathcal{D}_T$ is the SGS eddy diffusivity. In this equation, $\overline{\omega_c c}$ and $\tilde{c}$, require closures and the former is closed using a model similar to that in Eq. (5.3) as noted in [108, 110]. The SGS
5.2 SGS combustion modelling investigated

scalar dissipation rate (SDR), $\tilde{\varepsilon}_c$, is modelled using an algebraic expression investigated in earlier studies [45, 57, 108], see also (2.57):

$$\tilde{\varepsilon}_c = \mathcal{F} \left[ 2K_c \frac{s_L}{\delta_{th}} + (C_3 - \tau C_4 D_{a\Delta}) \left( \frac{2 u'_{a\Delta}}{3 \Delta} \right) \right] \frac{\epsilon_{SGS}^{\mu^2}}{\beta_c},$$  \hspace{1cm} (5.5)

where $\mathcal{F} = [1 - \exp(-0.75\Delta^+)]$ with $\Delta^+$ as the LES filter width, $\Delta$, normalised by the laminar flame thermal thickness, $\delta_{th}$, and $u'_{a\Delta}$ is a SGS velocity scale. The laminar flame speed is $s_L$ and the thermochemical parameter is $K_c = 0.79 \tau$, where $\tau$ is the temperature rise across the flame normalised by $T_u$.

The other parameters are defined as $C_3 = 1.5 \sqrt{K a_{\Delta}}/(1 + \sqrt{K a_{\Delta}})$, $C_4 = 1.1/(1 + K a_{\Delta})^{0.4}$, where $Ka_{\Delta} = (u'_{a\Delta}/s_L)^{3/2}(\delta_{th}/\Delta)^{1/2}$, and $D_{a\Delta} = \Delta s_L/(u'_{a\Delta} \delta_{th})$. It has been established in past studies that the above parameters and their values for Eq. (5.5) are closely connected to certain physical aspects of the scalar dissipation rate transport and elaborate detail can be found in [45, 56, 98]. The term $\epsilon_{SGS}^{\mu^2}/\beta_c$ comes from influences of flame front curvature induced by turbulence and spatial variations in thermo-chemical processes. Thus, $\beta_c$ is a scale dependent parameter.

In order to calculate $\tilde{\varepsilon}_c$ using Eq. (5.5) in LES, one needs to prescribe $u'_{a\Delta}$ and $\beta_c$. For this study, the velocity scale is obtained directly from the DNS data, to be described in the next section, while it may be modeled as in [108–110] for LES. A dynamic procedure for $\beta_c$ was developed in past studies using scale similarity [57, 108]. Following the procedure described in [106], the filtered SDR can be written as

$$\overline{p \tilde{N}_c} = \overline{p \tilde{D} (\nabla c \cdot \nabla c)} + \overline{p \tilde{\varepsilon}_c} = \psi_1 + \frac{\psi_2}{\beta_c},$$  \hspace{1cm} (5.6)

where $\psi_2$ is defined by equating $\psi_2/\beta_c$ to Eq. (5.5). By applying a test filter to the above equation one gets

$$\overline{p \tilde{N}_c} = \psi_1 + \psi_2/\beta_c,$$  \hspace{1cm} (5.7)

and

$$\tilde{\overline{p \tilde{N}_c}} = \tilde{p} \tilde{D} \left( \nabla \tilde{c} \cdot \nabla \tilde{c} \right) + \psi_2/\beta_c.$$  \hspace{1cm} (5.8)

The notation $\tilde{\psi}_2$ implies that $\psi_2$ must be evaluated using the test filtered quantities. The scale similarity concept suggests that $\tilde{\overline{p \tilde{N}_c}} \approx \tilde{p} \tilde{\tilde{N}_c}$ and hence, by using Eqs. (5.7) and (5.8) one gets

$$\beta_c = \frac{\tilde{\psi}_2}{\psi_1 + \psi_2/\beta_c - \tilde{p} \tilde{D} \left( \nabla \tilde{c} \cdot \nabla \tilde{c} \right)}.$$  \hspace{1cm} (5.9)
The dynamic procedure tested in [57, 108] assumed that $\beta_c$ did not change during test filtering operation, which is relaxed in the above description [106]. However, if one retains that assumption then the above procedure gives

$$\beta^*_c = \frac{\psi_2 - \psi_5}{\psi_1 - \bar{p} \nabla \cdot (\nabla \hat{c} \cdot \nabla \hat{c})}.$$  \hspace{1cm} (5.10)

Equation (5.9) can be solved iteratively to obtain $\beta_c$ if other quantities in this equation are known and these are readily available in LES. For this study, they are extracted from the DNS data described next.

### 5.3 DNS data

Yenerdag et al. [200, 201] directly simulated isochoric turbulent combustion of stoichiometric hydrogen-air mixture inside a vessel. The size of this vessel (computational domain) is $L_x \times L_y \times L_z = 20 \times 5 \times 20 \text{ mm}^3$ and is discretised using $N_x \times N_y \times N_z = 1025 \times 257 \times 1025$ grid points ensuring that enough points are in the Kolmogorov lengthscale, $\eta$, and the flame thickness. This rectangular box is a simple idealized model of an IC engine combustion chamber when the piston is at the TDC. Although this combustion volume is smaller than that in a practical engine, the present configuration is chosen to keep the DNS computationally affordable allowing one to investigate the effects of time-varying reactant mixture temperature and pressure on flame propagation and its interaction with turbulence. The vessel’s walls are specified to have a temperature of $T_w = 450 \text{ K}$ and the initial pressure in the vessel is set to be 0.1 MPa.

The flame is initiated using a spherical ignition kernel placed at the centre of the computational domain and has an initial temperature, $T_{ini}$, distribution given by

$$T_{ini} = T_u + (T_p - T_u) \exp \left( -\frac{r^2}{2R^2} \right),$$  \hspace{1cm} (5.11)

where $T_u = 700 \text{ K}$ is the preheated reactant initial temperature, $T_p = 2000 \text{ K}$ is the assumed peak temperature near the ignition location, after the plasma energy is converted into thermal energy, $r$ is the radial distance from the centre of the ignition kernel, $R = r_c / 3$ is the radial position at which the temperature gradient is maximum and $r_c = 0.5 \text{ mm}$ is the radius of the ignition kernel. The flame initiated thus propagates in fully developed homogeneous isotropic turbulence specified initially inside the domain. This turbulence field, precomputed in a separate simulation, has the following characteristics. The turbulent Reynolds number
is $Re_t = u'\ell/\nu = 516$ and $Re_\lambda = 97.1$, where $u'$ is the root-mean-square of the turbulent velocity fluctuations, $\ell$ is the integral length scale, $\lambda$ is the Taylor micro-scale, and $\nu$ is the kinematic viscosity. This yields $u'/s_L = 1.8$ and $\ell/\delta_F = 281$, where $\delta_F$ is the Zeldovich thickness, at the initial time. Hence, the condition of this isochoric combustion is in the corrugated flamelets regime of the turbulent combustion diagram [143] and this regime of combustion is representative for spark-ignited IC engines [137]. The combustion kinetics is modelled using a detailed kinetic mechanism with 12 species and 27 reactions [72]. Further detail on the numerical simulation such as conservation equations, numerical scheme, etc., can be found in [200, 201].

