Detailed Numerical Simulations of Turbulent Premixed Flames at Moderate and High Karlovitz Numbers

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Abstract

In generally accepted and applied flamelet combustion models, flame is mainly assumed distorted by large scale turbulent structures, whereas small scale turbulent effects are neglected. However, in a lot of industrial applications quite high turbulent intensities are often imposed, which induces turbulence scales at a range smaller than the flame thickness. Flame/turbulence interaction appears quite different at these small scales, which is why combustion model improvement to account for these phenomena is required.

In this thesis, direct numerical simulations (DNS) and large eddy simulations (LES) have been utilized for studies of lean premixed turbulent reactive flows at various turbulent intensities. DNS has been applied for small scale detailed studies of flame/turbulence interaction with theoretical turbulence to show flame structure and differential diffusion effects at high Karlovitz numbers. Hydrogen and methane flames have been considered, for which detailed chemistry has been used. Formation of pockets of unburned fuel/air mixture in burned gases as well as straining of flame segments into unburned gases until quenching from severe heat losses have been shown. Broadening of both preheat zone and reaction zone layers in the distributed reaction zone regime is also evidenced. The effect of differential diffusion for distributed flames was found significant also in this combustion regime.

LES was applied to a low swirl stabilized flame utilizing a flamelet combustion model approach. The simulations have shown high sensitivity of the prediction of turbulent flame fluctuations as well as ambient air entrainment rate into burned gases to inflow conditions. Overall the model showed good comparison with the temperature validation data in the thin reaction zone regime.
Acknowledgements

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At last I thank my parents Bernt-Ove and Karin for always encouraging and believing in me. I also thank my brothers Magnus and Tommy for giving me valuable love and joy.
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## Nomenclature

### Latin Characters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_L )</td>
<td>instantaneous turbulent flame front area ([m^2])</td>
</tr>
<tr>
<td>( A_M )</td>
<td>laminar flame area ([m^2])</td>
</tr>
<tr>
<td>( A_s )</td>
<td>Arrhenius constant [depending on reaction]</td>
</tr>
<tr>
<td>( C_p )</td>
<td>mixture averaged heat capacity at constant pressure ([J/(kg \cdot K)])</td>
</tr>
<tr>
<td>( C_{p,s} )</td>
<td>heat capacity of species ( s ) at constant pressure ([J/(kg \cdot K)])</td>
</tr>
<tr>
<td>( C_s )</td>
<td>Smagorinsky constant ([-])</td>
</tr>
<tr>
<td>( C_\mu )</td>
<td>turbulent viscosity constant in the RANS framework ([-])</td>
</tr>
<tr>
<td>( D )</td>
<td>diffusivity of mass ([m^2/s])</td>
</tr>
<tr>
<td>( D_s )</td>
<td>diffusion coefficient for species ( s ) ([m^2/s])</td>
</tr>
<tr>
<td>( D_0 )</td>
<td>mass diffusion constant ([kg/(m \cdot s)])</td>
</tr>
<tr>
<td>( E )</td>
<td>specific turbulent kinetic energy ([m^2/s^2])</td>
</tr>
<tr>
<td>( E_a )</td>
<td>activation energy ([J])</td>
</tr>
<tr>
<td>( G )</td>
<td>flame coordinate ([m])</td>
</tr>
<tr>
<td>( L_c )</td>
<td>characteristic length scale ([m])</td>
</tr>
<tr>
<td>( N_{sp} )</td>
<td>total number of species ([-])</td>
</tr>
<tr>
<td>( P )</td>
<td>thermodynamic pressure ([\text{Pa}])</td>
</tr>
<tr>
<td>( \dot{Q} )</td>
<td>radiative heat transfer rate ([J/(m^3 \cdot s)])</td>
</tr>
<tr>
<td>( \mathcal{R} )</td>
<td>universal gas constant ([J/(\text{mole} \cdot K)])</td>
</tr>
<tr>
<td>( S )</td>
<td>flame propagation speed ([m/s])</td>
</tr>
<tr>
<td>( S_{ij} )</td>
<td>symmetric rate of strain tensor ([m/s])</td>
</tr>
<tr>
<td>( S_l )</td>
<td>laminar flame speed ([m/s])</td>
</tr>
<tr>
<td>( S_T )</td>
<td>turbulent flame speed ([m/s])</td>
</tr>
<tr>
<td>( T )</td>
<td>temperature ([K])</td>
</tr>
<tr>
<td>( T_0 )</td>
<td>reference temperature ([T_0 = 298 , K])</td>
</tr>
<tr>
<td>( U_c )</td>
<td>characteristic velocity ([m/s])</td>
</tr>
<tr>
<td>( V_{s,j} )</td>
<td>diffusion velocity for species ( s ) in direction ( j ) ([m/s])</td>
</tr>
<tr>
<td>( W_i )</td>
<td>molar mass of species ( i ) ([kg/mole])</td>
</tr>
<tr>
<td>( Y_s )</td>
<td>mass fraction of species ( s ) ([-])</td>
</tr>
<tr>
<td>( Y_{s,0} )</td>
<td>mass fraction of species ( s ) in unburned gases at equilibrium ([-])</td>
</tr>
<tr>
<td>( Y_{s,b} )</td>
<td>mass fraction of species ( s ) in burned gases at equilibrium ([-])</td>
</tr>
<tr>
<td>( Y_{e,a} )</td>
<td>total mass fraction of element ( e ) ([-])</td>
</tr>
<tr>
<td>( Z )</td>
<td>mixture fraction ([-])</td>
</tr>
<tr>
<td>( a )</td>
<td>speed of sound in medium ([m/s])</td>
</tr>
<tr>
<td>( c )</td>
<td>reaction progress variable ([-])</td>
</tr>
<tr>
<td>( f_{s,j} )</td>
<td>specific volume force acting on species ( s ) in direction ( j ) ([N/kg])</td>
</tr>
<tr>
<td>( g_{i,j} )</td>
<td>velocity fluctuation correlation function for velocity fluctuation components ( i ) and ( j ) ([-])</td>
</tr>
<tr>
<td>( h )</td>
<td>enthalpy ([J/kg])</td>
</tr>
<tr>
<td>( h_{s,0} )</td>
<td>enthalpy of formation of species ( s ) ([J/kg])</td>
</tr>
<tr>
<td>( k )</td>
<td>wave number ([1/m])</td>
</tr>
<tr>
<td>( l )</td>
<td>integral length scale ([m])</td>
</tr>
<tr>
<td>( n_c )</td>
<td>sgs wrinkling factor model constant ([-])</td>
</tr>
<tr>
<td>( n_A )</td>
<td>Arrhenius exponent ([-])</td>
</tr>
</tbody>
</table>
\( \vec{n} \) flame normal vector [\text{-}]

\( p \) pressure [\text{Pa}]

\( p_h \) hydrodynamic pressure [\text{Pa}]

\( p' \) pressure correction [\text{Pa}]

\( q_i \) energy flux [\text{J/(m} \cdot \text{s)}]

\( r \) spatial distance [\text{m}]

\( t \) time [\text{s}]

\( u_i \) velocity component \( i \)

\( u'_i \) velocity fluctuation of velocity component \( i \) [\text{m/s}]

\( u_i \) integral scale velocity fluctuation [\text{m/s}]

\( u_{sgs} \) sgs velocity fluctuation [\text{m/s}]

\( x_i \) space coordinate in direction \( i \) [\text{m}]

**Greek Characters**

\( \Delta \) filter width [\text{m}]

\( \Delta t \) CFD time step [\text{s}]

\( \Delta x \) grid spacing [\text{m}]

\( \Xi \) flame wrinkling factor [\text{-}]

\( \Xi_{\lambda} \) sgs flame wrinkling factor [\text{-}]

\( \Omega_E \) external energy source term [\text{K/s}]

\( \alpha \) sgs wrinkling factor model constant [\text{-}]