Fig. 5.1 Visualisation of flame and flow features at $\hat{t} = 0.73$ (left) and 0.91 (right), where $\hat{t}$ is time normalised using the turbulence integral eddy turnover time. Blue isosurfaces represent $Q = \langle Q \rangle + 3\sigma_Q$ and red iso-surface is for 60\% of the maximum $\hat{\omega}_c$.

Typical flame surface and turbulence characteristics extracted at two different times, normalised using the initial eddy turnover time $t_{ed} = \ell/u'$, are shown in Fig. 5.1. The flame surface is marked using a reaction rate, $\hat{\omega}_c$, of 60\% of the maximum value at a given instant. The turbulence structure is visualised using $Q = \left(\Omega_{ij}\Omega_{ij} - S_{ij}S_{ij}\right)/2$, where $\Omega_{ij}$ and $S_{ij}$ are the anti-symmetric and symmetric part of the strain tensor $\partial u_i/\partial x_j$. The fluid velocity in the direction $i$ is denoted using $u_i$. The iso-surfaces of $Q$ shown in the figure are for $\langle Q \rangle + 3\sigma_Q$, where $\langle Q \rangle$ is the volume averaged value of $Q$ and $\sigma_Q$ is its standard deviation. The turbulent structures are seen typically outside the flame because of the effects of heat release rate and pressure variation across the flame front. Also, these structures are not seen in the burnt
mixture because of increase in the viscosity due to high temperature. The flame surface wrinkling are produced by the fine scale turbulence structures as noted in [200]. The flame propagation with time is obvious in Fig. 5.1 and it has not interacted with the walls yet.

Fig. 5.2 Temporal variation of mean pressure (○) and reactant temperature (□) inside the vessel is shown on the left. The picture on the right compares the \( P_u - T_u \) map from the DNS (symbols) to that of isentropic theoretical curve (line).

Figure 5.2 shows the temporal variation of mean pressure and reactant temperature inside the vessel. The DNS is conducted for about 1.5 eddy turnover time by which time the entire charge in the vessel is consumed by the turbulent combustion. The 1.5 eddy turnover time corresponds to about 24 laminar flame time and thus the turbulence-chemistry interaction has evolved sufficiently for model testing. The pressure, \( P_u \), shown in the figure is averaged over the entire volume but the temperature is conditionally averaged for \( c \leq 0.05 \) to include only the unburnt mixture. The reactant temperature decreases initially by about 30 to 40 K and increases after \( \hat{t} \approx 0.4 \). The mean pressure also shows a similar tendency as one would expect for isochoric combustion. This is because the heat release rate is relatively smaller than the heat loss through the walls in the initial stages. The increase in \( P_u \) is because of the compression caused by the expanding hot gases which is ideally an isentropic process, but the heat loss through the walls makes it to be non-isentropic. A comparison of \( P_u - T_u \) map with the theoretical curve is also shown in Fig. 5.2. The approximation of isentropic compression is quite good at the very early stages. The irreversible chemical changes and viscous heating causes \( \partial P_u / \partial T_u \) to be larger for the DNS compared to the theoretical value. The irreversibilities increase with temperature which leads to progressively, in time, increased deviation from the idealised behaviour. Also, the increase in \( T_u \) for a given increase in pressure is smaller for the DNS because of heat loss through the walls. This heat flux predominantly coming from the burnt mixture was shown to increase with \( \hat{t} \) in the earlier
study [201] and thus the $P_u-T_u$ curve from the DNS deviates progressively, with deviations increasing with time, from the theoretical curve as seen in Fig. 5.2.

To summarise, the DNS data captures the thermo-chemical processes and their interaction with turbulence which are expected inside an IC engine although the pressure rise is not as high as in a practical engine. This is because of smaller total energy released in the DNS compared to that in an engine. Since the fundamental processes are captured in the DNS, one can use it to investigate SGS combustion process and its interaction with turbulence. Hence, this data is post-processed using the steps described next to extract SGS information relevant for the modeling discussed in the previous section.

### 5.4 Data processing

Since the interest is on the SGS combustion processes and their modeling, the DNS data is filtered explicitly using a Gaussian filter to extract various quantities of interest and density weighted filtering is used here. This filtering is performed within a region of size $2\Delta \times 2\Delta \times 2\Delta$ centred at a filtering point, $\mathbf{x}$. A filtered quantity of interest, $F$, is then computed as

$$
\tilde{F}(\mathbf{x}, t) = \frac{1}{\overline{\rho}(\mathbf{x}, t)} \int_{\mathbf{x} - \Delta}^{\mathbf{x} + \Delta} \rho(\mathbf{x}', t) F(\mathbf{x}', t) \mathcal{G}(\mathbf{x} - \mathbf{x}'; \Delta) \, d\mathbf{x}'
$$

(5.12)

where $\rho$ and $\overline{\rho}$ are respectively the unfiltered and filtered density and $\mathbf{x}'$ is the sampling point in the filter sub-space. The Gaussian filter kernel, $\mathcal{G}$, is [155]

$$
\mathcal{G}(\mathbf{x} - \mathbf{x}') = \left( \frac{6}{\pi \Delta^2} \right)^{3/2} \exp \left( -\frac{6(\mathbf{x} - \mathbf{x}')^2}{\Delta^2} \right).
$$

(5.13)

The SGS Favre variance of $F$ is obtained using

$$
\sigma_{F,\text{sgs}}^2(\mathbf{x}, t) = \tilde{F}^2 - \overline{\tilde{F}}^2.
$$

(5.14)

The test filtered quantities required for Eqs. (5.9) and (5.10) are obtained following the above procedure but with a filter of size $\Delta = 2\Delta$.

### 5.5 Results and discussion

Figure 5.3 shows typical reaction rate, $\dot{\omega}_c$, contours extracted from the DNS data at $\hat{t} = 0.73$ for three different values of the filter width, $\Delta^+ = \Delta/\delta_{th} = 0.5, 1$ and 2. The reaction rates are normalised using $\rho_u, s_L$ and $\delta_{th}$ for the reactant mixture with $T_u$ and $P_u$ observed in the
DNS at $\hat{t} = 0.73$ and the contours are shown for the middle $x$-$z$ plane of the computational domain. The filtering operation does not alter the relatively larger wrinkling of the flame but the smaller wrinkling is smeared when large filter width is used and this is an expected behaviour. The peak reaction rate is observed to decrease with increase in the filter width. This is because the filtered flame thickness increases with $\Delta^+$ and thus the peak reaction rate must drop to conserve the overall reaction rate. Similar behaviour is observed for another time, $\hat{t} = 0.91$, as it can be seen in Figure 5.3. However, the peak reaction rate increases with time because of the increase in $T_u$ and $P_u$ (see Fig. 5.2). The contours on the right column are for the filtered reaction rate obtained using Eq. (5.3). This flamelet model seems to capture the spatial variations of the filtered reaction rate and also the flame wrinkles observed in the DNS. The trend of drop in the peak reaction rate with $\Delta^+$ is also observed for the modelled value as for the DNS results and the comparison shown in Fig. 5.3 is quite good in general. However, if one makes a closer comparison of the modelled reaction rate to those extracted from the DNS then some over predictions can be seen, which is discussed further below.

The contours shown in this figure suggest that $\Delta^+ \leq 0.5$ may be required for isochoric (IC engine) combustion modelling using unstrained flamelets. If this condition is applied for the largest $P_u$ and $T_u$ expected during the combustion process then it is satisfied automatically for earlier times. Further quantitative evaluation of this combustion model is discussed below.

### 5.5.1 SGS reaction rate closure

The reaction rate closure given in Eq. (5.3) uses unstrained laminar flames to build a look-up table which has $\bar{c}$ and $\bar{c}_{_{\text{SGS}}}^{n2}$ as two controlling variable for a given thermo-chemical condition ($T_u$ and $P_u$). Since the range of these two controlling variables are known the look-up table can be constructed a priori. The top row of Fig. 5.5 shows the variations of this modelled reaction rate for two instances, $\hat{t} = 0.73$ and 0.91 along with the corresponding filtered reaction rate extracted from the DNS data in the bottom row. The reaction rates are normalised using $\rho_u = 0.505$ kg/m$^3$, $s_L = 11.71$ m/s and $\delta_{th} = 3.49 \times 10^{-4}$ m for $\hat{t} = 0.73$, and $\rho_u = 0.713$ kg/m$^3$, $s_L = 14.36$ m/s and $\delta_{th} = 2.13 \times 10^{-4}$ m for $\hat{t} = 0.91$. Since $T_u$ and $P_u$ are increasing with time the reactant density, burning velocity increases while the laminar flame thermal thickness decreases. This is the reason why the normalised reaction rates at $\hat{t} = 0.91$ is seen to be smaller than those at an earlier time. Indeed, the dimensional values are larger for the later time.

The modelled normalised reaction rate, $\overline{\omega}_{\text{Model}}$, has its maximum value for $\bar{c}_{_{\text{SGS}}}^{n2} = 0$ which corresponds to quasi-steady and quasi-laminar flames. As the SGS variance increases the reaction rate drops for a given $\bar{c}$ value because the burning mode part of the SGS pdf, $\bar{p}(0.1 \leq \zeta \leq 0.9)$, decreases. Physically, this implies that the flame fronts are thin and thus
Fig. 5.3 Contours of filtered reaction rate from the DNS (left column) for $\Delta^+ = 0.5, 1$ and 2 (from top to bottom) at $\tilde{t} = 0.73$ and the corresponding modelled reaction rate (right). The reaction is normalised using $\rho_u, s_L$ and $\delta_h$. 
Fig. 5.4 Contours of filtered reaction rate from the DNS (left column) for $\Delta^+=0.5$, 1 and 2 (from top to bottom) at $\tilde{t}=0.91$ and the corresponding modelled reaction rate (right). The reaction is normalised using $\rho_u$, $s_L$ and $\delta_{th}$. 
the SGS pdf is bimodal. The peak value seen around $\bar{c} = 0.5$ for a given value of SGS variance is because the reactant mixture is stoichiometric hydrogen-air. A similar behaviour is seen for the DNS results also and these results are constructed by collecting the reaction rate from every point within the flame (identified by using the instantaneous reaction rate to be larger than 5% of its maximum value) and then conditionally averaging these samples. The maximum value of $c_{\text{sgs}}''$ for a given $\bar{c}$ is limited by $\bar{c}(1 - \bar{c})$ when the flame front is very thin. The value observed in the DNS is well below 0.25 clearly suggesting that the bimodal limit (thin flame front) is not observed for the conditions of the DNS, despite the initial turbulence characteristics seem to suggest corrugated flamelets regime combustion. This difference is because of the effects of heat release on the local turbulence which has been recognised in many past studies on constant pressure combustion, for example see [150, 178]. The DNS results also show that there is a lower limit for $c_{\text{sgs}}''$ for a given value of $\bar{c}$. The absence of very low $c_{\text{sgs}}''$ values implies that there are no (in a statistical sense) quasi-steady
and quasi-laminar flames in the DNS. A comparison of the results in Fig. 5.5 shows that the general variation of the filtered reaction rate with $\tilde{c}$ and $\epsilon_{\text{sgs}}^2$ is captured quite well by the unstrained flamelet model.

![Fig. 5.6 Joint pdf, $P$, of normalised DNS and modelled filtered reaction rate for $\hat{t} = 0.73$ (left) and 0.91 (right). The results are shown for $\Delta^+ = 0.5$. The colour scale is for log($P$).](image)

Figure 5.6 shows the contours of joint pdf, $P$, of modelled and DNS values of reaction rates normalised using $\rho_u$, $s_L$ and $\delta_h$. The contours are shown for $\Delta^+ = 0.5$. If there is perfect match between the modelled and DNS values of the filtered reaction rate at every point inside the flame then all the data points, thus $P$, would lie along the diagonal line. The joint pdf is shown here rather than the scatter plot of $\tilde{\omega}_{\text{Model}}^+$ vs $\tilde{\omega}_{\text{DNS}}^+$ so that the model performance can be evaluated in a statistical sense. The joint pdf contours are observed to align along the diagonal line and the peak of the pdf is close to the origin. It is also worth to note that log($P$) is shown and thus there is four orders of magnitude difference between the brighter and darker regions. The values of log($P$) having large values of $\tilde{\omega}_{\text{Model}}^+$ are smaller than 1 while the peak value is seen to be larger than 5. Thus, there is a long tail for the larger value of $\tilde{\omega}_{\text{Model}}^+$, which is not statistically important. Hence, one can conclude that the unstrained flamelet model works quite well for stoichiometric hydrogen-air premixed combustion at constant volume and the results discussed above offer good support for this. However, the SGS variance of the reaction progress variable needs to be obtained from its transport equation, Eq. (5.4), in the LES for the reaction rate modelling and thus, one must use closures for $c\tilde{\omega}_c$ and the SGS SDR $\bar{\epsilon}_c$. The former term can be modelled in a manner
similar to the unstrained flamelet closure in Eq. (5.3) and the later quantity can be modelled using Eq. (5.5), which is evaluated in the discussion below.