\( \alpha_{\lambda} \) thermal diffusion coefficient [\text{m}^2/\text{s}]

\( \beta \) sgs wrinkling factor model constant [\text{m/s}]

\( \delta_{ij} \) Kronecker delta [1 if \( i = j \), else 0]

\( \delta_{ik} \) laminar flame thickness [\text{m}]

\( \varepsilon \) dissipation rate of turbulent kinetic energy per unit mass [\text{m}^2/\text{s}^3]

\( \eta \) Kolmogorov length scale [\text{m}]

\( \kappa_s \) mass diffusion coefficient for species \( s \) [\text{m}^2/\text{s}]

\( \rho_0 \) density of unburned fuel air mixture [\text{kg/m}^3]

\( \lambda \) thermal heat conductivity [\text{J/(s} \cdot \text{m} \cdot \text{K)}]

\( \lambda_\varepsilon \) eigenvalue [\text{varying}]

\( \lambda_T \) Taylor length scale [\text{m}]

\( \mu \) dynamic viscosity [\text{kg/(m} \cdot \text{s)}]

\( \mu_\Delta \) turbulent viscosity [\text{kg/(m} \cdot \text{s)}]

\( \nu \) kinematic viscosity [\text{m}^2/\text{s}]

\( \nu_T \) turbulent kinematic viscosity [\text{m}^2/\text{s}]

\( \rho \) density [\text{kg/m}^3]

\( \tau_c \) chemical time scale [\text{s}]

\( \tau_i \) integral time scale [\text{s}]

\( \tau_\eta \) Kolmogorov time scale [\text{s}]

\( \tau_{ij} \) viscous stress tensor [\text{kg/(m} \cdot \text{s}^2)]

\( \tau_{ij}^T \) LES viscous stress tensor [\text{kg/(m} \cdot \text{s}^2)]

\( \varphi \) local equivalence ratio [\text{-}]

\( \dot{\omega}_T \) heat release rate per unit volume [\text{J/(m}^3 \cdot \text{s)}]

\( \dot{\omega}_s \) reaction rate of species \( s \) per unit volume [\text{kg/(m}^3 \cdot \text{s)}]
Non-dimensional Numbers

\[ Le = \frac{\sigma_L}{\rho} \] Lewis number
\[ Le_s = \frac{\sigma_s}{\rho_s} \] Lewis number of species \( s \)
\[ Ka = \frac{\tau_e}{\tau_\eta} \] Karlovitz number
\[ Ma = \frac{u_e}{\tau_\eta} \] Mach number
\[ Re = \frac{\rho u_e l_c}{\mu} \] Reynolds number
\[ Re_T = \frac{u_e l_c}{v} \] turbulent Reynolds number

Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDR</td>
<td>convection diffusion reaction</td>
</tr>
<tr>
<td>CFD</td>
<td>computational fluid dynamics</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy</td>
</tr>
<tr>
<td>DFT</td>
<td>discrete Fourier transform</td>
</tr>
<tr>
<td>DMD</td>
<td>dynamic mode decomposition</td>
</tr>
<tr>
<td>DNS</td>
<td>direct numerical simulation</td>
</tr>
<tr>
<td>DVODE</td>
<td>variable-coefficient ordinary differential equation</td>
</tr>
<tr>
<td>HAB</td>
<td>height above burner</td>
</tr>
<tr>
<td>HOT</td>
<td>higher order terms</td>
</tr>
<tr>
<td>ILES</td>
<td>Implicit LES</td>
</tr>
<tr>
<td>JPDF</td>
<td>joint probability density function</td>
</tr>
<tr>
<td>LES</td>
<td>large eddy simulation</td>
</tr>
<tr>
<td>LIF</td>
<td>laser induced fluorescence</td>
</tr>
<tr>
<td>POD</td>
<td>proper orthogonal decomposition</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds averaged Navier-Stokes equations</td>
</tr>
<tr>
<td>RCARS</td>
<td>rotational coherent anti-Stokes Raman spectroscopy</td>
</tr>
<tr>
<td>PIV</td>
<td>particle image velocimetry</td>
</tr>
<tr>
<td>PLIF</td>
<td>planar LIF</td>
</tr>
<tr>
<td>SGS</td>
<td>sub-grid scale</td>
</tr>
<tr>
<td>TVD</td>
<td>total variation diminishing</td>
</tr>
<tr>
<td>WENO</td>
<td>weighted essentially non-oscillating</td>
</tr>
</tbody>
</table>

Chemical Compounds

<table>
<thead>
<tr>
<th>Compound</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>methane</td>
</tr>
<tr>
<td>CO</td>
<td>carbon monoxide</td>
</tr>
<tr>
<td>CO₂</td>
<td>carbon dioxide</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>propane</td>
</tr>
<tr>
<td>H</td>
<td>hydrogen atom</td>
</tr>
<tr>
<td>H₂</td>
<td>hydrogen</td>
</tr>
<tr>
<td>HO₂</td>
<td>hydrodioxide</td>
</tr>
<tr>
<td>H₂O</td>
<td>water</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>hydrogen peroxide</td>
</tr>
<tr>
<td>N₂</td>
<td>nitrogen</td>
</tr>
<tr>
<td>NO₅</td>
<td>nitrogen oxides</td>
</tr>
<tr>
<td>O₂</td>
<td>oxygen</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>-------------------------</td>
</tr>
<tr>
<td>OH</td>
<td>hydroxide</td>
</tr>
<tr>
<td>UHC</td>
<td>unburned hydrocarbons</td>
</tr>
</tbody>
</table>
Chapter 1
Introduction

Combustable fuels have for a long time been the primary source of the human energy supply and with increasing living standard and a growing population of the planet earth, the energy demand is rising. Combustion of fossil as well as renewable fuels will therefore be of high importance also in the future and to assure energy access at the same time as pollution limitations has to be met, a comprehensive research within the field of combustion needs to be conducted. The important combustion emissions are unburned hydrocarbons (UHC), nitrogen oxides (NO\textsubscript{x}), carbon monoxide (CO) and soot. UHC is lowering the efficiency of the combustion device as the fuel is not completely oxidized. UHC origin typically from quenched flame or from fuel hiding at inflammable locations in the combustor. NO\textsubscript{x} is a toxic gas primary formed at high flame temperatures, whereas on the contrary CO is a toxic gas formed at low flame temperatures. Soot is a collective term for larger (read >10 nm) carbon-rich particles formed in fuel rich, low temperature reactions. The desire is of course to minimize all these emissions simultaneously, but also to maintain high combustion efficiency. This is important both for economical reasons, but also since the combustion product CO\textsubscript{2} is a green house gas, the fuel consumption should be kept low. Combustion control is therefore of major importance to ensure the system to operate at suitable conditions in terms of flame temperature, fuel/oxidizer composition and flame/flow interaction.

Studies and development of combustion systems have for centuries been performed through experimental investigations where parameters have been tuned until desired features have been obtained. It was not until the invention of computers that computational fluid dynamics (CFD) became a scientific tool for studies of flow and combustion properties. As computational power has become greater and cheaper, CFD has become applicable to industrial applications involving combustion where trends of e.g. geometry or fuel composition changes can be determined without experiments. Especially in regards to the former, great economical benefits can be found. Instead of constructing several test vessels, CFD can determine the trends at a much lower cost.