### 5.5.2 Evaluation of $\tilde{\varepsilon}_c$ closure

Figure 5.7 compares the SGS SDR computed directly from the DNS data and its modelled value obtained using Eq. (5.5) for two different times. The values are normalised using the respective $s_L$ and $\delta$. The model parameter $\beta_c$ is chosen specifically to get a good correspondence with the DNS data and its value changes with time, 0.6 for $\tilde{t} = 0.73$ and 0.3 for 0.91. This is because, the objective here is to evaluate this model expression by feeding the required quantities, except $\beta_c$, obtained directly from the DNS. If the model performs well then all the data points must lie along the diagonal line. The results in the figures suggest that the model captures the DNS values quite well for both times and there is some scatter which is typical of turbulent flows involving some inherent randomness. Most of the data points are close to the diagonal line, which is confirmed by constructing the joint pdf of modelled and DNS values. This joint pdf is not shown here for brevity. One needs to specify $\beta_c$ to use this $\tilde{\varepsilon}_c$ model in LES and it can be evaluated using the dynamic procedures given by Eqs. (5.9) and (5.10). Before discussing these results, let us understand why $\beta_c$ value varies with time.

![Fig. 5.7 Comparison of DNS and modelled SGS scalar dissipation rate at $\tilde{t} = 0.73$ (left) and 0.91 (right) for $\Delta^+ = 0.5$. The modelled value is obtained using Eq. (5.5) with $\beta_c = 0.6$ and 0.3 respectively for $\tilde{t} = 0.73$ and 0.91.](image)
The parameter $\beta_c$ in Eq. (5.5) is related to the behaviour of $(T_4 - D_2)$ [31, 58] which involve $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$. The symbols $T_4$ and $D_2$ are defined as

$$T_4 = 2 \partial (\nabla c \cdot \nabla \dot{\omega}_c) \quad \text{and} \quad D_2 = 2 \rho \partial^2 (\nabla \nabla c : \nabla \nabla c). \quad (5.15)$$

Thus, one sees that $\beta_c$ behaviour is strongly related to $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$, which are scale dependant quantities and also the changes in $T$ and $P$ with time in isochoric combustion influence these gradients strongly. There is about 136 percent increase in the peak value of $\dot{\omega}_c$ at $\hat{t} = 0.91$ compared to that at $\hat{t} = 0.73$. This is because the temperature and pressure inside the domain increase as the flame propagates. It is well known that increasing $T$ and $P$ result in thinner flame and higher reaction rate as noted earlier in section 5.5.1. This consequently results in increase of $\nabla \dot{\omega}$, $\nabla c$ and $\nabla^2 c$. Thus, one expects that $\beta_c$ will change with time and this change is in addition to the spatial variation at a given time and these changes can only be captured using dynamic procedures in LES. These procedures have been developed in past studies and are briefly reviewed in section 5.2. Two dynamic methods for evaluating this model parameter are given by Eqs. (5.9) and (5.10). The various, including the test filtered, quantities involved in those two equations are obtained directly from the DNS data. The PDFs of this model parameter obtained using the dynamic approaches are shown in Fig. 5.8 for both the equations. These results are shown for two different times using the samples collected from locations having $\dot{\omega}_c \geq 0.05 \langle \dot{\omega}_c \rangle_{\text{max}}$, where the angle brackets denote time averaging. This condition allows to pick regions with considerable reaction since the dynamic procedures in Eqs. (5.9) and (5.10) do not make sense outside the flame.

When the model parameter is assumed to be constant for the test filtering then the range of $\beta^*_c$ obtained using Eq. (5.10) is considerably shorter than for $\beta_c$ from Eq. (5.9) as shown in Fig. 5.8 for $\hat{t} = 0.73$. The most probable values of $\beta^*_c$ and $\beta_c$ are respectively 0.63 and
0.88. The constant value used for the results in Fig. 5.7 for this time is very close to the most probable value of $\beta^*_c$. When the reaction is stronger (flame is thinner) then the difference between $\beta_c$ and $\beta^*_c$ is negligible as seen in Fig. 5.8 for $\hat{\tau} = 0.91$ and the most probable value is about 0.31 which is almost the same as that used for the corresponding time in Fig. 5.7. Since the reaction rates are larger at this time the SDR will be larger and thus one gets smaller $\beta_c$ values compared to those for $\hat{\tau} = 0.73$. Thus, it is quite clear that if this model parameter, irrespective of $\beta_c$ or $\beta^*_c$, is chosen carefully then the $\tilde{\epsilon}_c$ model in Eq. (5.5) works well.

The performance of this model with its parameter obtained using Eqs. (5.9) and (5.10) are evaluated in a statistical sense by calculating the joint pdf of the modelled and DNS values of the sub-grid scale SDR. This joint pdf is shown in Fig. 5.9 for both $\beta_c$ and $\beta^*_c$ evaluations at two different times. The model with $\beta^*_c$ works well and for the earlier time whereas the SDR model with either $\beta^*_c$ or $\beta_c$ works equally well for later time. There is some over prediction of the SDR, however the pdf values for these over predictions are small.
and thus it can be neglected. It is clear that the SDR model in Eq. (5.5) with the dynamic procedure in Eq. (5.10) works well and can be used in LES of engine simulations, which will be explored in a future study.

5.6 Summary

DNS data of stoichiometric hydrogen-air turbulent premixed flame propagating inside a constant volume chamber has been analysed to shed physical insight on the effects of pressure and temperature rising conditions on flamelets based combustion closure for sub-grid scale reaction rate. The computational domain for the DNS is representative of the combustion chamber in an IC engine when its piston is at the top dead centre. The reaction rate closure using FlaRe (Flamelets Revised for physical consistencies) approach is investigated. This approach is based on the unstrained flamelets and gives appropriate emphasis on the SGS variance of reaction progress variable, various physical processes influencing the evolution of this variance and their modelling. Two specific terms, the reaction rate and the SGS scalar dissipation rate, are investigated in detail using the DNS data. Since the temperature and pressure increase with time in constant volume combustion process, the reactions become stronger with time leading to larger dissipation rates and thus the scalar dissipation rate model parameter must be evaluated dynamically. Two variants of a dynamic procedure studies in the past are investigated. It has been shown that the unstrained flamelet closure for the reaction rate and the SDR model in Eq. (5.5), along with the dynamic procedure in Eq. (5.10), work quite well for constant volume combustion of stoichiometric hydrogen-air mixture. Although this modelling approach using URANS paradigm has been explored in the chapter 4, its application in LES framework for engine flow simulations will be explored in future.
Chapter 6

Swirling combustion inside a closed vessel

6.1 Introduction

The choice between URANS and LES for IC engine simulations depends on the objective of the investigation. LES is suitable to study cycle-to-cycle variations while URANS is adequate to capture the statistics such as cycle averaged pressure rise with crank angle, temperature and heat release rate variations, etc. The ability of LES to investigate cycle-to-cycle variation is because the dynamic large structures, which depend on the flow configuration, are tracked and thus their temporal and spatial variations are captured quite well in LES. The URANS simulations discussed in Chapter 4 identified that the results are sensitive to the choice of the value for the FlaRe model parameter $\beta_c$, see Eq. (2.57). Its dynamic evaluation using DNS data was explored in Chapter 5 and thus the next step is to investigate in-cylinder combusting flows using LES with dynamic evaluation of the parameter $\beta_c$. This task is not quite straightforward in a commercial code such as STAR-CD because the access to source code is unavailable to implement the dynamic procedures and the test filtering required to evaluate other quantities needed for this. As an attempt towards this goal of conducting LES of IC engine flows and also as a first step, LES of a swirling premixed flame under pressure rising condition is investigated in this chapter. It is hoped that this attempt will assist to identify the ups and downs of the FlaRe-LES approach and its implementation in a complex code such as STAR-CD.

This chapter is organised as follows. The experiments of swirling premixed flame under pressure rising conditions are discussed briefly in section 6.2 and its numerical modelling is
presented in section 6.3 along with various computational detail. The results are discussed in section 6.4 and conclusions are summarised in the last section.

6.2 Experimental test case

Hamomoto et al. [74] investigated the evolution of stoichiometric propane-air premixed flame in a swirling turbulent flow established inside a closed vessel. This experimental setup is shown schematically in Fig. 6.1. The combustion chamber was a short cylindrical vessel with optical access and the premixed mixture enters the vessel tangentially creating a swirling flow, with azimuthal velocity of $U_2$, as depicted in the figure. The radial velocity inside the combustion chamber was $U_1$. The coordinate directions, $x$ and $y$, are also marked and $z$ direction is along the length of the cylindrical chamber of diameter 125 mm and a height of 35 mm. The chamber was initially at a pressure of 50 kPa and this pressure increased to about 300 kPa as the chamber was filled with the stoichiometric mixture. Another case in which the chamber pressure rose to 400 kPa was also investigated but the case of 300 kPa is considered for this work. This pressure was before ignition at the chamber centre and the mixture temperature was at about the room temperature.

![Schematic diagram of the experimental setup](image)

Fig. 6.1 Schematic of the experimental test case with the representative computational domain used for the simulations. A schlieren picture is also shown.

Hamomoto et al. [74] conducted the experiments by spark igniting the mixture at different times after the chamber-filling valve was closed. This delay time (between the sparking and valve closure) was used to subject the initial kernel and thus the subsequent flame to different turbulence intensities and flow fields. The swirling motion inside the chamber decayed with time because of viscous effects and thus the turbulent intensity decreased with time. This was used to create different flow fields when the mixture was ignited. Using the radial
distribution of the mean tangential velocity at about the sparking time, an angular velocity, \( \Omega \), was calculated. The case of \( \Omega = 139.1 \text{ rad/s} \) corresponding to \( t_v = 10 \text{ ms} \), which is the time between the valve closure and spark ignition, is considered for this work.

High-speed schlieren photography and an ion-current probe were used to investigate the flame propagation. The flow velocities (in the non-reacting case) were measured using a 2D laser Doppler anemometer. The chamber pressure rise due to combustion was measured using a pressure transducer as marked in Fig. 6.1. A typical schlieren picture taken at about 11 ms after the spark ignition is also shown in the figure.

### 6.3 Numerical setup

The detail of numerical setup used for simulations of the experiment is described in this section. These simulations are performed using STAR-CD v4.18, which is a multidimensional commercial CFD code. The LES approach is used in this work and the necessary Favre-filtered conservation equations for mass, momentum, total enthalpy, progress variable and its sub-grid variance are discussed in section 2.2.2.

Fig. 6.2 Numerical domain considered for the simulations. The red sphere represents the sparking region.

#### 6.3.1 Computational details

The numerical domain consist of a simple cylindrical volume corresponding to the combustion chamber used in the experiment. This domain is shown schematically in Fig. 6.2 and this volume is discretised using about 750,000 block-structured cells. Although the domain and the expected mean flame propagation are axisymmetric, one needs to keep the three
dimensionality for LES and so the whole chamber volume is retained in the CFD model. This grid gives a filter width, normalised by the laminar flame thermal thickness, of about 1.5 which is quite good for turbulent premixed flame calculations. The filter width is calculated as the cube root of the smallest cell volume in the computational domain. The edges of the domain are specified to be no slip walls at $T_{\text{wall}} = 450$ K and the fluxes of $\bar{c}$ and $c'^2$ in the wall normal directions are specified to be zero for these walls. A time step size of $10^{-6}$ is used for the simulations reported here.

The momentum equations as well as the other scalar equations are discretised with a second order monotone advection and reconstruction scheme (MARS) available in the CFD code. The PISO algorithm is used for the pressure velocity coupling. The unresolved sub-grid stresses are closed using the Smagorinsky model with a static SGS viscosity model having $C_S = 0.167$ (see section 2.2.2). The filtered density is calculated using the state equation and the temperature is obtained from the enthalpy equation carried in the simulation.

### 6.3.2 SGS combustion modelling

The combustion is a SGS phenomenon in LES and it is modelled using the FlaRe approach described in section 2.5.8 This model is based on the unstrained flamlet approach and it is implemented in STAR-CD for LES through user subroutines and scalars. Thus, the combustion models available in STAR-CD are de-activated during the simulations. The implementation for LES is similar to that described in section 4.2.1 for RANS except that the variance of the progress variable to be transported is the SGS variance and the reaction rate to be obtained from the lookup table is the filtered reaction rate. The temperature rise during combustion is achieved by including an appropriate source term for the heat release rate, $\dot{\omega}_T$.