When CFD methods are utilized in industrial applications, usually through Reynolds averaged Navier-Stokes (RANS) approach or large eddy simulations (LES), modeling difficulties to account for interaction of turbulent eddies at scales much smaller than the laminar flame thickness arise. Due to complex flame/flow interaction at these scales [1] several phenomena, which are not well known, arise, e.g. fuel diffusion characteristics can cause differences along the flame due to turbulence induced curvature, turbulence caused flame strain will alter both structure and propagation speed of the flame and at high straining, local flame extinction as well as reignition can occur [1]. These effects should ideally be accounted for in the flame model. With acceptable accuracy the flames are often assumed undisturbed at these scales through utilization of so called flamelet models. This is not solely due to desired computational speed up, but also since well verified combustion models for the thin-reaction zone and distributed reaction zone combustion regimes are lacking to this date. Flamelet models assume flame to be representative by a single connected iso-surface which is transported through convection and self-propagation. Modifications of these models can be made to account for e.g. local extinction to some extent; however, since the basic assumptions of the models are not valid in high turbulent intensity combustion regimes, a different approach is most likely a necessary option.
When models for thin-reaction zone and distributed reaction zone regimes are to be developed sufficient reference data is required. Experimentally it is difficult to achieve high turbulent intensities in a laboratory combustion environment [2] and as it is achieved, simultaneous multi-species and temperature measurements are to be conducted, which demands access of complex, expensive equipment. Multi-species measurements in these types of flames have not been conducted until very recently [3, 4, 5, 6], where [6] is able to show a rather comprehensive set of radicals. However, for a complete picture, simultaneous temperature measurements and preferably 3D measurements would be preferred. This is probably not feasible in the near future, which is why direct numerical simulations (DNS) has due to the massive increase of computer power access during recent years come to play an important role since it is able to supply this kind of data.

The scope of this thesis is to apply CFD to studies of turbulent premixed combustion at moderate and high turbulent intensities, where the interaction between a turbulent flow and a flame appears quite different depending on the size and speed of the turbulent vortices. Premixed combustion is conventionally used in spark ignition engines and stationary gas turbines. This thesis is directly related to applications to gas turbines where swirl stabilized flames are successfully applied to achieve ultra low emissions of NOx. Practical difficulties still remaining are e.g. flashback, blow-off, thermo-acoustic oscillations and combustion noise. Here the focus is not on these issues per se, but instead the modeling difficulties arising during simulations of these types of flames such as: differential diffusion effect and flamelet model validity in thin-reaction zone regime. DNS is applied for studies of flames interacting with very high intensity turbulence to both improve understanding of the complex phenomena mentioned above as well as providing data-base for future model development and validation. The experimental low swirl burner [7] is studied utilizing LES with the flamelet G-equation model. The experimental data are used to evaluate the model performance.

Structures of premixed flames at moderate and high Karlovitz numbers are presented. Reaction zone broadening is shown, whereas global flame extinction is not significant. The effect of differential diffusion at moderate Karlovitz numbers is shown to be important, which is also true in the high Karlovitz number distributed reaction zone regime. In the low swirl burner set-up the temperature and oxygen fields simulated using the levelset G-equation flamelet model is validated using experimental data. Using dynamic mode decomposition analysis it is found that strong frequency specific modes exist in inner and outer shear layer of the burner, which plays an important role in the flame stabilization process in the low swirl flame.

Following this short introduction, the theory of premixed turbulent combustion is summarized in chapter 2. The methods utilized are described in chapter 3, a summary of obtained results is presented in chapter 4, and chapter 5 contains relevant conclusions and an outlook towards future work. Further details of the results are given in the papers listed in the appendix.
Chapter 2
Turbulent reactive flows

2.1 Turbulence

2.1.1 Laminar and turbulent flows

Turbulent flows are characterized by irregularity, randomness and chaos, whereas laminar flows are characterized by streamlines of parallel layer and transport in the transversal direction to the flow direction is simply governed by diffusion. Compared with turbulent diffusion, laminar diffusion is very slow and in most industrial applications mixing needs to be fast and the flows are therefore usually kept turbulent. Turbulence is often characterized through the Reynolds number:

\[ Re = \frac{\rho U_c L_c}{\mu}, \]

where \( \rho \) is density, \( U \) is characteristic velocity, \( L \) is characteristic length scale and \( \mu \) is dynamic viscosity. The Reynolds number is given by the ratio between inertial forces and viscous forces and tells the characteristics of the flow independent of fluid or geometry. Turbulent flows are associated with large Reynolds numbers.

2.1.2 Scales of turbulence

Turbulent energy cascading is of central importance in turbulent theory. Richardson stated the first turbulence concept, where turbulence can be considered composed of turbulent eddies of different size. The length scale of the large scale motion is on the same order as the apparatus generating the turbulence, and turbulent kinetic energy is thereafter cascaded from larger to smaller scales until finally dissipated by viscosity at the smallest scales. For characterization of turbulent scales in homogeneous turbulence, the correlation function for \( u_1 \) component can be defined as:

\[ g_{11}(r) = \frac{u_1'(x)u_1'(x + r)}{u_1'(x)u_1'(x)}, \]

where \( u_1' \) is the velocity fluctuation for velocity component 1 and \( r \) is distance from point \( x \). In isotropic turbulence, the correlation function is independent of direction \( (g_{11} = g_{22} = g_{33} = g) \), which for simplicity will be used here. The integral length scale, \( l \), describing the large scale structures, is defined through integration of this autocorrelation function:

\[ l = \int_0^\infty g(r)dr. \]

At this scale, the characteristic velocity, \( u_1' \), often referred to as turbulent intensity is a very important property for characterization of turbulence. Based on these length and velocity scales a turbulent Reynolds number is also defined:

\[ Re_T = \frac{u_1'l}{v}. \]
For large enough Reynolds numbers, in-between the smallest and largest scales of turbulence there is a cascading range where energy is transferred from larger to smaller scales. This range is called the inertial sub-range, for which it can be shown that the following relation for distribution of turbulent kinetic energy amongst scales, $E(k)$, holds:

$$E(k) \propto \varepsilon^{2/3} k^{5/3},$$

(5)

where $k$ is wave number. Related to this range is the Taylor scale, $\lambda_f$. This scale is also based on the autocorrelation function $g(r)$. It is defined through:

$$\lambda_f = -\frac{2}{d^2 g / dr^2 |_{r=0}}.$$  

(6)

The Taylor scale has no obvious physical interpretation, but it is a good estimation of the inertial sub-range. Later, in two similarity hypotheses from Kolmogorov, the turbulent theory for small scale turbulence was stated. The small scales of turbulence are solely governed by kinematic viscosity $\nu$ and rate of dissipation, $\varepsilon$. Based on these two quantities, through dimension analysis, the Kolmogorov length and time scales were defined:

$$\eta = (\nu^3 / \varepsilon)^{1/4}$$

$$\tau_\eta = (\nu / \varepsilon)^{1/2}$$

(7)

which are characteristic for the smallest scales of turbulence. The Kolmogorov length scale can be estimated through the turbulent Reynolds number:

$$\eta = \frac{l}{Re_t^{3/4}}.$$  

(8)

A schematic sketch of an energy spectrum for a homogeneous high Reynolds number turbulent flow is shown in Fig. 2.1.
This type of turbulence is theoretical and may be termed “Kolmogorov turbulence”. The turbulence found in most practical application does not follow this theory, and are not fully homogenous and isotropic.

2.2 Combustion

2.2.1 Premixed and non-premixed combustion

Combustion is a collective term for all types of exothermic reaction process where fuel is oxidized and releasing heat. Combustion is generally divided into two large classes: non-premixed and premixed combustion.

In non-premixed combustion fuel and oxidizer are separated prior to reaction and are later reacting simultaneous with the mixing process. The reaction is conducted around stoichiometric proportions with high flame temperature and is governed by diffusion and eventual turbulent mixing. Non-premixed flame temperature is therefore difficult to control. On the other hand non-premixed flames also provide desirable characteristics. Non-premixed flames are easy to stabilize and the separation of fuel and oxidizer prior to combustion provides secure handling. Typical applications for non-premixed flames are candles, solid combustion and typical diesel engines.