The SGS dissipation rate required for the SGS variance equation, see Eqs. (5.5) and (5.4), (see chapter 5) needs some care for its LES implementation. The sub-grid velocity scale, $u'_\Delta$, required for Eq. (5.5) must be modelled and it is modelled using a simple model [155]:

$$u'_\Delta = C_p \sum |\bar{u}_i - \bar{u}|$$

by using the computed filtered velocities and their test filtered values. Although the test filtering task is mathematically simple, its implementation in a commercial CFD code such as STAR-CD is a daunting exercise since there is no access to the source code. Here, an adhoc approach by using cell connectivity table is followed. The cell information for each and its neighbouring cells is unavailable in STAR-CD, therefore a connectivity table is constructed at the start of each time step with each cell number and its neighbouring cell. This information then is used to construct the required test filtered quantity. Although this approach worked for the velocities, it did not work for the quantities required for the dynamic evaluation of the model parameter $\beta_c$ (see Eqs. (5.9) and (5.10). Hence, static values for this model parameter are used to investigate the results’ sensitivity.
The lookup tables containing filtered reaction rates and various other sources and sinks are constructed using the presumed pdf approach. This table has two control variables, the filtered progress variable and the SGS variance for the premixed combustion of interest here. The SGS variance can be normalised as \( g \equiv \hat{\epsilon}^2/(1 - \hat{c}) \). Since the reactant temperature, \( T_u \) and pressure, \( p_u \), varies in isochoric combustion systems, a number of stoichiometric propane-air flamelets are computed to cover the expected range of these two thermodynamic quantities. Figure 6.3 shows the typical variation of the filtered reaction rate in the table for two different pressures, 8 and 20 bars, of the stoichiometric propane-air mixture at a temperature of 400 K. Quasi-steady and quasi-laminar flames are denoted by \( g = 0 \), which will have a peak reaction rate around \( c = 0.75 \) as in the laminar premixed flames which can be seen in the figure. As \( g \) increases, the peak of the filtered reaction rate moves towards the middle of \( \hat{c} \) space. Since the reactivity increases with pressure, the filtered reaction rates are larger for the 20 bar case shown in the figure. The values of filtered reaction rate and other sources required for each numerical cell in the LES are retrieved for the lookup tables depending on the cell values of \( \hat{c} \) and \( g \). A bi-linear interpolation having an accuracy of about 1\% is used for the table lookup.

Fig. 6.3 Variation of filtered reaction rate for stoichiometric propane-air mixture at \( T = 400 \) K for (a) \( p = 8 \) bar and (b) 20 bar pressures.

### 6.3.3 Initialization

The initial temperature and pressure inside the combustion chamber are specified to be 325 K and 243 kPa as in the experiment. The mean velocity fields are initialised using the measured values while the velocity fluctuations are obtained from a separate cold flow DNS by specifying an initial turbulence spectrum. The DNS has zero mean velocity and its
fluctuating velocities matching the measured statistics such as turbulence intensity and the integral length scale are chosen to specify the velocity fluctuations required for LES. The characteristics of this computed turbulence field are integral length scale, $\Lambda$, is 0.19 cm, Taylor micro scale is 0.14 cm and $u'$ is 0.39 m/s. These values suggests that $u'/s_L \simeq 1$ and $\Lambda/\delta_L \simeq 3$ and thus the turbulent premixed combustion is expected to be in the border among the wrinkled flamelets, corrugated flamelets and quasi-laminar flames regimes initially and the conditions will move into the wrinkled flamelets regime since $u'$ decays and $\Lambda$ grows with time.

The filtered progress variable and the SGS variance are specified to be zero initially for the entire domain, except in the region of ignition. These two fields are generated by the combustion which is initiated using a kernel. Thus, the kernel definition and its treatment determines the initial spatial variation of $\bar{c}$ and $e''^2$.

6.3.4 Spark treatment

The spark treatment used here follows the earlier work [2] on URANS. Certain number of cells are selected for spark ignition. The dynamics of the spark plasma and its run-away are not treated here but the spark is specified to be a small spherical kernel of burnt gases having a temperature of $T_b$. The temperature varies smoothly from $T_b$ at the centre of the kernel (see Fig. 6.2) to $T_a$ in the rest of the domain. The corresponding variations of $\bar{c}$ and the SGS variance are specified. Out of the two energy levels, 2 and 5 mJ, investigated in the past study [2], the case of 2 mJ is chosen. It is worth to note that the spark energy used in the experiments was not reported and thus there could be some uncertainty here, but the previous URANS study [2] suggests that 2 mJ may be a reasonable value.

6.4 Results and discussions

The kernel initialised as above is allowed to evolve in space and time establishing a self propagating premixed flame interacting with the swirling flow. There are in total four, one non-reacting and three reacting, simulations are conducted and their results are discussed below.

6.4.1 Cold flow validation

The cold flow simulations are conducted to validate the grid and numerical methodology used for LES. In the FlaRe model, the grid requirement is determined using the cold flow results which is inline with the original LES philosophy, which suggests that the smallest resolved
scale corresponds to the beginning of the universal (or $\kappa^{-5/3}$, where $\kappa$ is the wavenumber) range. The grid required to resolve the flame is not an issue because the combustion is a SGS phenomenon and typically occurs in small scales which are well beyond the universal range. Thus, if one can capture the cold flow statistics quite well using a grid then that grid is adequate for reacting flow for LES using FlaRe approach and this is followed here.

Figure 6.4 shows contours, as a colour map, of the three velocity components computed in the LES. This result is shown for the mid $x$-$y$ plane inside the chamber (see Fig. 6.2) at about 10 ms. The transverse velocity is very small and its colour map depicted in Fig. 6.4c shows that the net transverse velocity is close to zero. Its instantaneous values are smaller than the radial component in Fig. 6.4a and are nearly an order of magnitude smaller than the azimuthal velocity in Fig. 6.4b. Also, the net (averaged over the plane) radial velocity is very small and the predominant motion is in the azimuthal direction. The variation of this velocity is more or less uniform inside the chamber and it is close to zero as one would expect for this kind of flows. The variations of these velocities with $z$, along the length of the combustion chamber, is observed to be small and thus it is not shown here.

A radial cut of the computed azimuthal velocity is shown in Fig. 6.5a for two different times, $t_1 = 10$ ms and $t_2 = 100$ ms, and this 1D cut is taken along $y = 0$. The experimental data are also shown for comparison and the computed results agree quite well with the measurements with some difference for $t_2$. The corresponding turbulence intensity (TI) comparison is shown in Fig. 6.5b. The experimental data is sparse in general but it shows the trend for $t_1$. The computational results agree well with the measurements except for $x \leq 20$ mm where some over prediction is observed. For $t_2$, the measurements suggests that TI increases up to $x \leq 15$ mm and then drops before increasing again at about $x = 35$ mm. This trend is captured quite well in the LES although there is some quantitative differences. However, the general agreement between the computational results and the measurements are quite good. So this grid is used for subsequent reacting flow calculations.

6.4.2 Reacting flow

The contours of velocity magnitude are shown in Fig. 6.6 for the mid $x$-$y$ and $x$-$z$ planes. The results are shown for two different times, 4.2 and 9 ms, after the spark was initiated. The effects of combustion is reflected on the velocity field showing a strong acceleration in the flame region. This thin region is approximately spherical at the earlier time shown. Also, the flame starts to interact with the top and bottom walls by about 4.2 ms (see the velocity contours shown in the $x$-$z$ plane for this time in Fig. 6.6). After this, the flame moves laterally along the wall with no reaction rate occurring on the wall as one shall see later while
Fig. 6.4 Contours of (a) radial, (b) azimuthal and (c) transverse velocities computed in the LES. The results are shown in the mid $x$-$y$ plane at about 10 ms.
6.4 Results and discussions

Fig. 6.5 (a) Radial variation of the azimuthal velocity in the mid $x$-$y$ plane at two different times and the corresponding variation of turbulence intensity is shown in (b).

discussing Fig. 6.9. The other quantities such as reaction rate, progress variable, etc., to be discussed later, also portray the picture described above.

A. Flame quantities

The iso-surface of filtered progress variable with a value of 0.7 is shown in Fig. 6.7 for two times, 4.2 and 9 ms, considered for the velocity magnitude contours in Fig. 6.6. The isosurface is coloured using the filtered reaction rate, $\dot{\omega}_c$, of the progress variable and these iso-surfaces looks similar to the schlieren picture shown in Fig. 6.1. It is quite clear that the reaction rate on this surface is not uniform and has a large variation as shown in the figure. A close study of this figure suggests that the peak reaction rates are occurring in regions which are concave to the unburnt mixture because of non-unity Lewis number, $Le > 1$, for the propane-air mixture. Also the variations of the reaction rate in $z$ direction on this surface seems to be non-negligible as one shall see later. The wrinkling of the surface is quite substantial at both times and it can be created by the turbulence as well as the thermo-diffusive effects since the propane-air mixture has Le larger than unity. It is quite likely that turbulence effects may be relatively small because the combustion is in the wrinkled flamelets regime for the experimental conditions as noted earlier.

Two-dimensional cuts of the filtered progress variable and reaction rate fields are shown in Figs. 6.8 and 6.9 respectively. These contours are shown for two different times in the mid $x$-$y$ and $x$-$z$ planes. The centre region has burnt products and the flame is propagating outwardly. These contours are consistent with the observations discussed earlier using the velocity contours and iso-surface of the reaction progress variable. The reaction rate contours plotted in Fig. 6.9 show that this quantity is more or less uniform along the azimuthal
direction but there is non-negligible variation of it along $z$. The asymmetry in the flame propagation is also seen clearly in the reaction rate contours.

The SGS dissipation rate is an important quantity in the FlaRe approach. In premixed flames, the scalar gradients are produced predominantly by the chemical reaction rate and thus the dissipation rate is expected to follow the variation of reaction rate. The contours of SGS scalar dissipation rate shown in Fig. 6.10 corresponds to the reaction rate depicted in Fig. 6.9. The variations of $\tilde{\varepsilon}_c$ mimics the reaction rate variations well, including the wrinkles. This behaviour is expected strongly for the wrinkled flamelets regime combustion and the modelling framework used in this study seems to capture this well. The reason for this is because the dissipation rate model used is built considering the fundamental aspects of turbulent premixed combustion.

The structure of the filtered flame is expected to be similar to the laminar flame. This is verified in Fig. 6.11 by cross plotting the filtered reaction rate with the filtered progress
Fig. 6.7 Iso-surface of $\tilde{c} = 0.7$ coloured with $\overline{\omega_k}$ (in kg/m³ s) at 4.2 (top) and 9 ms (bottom)
variable and also $\tilde{\epsilon}_c$ vs $\tilde{c}$. The results are shown for two different times. The scatter is the LES data points and lines are the corresponding conditional averages. The peak reaction rate is expected to be around $\tilde{c} = 0.8$, which seen for the LES results shown in the figure and this behaviour is as expected for the wrinkled flamelets regime combustion. All of the results discussed so far are obtained using $\beta_c = 6$. Hence, it is important to understand the sensitivity of the LES results to this model parameter. Ideally, this parameter should be evaluated dynamically as noted in Chapter 5 but the implementation of the dynamic procedure in a commercial CFD code is not possible because of the access to the source code is not available. So, alternative approach is to investigate the sensitivity of the LES results using various values of $\beta_c$.

**B. Sensitivity to parameter $\beta_c$**
The results discussed in section 4.3.6 showed that the cylinder peak pressure and thus the burn rate is sensitive to the $\beta_c$ value for the URANS. Based on those results, three values, $\beta_c = 6, 6.7$ and $7.5$, are chosen to test the sensitivity of LES results to this parameter. The results for $\beta_c = 6$ are discussed above. The flame propagation in time and space can be extracted from these results and these flame positions can be compared to the measured values. Hamamoto et al. [74] used ion probes to determine the position of the flame front by repeating the experiments with the ion probes fixed at several locations. Schlieren photographs were also used to visualise the flame propagation and it was noted by Hamamoto et al. that the two techniques agreed quite well with each other for flame locations. The Schlieren technique is based on the density gradient, which is typically high at the leading edge of the flame and thus a value of $\tilde{c} = 0.05$ is used to define flame position in the LES.

By appropriately averaging the spatial variation of $\tilde{c}$ at a given time, the flame location in $x$-$z$ space can be obtained. This is shown in Fig. 6.12 for three different values of $\beta_c$ along
with the experimental data. For $\beta_c = 6$, the agreement is quite good in the middle ($z = 0$) and the computational flame starts to deviate from the measured flame as one moves towards the top or bottom wall. This result suggests that the flame propagation is relatively faster in the computations compared to those in the experiments. As the $\beta_c$ value is increased the rate of flame propagation also increases and this observation is in agreement with the results discussed in section 4.3.6 for the URANS paradigm. The variation of chamber pressure with time depicted in Fig. 6.13 shows that the initial burn rate in the computation agrees quite well with the measurements in the initial stages and once the flame starts to interact with the top and bottom walls the burn rate in the computations are larger than in the experiments. This leads to quicker rise of the chamber pressure. For the other two values of $\beta_c$, the chamber pressure rises quickly suggesting faster burn rate. All of these are consistent with the flame propagation comparison shown in Fig. 6.12.
6.4 Results and discussions

Fig. 6.11 Variations of (a) filtered reaction rate and (b) SGS dissipation rate with $\tilde{c}$ at 4.2 and 9 ms. The scatter is from LES and the lines are the corresponding conditional averages.