In premixed combustion the fuel and oxidizer is mixed prior to reaction. Contrary to non-premixed flames premixed flames has a distinct reaction zone with characteristics such as a laminar flame thickness and flame speed. Premixed combustion allows direct control of the flame temperature through the mixture ratio between fuel and oxidizer and thereby control of emissions. On the other hand premixing gives rise to problems of stabilization, blow-off and flashback. Typical applications for this are Bunsen burners, spark-ignition engines and stationary gas turbines.

2.2.2 Turbulent premixed combustion

As previously mentioned, in laminar premixed flames the flame is characterized by a laminar flame thickness, $\delta_L$, and a laminar flame speed, $S_L$. For hydrocarbon fuel/air mixture at stoichiometric proportions and room conditions the laminar flame speed is typically on the order of half a meter per second. This speed is very much too low to be useful in industrial applications, which is why most combustion systems are turbulent. Turbulence wrinkles flames and increase the flame area and thereby the fuel consumption speed. Instead a turbulent burning velocity, $S_T$, can be defined through a relationship of flame area:

$$S_T = A_L/A_M \cdot S_L = \Xi \cdot S_L,$$

where $A_L$ is instantaneous turbulent flame front area, $A_M$ is the corresponding meant turbulent flame area and $\Xi$ is the flame wrinkling factor. In applied turbulent premixed combustion the mean flame is therefore propagating at a much higher velocity than a corresponding laminar flame ($S_T \sim 10 \cdot S_L$). This relation is shown in a schematic sketch in Fig. 2.2. However, as described in Section 2.1 turbulence consist of a range of turbulent scales. Flame wrinkling is mainly conducted by the highly energetic large scale eddies, whereas the small scale eddies can cause different types of interaction with the flame depending on their length scale. To show the structures of premixed flame, a 1D flame profile for a lean methane/air flame computed with the Smooke mechanism [8] is presented in Fig. 2.3. Here it can be seen how
the flame profile can be divided into preheat zone, reaction zone (inner layer) and oxidation zone. In the preheat zone temperature is raised mainly due to diffusion of energy from reaction zone not due to significant heat release rate. The reaction zone is a thin layer where fuel and oxidizer are consumed through several chain branching and chain propagating reactions involving intermediate radicals such as: H, O, OH, CH and CH₂O for hydrocarbon flames. The oxidation zone is following the reaction zone and remaining heat is released through oxidation of residual radicals (mainly OH and CO). Relative the reaction zone, the oxidation zone is very wide and equilibrium burned gases are reached quite far downstream, cf. Fig. 2.3.

Interacting with premixed flames, the turbulent Reynolds number is modified based on the characteristic flame properties, $S_L$ and $\delta_L$, by assuming viscosity proportional to these:

$$Re_T = \frac{u' \cdot l}{S_L \cdot \delta_L}.$$  \hspace{1cm} (10)

The interaction between small scale turbulence and flame is quantified through the Karlovitz number:

$$Ka = \frac{\tau_{e}}{\tau_\eta} = \left(\frac{u'}{S_L}\right)^{3/2} \left(\frac{\delta_L}{l}\right)^{1/2} \sim \left(\frac{\delta_L}{\eta}\right)^2,$$ \hspace{1cm} (11)

where $\tau_e$ is the chemical time scale and $\tau_\eta$ is the Kolmogorov time scale. As seen in the right hand side of equation (11) the Karlovitz number behaves as the ratio between laminar flame thickness and Kolmogorov length scale squared. A Karlovitz number of unity therefore means that the flame thickness and the smallest scale of turbulence are of the same order and a Karlovitz number of 100 means that the smallest scale of turbulence is about one order of magnitude smaller than the flame thickness. This is typically the width of the inner reaction zone layer. The turbulent premixed combustion diagram proposed by Borghi [9] and later revised by Peters [10] is a generally accepted description of eddy/flame interaction premixed flames. The Peters-Borghi diagram is shown in Fig. 2.4 where the region of laminar flames is defined for turbulent Reynolds numbers smaller than unity. When Karlovitz number is smaller than one, the flame is considered a flamelet, which means that the flame can be locally considered one-dimensional as it is solely influenced at large scales by turbulence. Extensive experimental [5, 6, 11, 12, 13] and numerical [10, 14, 15, 16] investigations have been dedicated to study flames in the flamelet regime showing results consistent with theory and the flamelet regime can therefore be considered quite well understood [17].
According to theory, for Karlovitz number greater than one, the smallest scales of turbulence are able to penetrate into the flame preheat zone and cause preheat zone broadening. This combustion regime is called the thin reaction zone regime, as turbulence should be unable to penetrate the inner reaction zone layer. Preheat zone broadening has been shown experimentally [5, 6, 18, 19] as well as numerically [20, 21] and can be considered a well known feature. However, its effect on the turbulent burning rate is a less known phenomenon. During modeling of premixed flames in the thin reaction zone regime, the flamelet concept is often extended to be assumed valid at quite large Karlovitz numbers. The preheat zone is disturbed, however, since the inner reaction zone should be left unperturbed, flamelet models are often, with great success, also applied in this combustion regime. When the Karlovitz number is greater than 100 the smallest scale of turbulence is also smaller than the inner reaction zone layer and the hypothesis is therefore that increased mixing inside the inner reaction zone layer can cause flame quenching. This has been shown experimentally in jet flames [3, 4, 5, 6, 22]. The limit of Karlovitz number 100 separating the thin-reaction zone regime from the distributed reaction zone regime can also be considered highly theoretical. The Kolmogorov length scale is first of all within an order of magnitude from the smallest eddy in a turbulence field. Secondly, viscosity increase across a flame greatly raise the Kolmogorov length scale, which questions if the small scale turbulence survive for a sufficient time to cause the kind of expected interaction with the inner reaction zone layer before dissipated. Fundamental questions such as what can be considered distributed combustion, if distributed burning is reached and what kind of features expected in the distributed reaction zone regime can be found are of great importance for modeling of combustion systems where distributed burning is expected to occur, e.g. SI engines at high load.

Due to difficulties of reaching very high turbulent intensities in laboratory experimental rigs, DNS has risen as an excellent tool for detailed studies of this kind of questions. Structure of flames in the distributed reaction zone regime was investigated by Poludnenko and Oran [21] as dependant on resolution utilizing simple chemistry. Effects of both small and large turbulent scales on the flame were found highly resolution dependant and it was concluded that in their case, turbulent scales much smaller than the laminar flame thickness did not play a prominent role in terms of effect on flame brush properties and dynamics.
Figure 2.4 implies that effect of fuel does not need to be explicitly accounted for, but implicitly through its influence through $S_c$ and $\delta_L$. However, due to differences in mass diffusion speed relative to thermal diffusion speed combustion can appear quite different for different fuel. This ratio is presented through the Lewis number, $Le$:

$$Le = \frac{\alpha_\lambda}{D},$$

where $\alpha_\lambda$ is thermal diffusivity and $D$ is mass diffusivity, which for non-unity Lewis number will cause significant influence to the flame shape. A lot of species, $O_2$, $N_2$, $CH_4$, $CO$, $CO_2$ and $H_2O$, have Lewis number close to unity and can therefore for simplification be assumed unity. However, other common species e.g. $H$, $H_2$ and $C_3H_8$, have Lewis number quite far from unity, for which the same simplification cannot be made that easily. Non-unity Lewis number influences the flame front at species gradients and flame curvature. At a flame front both species and temperature gradients appear. Due to this gradient species and temperature diffuse in the opposite direction to the gradient at different speed relative each other. The equivalence ratio will therefore be locally different at different positions within the flame. This effect is not a problem modeling when using a flamelet concept. However, as in turbulent flames, flame curvature is induced. The effect of differential diffusion will cause focusing of rapidly diffusing species ($Le < 1$) in flame convex surfaces and defocusing in concave surfaces and vice versa for slowly diffusing species ($Le > 1$) [23, 24]. This effect is difficult to capture applying the flamelet concept and for its effect during interaction with turbulence, high resolution numerical studies need to be performed. For quantification of differential diffusion a local equivalence ratio, $\varphi$, is often computed. For a hydrocarbon fuel it can be expressed as [25]:

$$\varphi = \frac{\sum Y_{H,all} W_H}{\sum W_H} + \frac{2 \cdot Y_{C,all} W_C}{W_C},$$

$$\varphi = \frac{Y_{O,all}}{W_O},$$
where $Y_{H,all}$ is mass fraction of hydrogen element, $W_H$ is molar mass of hydrogen atom, $Y_{C,all}$ is mass fraction of carbon element, $W_C$ is molar mass of carbon atom, $Y_{O,all}$ is mass fraction of oxygen element and $W_O$ is molar mass of oxygen atom. Aspden et al. [26, 27, 28, 29] have in several publications studied Lewis number effects in flames in the distributed reaction zone regime. It was shown that the effect of differential diffusion both in the normal direction as well as the tangential direction of the flame was greatly reduced at high Karlovitz numbers. The studies were not claimed to utilize DNS as the turbulence field used was unresolved. Turbulent intensity was maintained using a density weighted forcing algorithm and chemistry was solved for using detailed mechanisms.

In a turbulent flame it is necessary to express reaction progress for quantification of flame structure. As previously described, fuel Lewis number can differ a lot and a reaction progress variable, $c$, is here therefore based on the close to unity Lewis number oxidizer oxygen:

$$c = \frac{Y_{O_{2,0}} - Y_{O_2}}{Y_{O_{2,0}} - Y_{O_{2,b}}}$$

(14)

where $Y_{O_{2,0}}$ is oxygen mass fraction in unburned mixture, $Y_{O_2}$ is local mass fraction of oxygen and $Y_{O_{2,b}}$ is oxygen mass fraction in burned mixture at equilibrium.

### 2.3.3 Mathematical description

In a reacting flow system the flow is governed by conservation equations for mass and momentum (the Navier-Stokes equations). In conserved form these equations can be written [14]:

$$ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 $$

(15)

$$ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho \sum_{s=1}^{N_{sp}} Y_s f_{s,j}, $$

(16)

where $u_i$ is velocity component $i$, $p$ is pressure $\tau_{ij}$ is the viscous tensor, $Y_s$ is mass fraction of species $s$, $N_{sp}$ is number of species and $f_{s,j}$ is specific volume force acting on $s$ in direction $j$. Pressure is determined through the equation of state:

$$ p = \rho \mathfrak{R} T \sum_{s=1}^{N_{sp}} \frac{Y_s}{W_s}, $$

(17)

where $\mathfrak{R}$ is the universal gas constant, $T$ is temperature and $W_s$ is molar mass of species $s$. The viscous stress tensor is defined through:

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

(18)

where $\delta_{ij}$ is the Kronecker delta.
Equations for handling combustion are conservation equations for energy and species. Energy can be expressed either through enthalpy or temperature. Both options have advantages and disadvantages. Through the use of enthalpy in the energy equation reaction rates are not explicitly accounted for in the equation since enthalpy is conserved during reaction. On the other hand temperature is commonly used quantity and to be extracted when the enthalpy equation is applied, post-processing needs to be performed. The enthalpy equation can be written [14]:

$$ \frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_j} = \frac{\partial p}{\partial t} + \frac{\partial u_i p}{\partial x_j} - \frac{\partial q_i}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{s=1}^{N_{sp}} Y_{s,j} V_{s,j} , \quad (19) $$

where $q_i$ is the energy flux, $\dot{Q}$ is heat source term and $V_{s,j}$ is diffusion velocity for species $s$ in direction $j$. The heat source term, e.g. spark ignition or radiative heat transfer, can through direct insert to the equation be given analytically.

Rewriting the energy equation in temperature form gives the conservation equation for energy in terms of temperature [14]:

$$ C_p \frac{\partial \rho T}{\partial t} + C_p \frac{\partial \rho u_i T}{\partial x_j} = \frac{\partial p}{\partial t} + \frac{\partial u_i p}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) - \left( \rho \sum_{s=1}^{N_{sp}} C_{p,s} Y_s V_{s,j} \right) \frac{\partial T}{\partial x_j} $$

$$ + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \dot{Q} + \rho \sum_{s=1}^{N_{sp}} Y_{s,j} V_{s,j} + \dot{\omega}_T , \quad (20) $$

where $C_p$ is mixture averaged heat capacity at constant pressure, $\lambda$ is thermal conductivity, $C_{p,s}$ is heat capacity for species $s$ at constant pressure and $\dot{\omega}_T$ is heat release rate. The conservation equation for mass fraction of species $s$, $Y_s$, can be written [14]:

$$ \frac{\partial \rho Y_s}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho (u_j + V_{s,j}) Y_s \right) = \dot{\omega}_s , \quad (21) $$

where $\dot{\omega}_s$ is reaction rate of species $s$. The species mass diffusion, $V_{s,j} Y_s$, that appears in both energy and species equations is often modeled using Fick’s law:

$$ V_{s,j} Y_s = \kappa_s \frac{\partial Y_s}{\partial x_j} - Y_s \sum_{s=1}^{N_{sp}} \kappa_s \frac{\partial Y_s}{\partial x_i} \quad (22) $$

where $\kappa_s$ is mass diffusion coefficient for species $s$. 
Chapter 3
Methods

3.1 Turbulence modeling

3.1.1 Direct Numerical Simulation (DNS)

By definition no turbulence model needed with DNS. The full range of turbulent kinetic energy should be resolved, from integral scale to Kolmogorov scale, so that both cascading and small scale dissipation by viscosity should be handled. This means that a very fine mesh is required. DNS is therefore limited to small computational domains and low Reynolds numbers, which means that it is not applicable for industrial applications. For fundamental research DNS has risen as a useful tool for detailed studies of flame/flow interaction. In this thesis it has been applied for studies of high Karlovitz number effects in premixed flames. Two different codes has been applied, an in-house code and an open source code, which will be presented separately.

3.1.1.1 In-house code

The DNS code employed here is of low Mach number (\(Ma\)) type. The pressure is split in two parts, \(P(t)\) and \(p_h(x,t)\) corresponding to thermodynamic and hydrodynamics pressure respectively. The thermodynamic pressure, applied in the equation of state, is constant in space whereas the smaller hydrodynamic pressure is the one applied in the momentum equation. To handle large density gradients the continuity equation is written in a material derivative form. For convenience of discretization, momentum, temperature and species equations are all written in a CDR (convection, diffusion, reaction) form [30]:

\[
\frac{\partial u_i}{\partial x_i} = -\frac{1}{P} \frac{\partial P}{\partial t} + \frac{1}{T} \frac{\partial T}{\partial t} + \sum_{k=1}^{N_{sp}} \frac{\bar{W}}{W_s} \frac{\partial Y_s}{\partial t} + \frac{1}{\Omega_E} \frac{\partial E_E}{\partial t} + \frac{1}{\rho C_p} \frac{\partial T}{\partial t} + \frac{1}{\rho} \frac{\partial p_h}{\partial x_i} + \frac{1}{\rho} \frac{\partial u_j}{\partial x_i} \frac{\partial u_j}{\partial x_j} - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}.
\]

\[
\frac{\partial \rho u_i}{\partial t} = C_M + D_M - \frac{\partial p_h}{\partial x_i},
\]

\[
\frac{\partial T}{\partial t} = C_E + E_E + \frac{1}{\rho C_p} \frac{\partial T}{\partial t} + \Omega_E + D_E + R_E
\]

\[
\frac{\partial Y_s}{\partial t} = C_s + D_s + R_s, \quad (s = 1, \ldots, N_{sp}),
\]

where \(\bar{W}\) is mixture averaged molar mass, \(C, D\) and \(R\) are convection, diffusion and reaction terms respectively, \(E_T\) is energy transport due to non-unity Schmidt number and \(\Omega_E\) is external energy source e.g. spark ignition which can be given analytically. The different terms are written as