Fig. 6.12 Comparison of measured (dashed line) and computed flame propagation for $\beta_c = 6.0$ (blue line), 6.7 (red), 7.5 (green).
6.5 Summary

Large eddy simulation is used to simulate turbulent premixed flame propagating in a swirling flow inside a closed vessel. The subgrid stress and fluxes are modelled using the standard practice available in STAR-CD CFD code and the SGS combustion is modelled using the flame model discussed in Chapter 2. The initial velocity fluctuations are obtained from a separate direct numerical simulation (DNS) and the statistics of these fluctuations are very close to those measured in the experiments when the flame was initiated. The plasma dynamics and its thermal run-away from the initial spark are not included but the flame is initiated using a kernel containing burnt gases. The cold flow statistics are used to select the numerical grid which is used for flame simulations. The cold flow statistics agree quite well with measurements and the flame simulations showed the right behaviour of the flame and flow inside the combustion chamber. However, the computed flame propagation agreed well with measurements in the initial stages (in terms of combustion chamber pressure rise), but the propagation is faster in calculations after the flame started to interact with the top and bottom walls of the chamber. The sensitivity of the results to $\beta_c$ parameter is also investigated and the results are quite similar to those reported in Chapter 4 for URANS.
Chapter 7

Cocluding remarks

7.1 Summery of findings

Flamelet based approach FlaRe model has been tested for IC engine conditions. In the first part of this work, freely propagating laminar premixed flames of stoichiometric mixtures of gasoline surrogate and iso-octane with air were computed in the view to understand their structures and burning velocities at conditions which are of interest for future IC engine combustion technologies such as PCCI and HCCI. These flames were computed using CHEMKIN-PRO software and the combustion kinetics were modelled using three different mechanism with varied level of detail and complexity. The reactant temperature and pressure of interest studied were $850 \leq T_u \leq 950$ K and 3 to 4 MPa. The burning velocities of these mixtures at temperature of $850 \leq T \leq 950$ was observed to decrease with pressure up to about 3 MPa and started to increase beyond this pressure. This contrasting behaviour was explained, which was related to the role of pressure dependent reaction involving OH and the influence of this radical on the fuel consumption rate. The results seem to suggest that the overall order of the combustion reaction is larger than two at pressures higher than 3 MPa.

Flare model was then applied in a spark ignited IC engine for five operating conditions, in RANS context. The predictive capabilities of the model were studied for a SI engine. The sensitivity of the model was assessed with respect to the chemical kinetics used for the flamelet library generation, for both a skeletal and a detailed iso-octane mechanisms. The results showed large discrepancies in the laminar flame speeds between the two kinetics – and also when compared to experimental data – which manifest themselves in significant differences in the pressure evolutions. Calculation of the un-burnt temperature was found to give differences of 5% when compared with measurements, while the temperature increment used for the tabulation of the library showed little sensitivity between 100 K, 50 K and 25 K. FlaRe model includes a parameter representing the effects of flame curvature on the burning
rate. Since the reactant temperature and pressure inside the cylinder are continually varying with time, the mutual influence of flame curvature and thermo-chemical activities may be stronger in IC engine, and thus the sensitivity of engine simulation results to this parameter was investigated for a range of engine speed and load conditions. The results indicated some sensitivity and so a careful calibration may be required for URANS calculation which can be avoided using dynamic evaluations for LES.

The DNS data of stoichiometric hydrogen-air turbulent premixed flame propagating inside a constant volume chamber were analysed to shed physical insights on the effects of pressure and temperature rising conditions on flamelets based combustion closure for subgrid scale reaction rate. Two specific terms, the reaction rate and the SGS scalar dissipation rate, were investigated in detail using the DNS data. Since the temperature and pressure increases with time in constant volume combustion process, the reactions become stronger with time leading to larger dissipation rates and thus the scalar dissipation rate model parameter must be evaluated dynamically. Two variants of a dynamic procedure studied in the past are investigated. It was observed that the unstrained flamelet closure for the reaction rate and the SDR model, along with the dynamic procedure, work quite well for constant volume combustion of stoichiometric hydrogen-air mixture. Although this modelling approach using URANS paradigm has been explored in the chapter 4, its application in LES framework for engine flow simulations were explored in chapter 6.

Intermittent combustion taking place inside a closed vessel was then explored in LES framework, for the unstrained FlaRe model. Experiments of [74] were used for validation. In these experiments turbulence was generated using swirling inflow of premixed fuel and air, where stoichio-meteric propane-air mixture was used. This setup is used as a test case for IC engine combustion and the simulations were conducted using STAR-CD. Different values of $\beta_c$ were explored, results observed, were quite similar to what was observed in chapter 4.

### 7.2 Future work

The work carried out in this study has identified the following areas for further investigations.

- Development of chemical mechanisms which are validated for pressures of 100 bar and beyond, and ultimately, the exploration and the need for experimental test cases for laminar flame speed, which represent IC engine conditions. These results show the importance of choosing a mechanism that can correctly predict the laminar flame characteristics of the mixture. None of the mechanisms used in this study has been validated for the high temperature and pressure conditions experienced inside the
cylinder. Thus it is imperative that one needs further measurements of laminar flame characteristics at un-burnt mixture temperature and pressure expected in future engines.

- The results presented in this chapter 4 indicate the importance of choosing a correct ignition model, since the subsequent flame propagation depends on the initial flame kernel growth. Although the simple ignition model used in chapter 4 gives reasonable pressure trace, it needs to be refined for improved treatment of the initial kernel growth and its interaction with local turbulence and thermochemical conditions. Other approaches to calculate $T_u$ would be to solve an additional transport equation for the un-burnt mixture enthalpy or to use the isentropic relation. Sensitivity of the results to these approaches could be explored in a future study. The results in chapter 4 indicated that the FlaRe modelling framework is promising for IC engine simulations. However, dynamic evaluation of $\beta_c$ is more appropriate for simulations of in-cylinder flow and combustion in modern environmentally friendly engines to investigate cycle-to-cycle variations and pollutants production using LES paradigm.

- The reaction rate closure using FlaRe approach investigated in chapter 5, could be analysed in DNS simulations with tumble and swirl in the domain, which could represent and ever more realistic IC-engine conditions. Additionally, higher hydrocarbon fuels such as n-heptane and propane could also be explored in future DNS simulations.

- LES calculations of the swirling combustion inside a closed vessel using LES, can be repeated in a future study using other more detailed mechanisms, to determine the effect of chemical mechanism. Also these calculations can be repeated using finer grid. Furthermore, testing this case with more values of $\beta_c$ could also bring more insight. Finally, the methodology could be extended to perform LES with dynamic $\beta_c$ for the closed vessel and ultimately for a real IC engine.
References


References


References