\[
C_M = -\frac{\partial \rho u_j u_i}{\partial x_j}, D_M = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij},
\]

\[
C_E = -u_j \frac{\partial T}{\partial x_i}, E_E = \frac{1}{\rho C_p} \left( \rho \sum_{s=1}^{N_{sp}} C_{p,s} V_{s,j} Y_s \right) \frac{\partial T}{\partial x_j}.
\]
\[
D_E = \frac{1}{\rho C_p} \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j},
R_E = -\frac{1}{\rho C_p} \sum_{s=1}^{N_{sp}} h_{s,0} \dot{\omega}_s,
\]
\[
C_s = -u_j \frac{\partial Y_s}{\partial x_j},
D_s = \frac{1}{\rho} \frac{\partial \rho V_{s,j} Y_s}{\partial x_j},
R_s = \frac{1}{\rho} \dot{\omega}_s,
\]

where \( \delta_{ij} \) is Kronecker delta, \( \lambda \) is mixture averaged thermal conductivity, \( h_{s,0} \) is enthalpy of formation of species \( s \) and \( V_{s,j} Y_s \) is the species mass diffusion.

### 3.1.1.2 The pencil code

The pencil code is a high-order fully compressible DNS code available at a public domain [31]. Originally, the pencil-code was developed for applications in astrophysics and magnetohydrodynamics, but is applicable in combustion since a transport/chemistry module was implemented [32]. In this compressible code, the set of governing equations solved are rewritten as:

\[
\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = -\frac{\partial u_j}{\partial x_j}
\]

\[
\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( 2 \rho \nu \left( S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial u_j}{\partial x_j} \right) \right)
\]

\[
\rho C_v \left( \frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} \right) = \dot{\omega}_T + \xi T \frac{\partial}{\partial x_j} \left( \rho \sum_{s=1}^{N_{sp}} \frac{D_S}{W_s} \frac{\partial Y_s}{\partial x_j} \right) + \rho \frac{\partial T}{\partial x_j} \sum_{s=1}^{N_{sp}} C_{p,s} D_s \frac{\partial Y_s}{\partial x_j}
\]

\[
+ \frac{\partial}{\partial x_j} \lambda \frac{\partial T}{\partial x_j} \left( S_{ij} - \frac{1}{3} \delta_{ij} \frac{\partial u_j}{\partial x_j} - \rho \delta_{ij} \right) \frac{\partial u_j}{\partial x_j}
\]

\[
\rho \left( \frac{\partial Y_s}{\partial t} + u_j \frac{\partial Y_s}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \rho D_s \frac{\partial Y_s}{\partial x_j} + \dot{\omega}_s
\]

where \( S_{ij} \) is the symmetric rate of strain tensor:

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

and \( D_s \) is mass diffusion coefficient for species \( s \). Fick’s law and Fourier’s law have been applied for the species diffusion and heat diffusion respectively. Species diffusion coefficients and heat conductivity are solved for in a simplified way compared with the in-house code. Species diffusion coefficients are evaluated following expression [8]:

\[
\rho D_s = \frac{D_0}{Le_s} \left( \frac{T}{T_0} \right)^n,
\]

where \( D_0 \) is a mixture specific constant (\( D_0 = 2.58 \times 10^{-4} \) kg/(m \cdot s) for CH\(_4\)/air mixture), \( Le_s \) is Lewis number of species \( s \), \( T_0 \) is reference temperature (\( T_0 = 298 \) K) and \( n = 0.7 \). Constant species Lewis numbers are assumed. Heat conductivity is computed through the expression [8]:

12
\[ \lambda = D_0 C_p \left( \frac{T}{T_0} \right)^n. \]  

### 3.1.2 Large Eddy Simulation (LES)

In LES a coarser grid than in DNS is used such that the spatial resolution is within the inertial sub-range and (much) larger than the Kolmogorov scale. The small turbulent scales are assumed to be local and are responsible for dissipation of turbulent kinetic energy. According to the turbulence spectrum, Fig. 2.1, the main part of the turbulent kinetic energy is contained in the large scales and the concept of LES is therefore to resolve those scales to be able to capture the dynamic features of the flow. The governing equations are filtered on an LES scale (usually the grid resolution scale), extracting small scales from the solution. For reacting flows, density is not constant. The filter applied is therefore of density weighting type, defined here for a general function \( g \):

\[ \tilde{g} = \frac{\rho g}{\rho}, \]  

where over-bar denotes averaging and over-tilde Favre density weighted averaging. The density weighting filter operator is expressed as:

\[ \tilde{g}(x) = \int \rho g(x') F_\Delta (x - x') dx', \]  

where \( F_\Delta \) is the LES filter kernel.

By assuming low pressure variation, i.e. low Mach number flow, neglecting viscous damping and radiation heat transfer and without volume forces, the filtered governing equations can be written:

\[ \frac{\partial \tilde{\rho} u_i}{\partial t} + \frac{\partial \tilde{\rho} u_i u_i}{\partial x_i} = 0 \]  
\[ \frac{\partial \tilde{\rho} u_i}{\partial t} + \frac{\partial \tilde{\rho} u_i u_i}{\partial x_i} = - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \mu \frac{\partial u_i}{\partial x_i} \right) - \frac{\partial \tau_{ij}^r}{\partial x_j} \]  
\[ \frac{\partial \tilde{h}}{\partial t} + \frac{\partial \tilde{u}_j \tilde{h}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial \tilde{h}}{\partial x_j} \right) \]  
\[ \frac{\partial \tilde{\rho} \tilde{Y}_s}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_j \tilde{Y}_s}{\partial x_j} = \frac{\partial}{\partial x_j} \rho D_s \left( \frac{\partial \tilde{Y}_s}{\partial x_j} \right) - \tilde{\omega}_s, \quad (s = 1, \ldots, N_{sp}), \]  

where \( \tau_{ij}^r \) is an additional unknown term that appears as the filtering is performed:

\[ \tau_{ij}^r = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j. \]

### 3.1.3 SGS models for LES

For closure of the filtered LES equations, modeling of the unclosed term \( \tau_{ij}^r \) needs to be performed. A large number of closure models have been developed through the years, e.g. Smagorinsky model [33], one-equation model [34, 35], scale similarity model [36] and
Germano dynamic model [37]. Here the only model presented will be the Smagorinsky model and also the concept of Implicit LES (ILES), where one is not using any explicit model at all.

3.1.3.1 Smagorinsky model

In the RANS framework, the Boussinesq’s hypothesis is used for introducing a turbulent viscosity. In analogy to that model, the Smagorinsky model is given by:

$$\tau_{ij}^T = \mu_\Delta \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right),$$

where $\mu_\Delta$ is the turbulent viscosity. The modeling of the turbulent viscosity is done through:

$$\mu_\Delta = \bar{\rho} (C_S \cdot \Delta)^2 \sqrt{2 \delta_{ij} \tilde{S}_{ij}},$$

where $C_S$ is the Smagorinsky constant, $\Delta$ is the filter width and $\tilde{S}_{ij}$ is the filtered symmetric rate of strain tensor. The Smagorinsky model is very commonly applied in LES due to its simplicity as well as its correct asymptotic behavior as the grid is refined ($\mu_\Delta \propto \Delta^2$).

3.1.3.2 Implicit LES (ILES)

If the discretization scheme applied to the convective term in the momentum equation is of odd order e.g. first order:

$$\frac{\partial u}{\partial x} = \frac{u^{(n+1)} - u^{(n)}}{\Delta x} - \frac{\Delta x}{2} \frac{\partial^2 u}{\partial x^2} + \text{HOT},$$

where the superscript $n$ denotes cellnumber, $\Delta x$ is the grid spacing and HOT is higher order terms, the lowest order term in the truncation error behaves as a dissipating diffusion term [38]. The idea of ILES is therefore to not employ any explicit SGS model but instead assume that the effect of dissipation of the small scale turbulence is accounted for by the truncation error [39].

3.2 Combustion modeling

Combustion modeling generally means determination of the number of species equations used as well as handling of the species reaction rate terms. In this thesis two methods has been applied, direct use of finite rate chemistry for DNS and the levelset G-equation based flamelet chemistry for LES.

3.2.1 Finite rate chemistry

In DNS the resolution is fine enough so that all flow related and chemistry related time scales are resolved. However, when several species are involved in a combustion system the time scales of those reactions are usually very different, leading to a stiff system. During a relatively large CFD time step the mass fraction of intermediate species with short chemical time scales may vary substantially, which makes direct use of Arrhenius reaction rates (here displayed for a $A + B \rightarrow C + D$ reaction):
$\dot{\omega}_c = [A][B]A_s T^{n_A} \exp(-E_a/RT)$, \hspace{1cm} (44)

induce large errors. $A_s$, $n_A$ and $E_a$ in equation (44) are reaction specific constants. A stiff solver is therefore needed which split the CFD time step into multiple sub-steps and then integrates the reaction rates for all sub-steps. This is computationally expensive, which is the first reason why the method is commonly avoided in LES studies. A more severe issue as finite rate chemistry is applied to LES is that the reaction rates are computed based on filtered quantities and integrated across huge CFD time steps (read $\Delta t \sim \mu s$). This direct use of finite rate chemistry in LES is generally not possible without case by case tuning of the chemical scheme and/or a well developed SGS model. In this thesis the $\text{H}_2$ sub-mechanism of Peters $\text{C}_3$ hydrocarbon mechanism [40] and the mechanism by Smooke and Giovangigli [8] were used for the $\text{H}_2$/air and the $\text{CH}_4$/air simulations respectively.

### 3.2.2 Levelset $G$-equation

There are a variety of alternative combustion models to finite rate chemistry. The one used in this thesis is called the levelset $G$-equation [10]. By assuming that the flame is of flamelet type and therefore can be described as a single connected isosurface, a transport equation for such an isosurface can be derived. By definition, the flame is characterized by the equation:

$$G(\hat{x}, t) = 0.$$ \hspace{1cm} (45)

Differentiating this equation gives:

$$\frac{\partial G}{\partial t} + \frac{\partial G}{\partial x_i} \frac{\partial x_i}{\partial t} = 0,$$ \hspace{1cm} (46)

where the term $\partial x_i / \partial t$ can be expressed through convection speed and self-propagation, $S$:

$$\frac{\partial x_i}{\partial t} = u_i + S \cdot n_i$$ \hspace{1cm} (47)

where $n_i$ is the component of the flame front normal. The equation is solely valid for the isosurface $G(\hat{x}, t) = 0$, however, by assuming that the equation is also valid in a narrow band around the flame, the $G$-field can be extended into this region. The flame front normal can then be expressed from the $G$-field:

$$n_i = -\frac{\partial G}{\partial x_i} / |\nabla G|.$$ \hspace{1cm} (48)

Insert of equations (47) and (48) in (46) gives the levelset $G$-equation:

$$\frac{\partial G}{\partial t} + u_i \frac{\partial G}{\partial x_i} = S \cdot |\nabla G|.$$ \hspace{1cm} (49)

The extended $G$-field in the narrow band around the $G = 0$ isosurface is defined by the signed closest normal distance to the flame. The sign is negative for unburned gasses and positive for burned gasses. This extension is called the reinitialization process and performed through solving of the equation:
When the G-equation is solved, the flame structure is described using a pre-computed library. This library can be computed based on several variables, e.g. $G$, mixture fraction ($Z$) and strain ($\sigma$). The sensitive part of the G-equation is self-propagation speed which requires modeling. In DNS it corresponds to the local flame speed and in LES it corresponds to an unresolved turbulent flame speed $S_T$. As previously described the turbulent flame speed is related to the laminar flame speed through the wrinkling factor, cf. eq (9). In LES context, the unresolved flame wrinkling is defined by the SGS wrinkling factor, $\Xi_{\Delta}$. The majority of the models used for the SGS wrinkling factor can be summarized by the expression:

$$\Xi_{\Delta} = \left( 1 + \alpha \left( \frac{u'_{SGS}}{S_L + \beta} \right)^{n_c} \right)^{1/n_c}, \quad (51)$$

where $\alpha$, $\beta$ and $n_c$ are modeling parameters and $u'_{SGS}$ is SGS fluctuation, which requires estimation. Combining estimations of turbulent viscosity from the Smagorinsky model with the one from the RANS framework results in the SGS fluctuation estimation according to:

$$\begin{align*}
\left\{ 
\nu_T = (C_s \Delta)^2 \sqrt{2 \cdot S_{ij} S_{ij}} \\
\nu_T = C_\mu \cdot \Delta \cdot u'_{SGS}
\end{align*} \Rightarrow u'_{SGS} = \frac{C_s^2}{C_\mu \Delta} \sqrt{2 \cdot S_{ij} S_{ij}}. \quad (52)$$

In this thesis, all modeling parameters are assigned constant values with $\alpha = 2.2$, $\beta = 0.01$ and $n_c = 1$. When employing the G-equation model within LES and RANS framework the equation is filtered and Favre averaged, resulting in:

$$\frac{\partial \rho \tilde{G}}{\partial t} + \bar{u}_i \frac{\partial \rho \tilde{G}}{\partial x_i} = \rho_0 S_T \cdot |\nabla G|, \quad (53)$$

where $\rho_0$ is density of unburned gas. The levelset G-equation has been applied and validated for a wide range of combustion applications [15, 16, 41, 42, 43].

3.3 Numerical discretization

3.3.1 DNS

3.3.1.1 Inhouse code

An in-house DNS code implemented in a vector form enabling 1D, 2D as well as 3D simulations has been used in this thesis. The code is of finite difference type with a Cartesian grid structure. Temporal integration of the CDR terms in the governing equations is performed using an operator splitting technique. The 2nd order symmetrical Strang splitting algorithm [44] is employed where the stiff integration of chemistry is performed between two half-step integrations of the diffusion and convection terms. Integration of the diffusion terms
is however quite sensitive and needs to be split into several additional sub-steps to satisfy the diffusion stability limit. In paper I in the appendix, a 3rd order Runge-Kutta [45] temporal discretization was employed, however it was found during strict grid dependency testing that 2nd order Strang splitting showed a more desirable accuracy. Discretization of spatial terms in the governing equations is done through utilization of 6th order central difference stencil except for the convective term in the species and energy equations. Due to large gradients of both species and temperature across the flame, these terms are chosen to be discretized using a 5th order WENO scheme [46] to avoid unphysical oscillations close to such gradients. Especially in the species equations such oscillations can cause mass fractions to be negative or larger than unity. The detailed chemical kinetic mechanisms employed are integrated by a stiff solver, the DVODE solver [47]. In this thesis hydrogen flames has been studied and two different H2/air mechanisms have been employed [40, 48].

Using low Mach number assumption makes the CFD time step solely limited by maximum convection speed with associated Courant-Friedrichs-Lewy (CFL) condition and not by acoustic waves (speed of sound). However due to the decoupling of mass and momentum equations, a variable coefficient Poisson equation for pressure correction, \( p' \), needs to be solved:

\[
- \frac{\partial}{\partial x_j} \left( \frac{1}{\rho^{n+1}} \frac{\partial}{\partial x_j} p' \right) = \frac{1}{\Delta t} \left( \frac{\partial}{\partial x_j} u_j^{n+1} - \frac{\partial}{\partial x_j} u_j^* \right),
\]

(54)

where \( \rho^{n+1} \) is updated density at time step \( n + 1 \), \( u_j^{n+1} \) is updated velocity at time step \( n + 1 \) and \( u_j^* \) is velocity at last fractional time step. This equation is discretized using 2nd order central difference, to avoid large discretization stencil, and solved implicitly using a multi-grid procedure. Details on the multi-grid can be found in [49, 50] and further details on the discretization can be found in [30].

For studies of flame/turbulence interaction an initial turbulence field has to be applied. Through superimposing of Fourier waves by assuming the turbulence spectrum described by an analytical function [51], a turbulence field characterized by specified turbulent intensity and integral length scale is obtained [52].

The DNS employed in this thesis is 2D due to the limited accessible computational resources available at the time of execution. The lack of vortex stretching in 2D and through it differences in turbulent cascading between 3D and 2D turbulence fields, 3D simulations would of course have been preferable, however, in several investigations [53, 54, 55] it has been shown that during flame/turbulence interaction, the eddies tend to have a cylindrical shape in a higher extent than spherical. Regardless of this, 2D DNS is here applied to study interaction of velocity field consisting of different scales with flame. This is assumed to be obtained in 2D similar as in 3D.

### 3.3.1.1 The pencil code

In the pencil-code the equations are discretized through 6th order central difference schemes for spatial derivatives on Cartesian grids. As mentioned in section 3.1.1.1 unphysical oscillations can occur due to high order central difference schemes, which is why 5th order upwind scheme was used for convective terms in energy and species equations. The equations were solved using explicit 3rd order Runge-Kutta [45] scheme.
The initial turbulence fields utilized in the simulations were generated through applied forcing at desired scale in a isothermal flow simulation which was run until statistically stationary turbulence was generated.

3.3.2 LES

Large eddy simulations were performed using a finite difference in-house solver. The code utilizes staggered Cartesian grid for discretization of the filtered governing equations, eq. (36-39, 53). Due to the application in non-homogenous premixed combustion species equations for fuel and mixture fraction needs to be solved. The fuel equation accounts for mixing of fuel/air mixture with ambient air prior to combustion, whereas mixture fraction is needed to also track mixing of burned gases with ambient air. Mixture fraction is a passive scalar without reaction rate. Fuel is equal to the mixture fraction in the unburned gases, where as it is unlike mixture fraction consumed across the flame. The consumption of fuel is controlled through tabulation close to the $G = 0$ levelset. For speeding up convergence, the code is using a multi-grid structure [56].

The convective term in the momentum equation is discretized using a 3rd order upwind scheme [57]. Due to the odd order discretization, the concept of ILES is applied with no explicit SGS model as described in section 3.1.3.2. Other spatial derivatives in equations (36-39) are discretized using a 4th order central difference scheme. Time integration is computed using a 2nd order implicit scheme. The G-equation requires a bit different treatment due to its correlation with high density gradient and a more stable discretization needs to be employed. Spatial derivatives are computed through a 3rd order WENO scheme [46] and time integration is performed using a 3rd order Runge-Kutta total variation diminishing (TVD) scheme [45].

3.4 Dynamic mode decomposition (DMD)

For determination of spatial structures characterized by frequencies and rate of growth or decay from a given set of data (numerical or experimental), dynamic mode decomposition (DMD) [58, 59] has been recently developed. The approach used in this thesis will be shortly presented here. A set of (column) data is provided \( \{u_k\}_{k=1}^{m} \). This can be several time sequences for a point measurement or \( \geq 1D \) measurements at several time instances. The last set of data \( (m) \) is replaced by a linear combination of the other datasets:

\[
\begin{align*}
  u_m &= \sum_{k=1}^{m-1} c_k u_k, \quad (55)
\end{align*}
\]

where the weight coefficients \( c_k \) are computed through least square fitting. The columns are combined to a matrix \( U \):

\[
U = [u_1 \ u_2 \ ... \ u_m]. \quad (56)
\]

If it is assumed that one set of data can be given by the previous through applying an operator \( A \ (u_{k+1} = Au_k) \), the expression:

\[
AU = UC \quad (57)
\]
is valid for the companion matrix $C$:

$$
C = \begin{bmatrix}
0 & c_1 \\
1 & 0 & c_2 \\
& \ddots & \ddots & \ddots \\
& & 1 & 0 & c_{m-2} \\
& & & 1 & c_{m-1}
\end{bmatrix}.
$$

(58)

From the companion matrix, an eigenvalue problem is stated:

$$
Cx = \sigma x,
$$

(59)

from which eigenvectors (dynamic modes) and eigenvalues, $\lambda_e$, are solved for. The eigenvalues are related to $\sigma$ through $\sigma = e^{\lambda_e t}$. Real part and imaginary part of $\lambda_e$ corresponds to growth/decay rate of the mode and oscillating frequency of the mode, respectively.
Chapter 4
Summary of results

In this chapter a summary of relevant published and unpublished results is presented. For further details on performed analysis the reader is referred to the papers appended at the end of the thesis.

4.1 Flame/turbulence interaction at high Karlovitz numbers: DNS study

The first part of the results covered in this thesis address DNS of turbulent reacting flows. As previously mentioned it is common to assume flamelet like behavior of a studied flame to simplify modeling. A $\phi = 0.6$, $Ka = 1$ $\text{H}_2/\text{air}$ flame propagating in an inflow/outflow configuration has been studied and a time evolution of the $\text{HO}_2$ mass fraction field is displayed in Fig. 4.1. The time step between the frames corresponds to 0.1 integral time scale for the turbulence field. During modeling of this kind of flames, the flame is commonly assumed locally 1D, which for the $\text{HO}_2$ field in Fig 4.1 is shown to be a good approximation. The effect of turbulence on flame is limited to large scale distortion and a resulting curved flame. The strong differential diffusion effect in lean $\text{H}_2/\text{air}$ flames makes convex flame segments propagate faster due to increased local equivalence ratio, which, as seen in Fig. 4.1, cause larger curvature magnitude for concave than for convex flame segments. As described in Section 2.2.2, the differential diffusion effect is modifying the flame structure both in the normal and tangential directions of the flame, not discernable in Fig. 4.1. For investigation of this effect to flamelet propagation, a statistical analysis will be presented.

Figure 4.1. Mass fraction of $\text{HO}_2$ for $\phi = 0.6$, $Ka = 1$ $\text{H}_2/\text{air}$ flame propagating towards a turbulent inflow on the left hand side.

Scatter plots of mass fractions of species $\text{HO}_2$, $\text{H}_2\text{O}_2$, OH, $\text{H}_2$, $\text{O}_2$ and $\text{H}_2\text{O}$ are visualized in Fig. 4.2. For all species, except OH, a quite unique correlation between temperature and species can be seen. In the reaction zone a larger effect due to flame curvature can be seen compared with the preheat zone, however, since the flame is often very thin compared with the grid resolution in both LES and RANS simulations, the error induced by applying a flamelet model for hydrogen combustion is overall minor. The errors that will be induced due to flamelet modeling will cause slight over or under-estimation of laminar flame speed, however, turbulent flame speed is governed by the relations presented in eq (9) and (51), where $u^*_\text{SGS} \gg S_L$ often is valid. Therefore, also for turbulent flame speed modeling, flamelet assumption to premixed hydrogen/air flames is applicable.
Figure 4.2. Scatter plots of mass fractions of HO₂, H₂O₂, OH, H₂, O₂ and H₂O as function of temperature for a $\phi = 0.6$, Ka = 1 H₂/air flame presented in Figs. (a)-(f) respectively.

Lean premixed flame interaction with decaying turbulence field at high turbulent intensities has been investigated for hydrogen and methane flames. Figure 4.3 shows a comparison of fields of reaction progress variable as well as normalized heat release rate for an H₂/air flame as well as a CH₄/air flame after flame propagation corresponding to one integral time scale.

![Figure 4.2](image1.png)

Figure 4.3. Instantaneous snapshots of turbulent H₂/air flame (column 1) and CH₄/air flame (column 2) of progress variable (row 1) and heat release rate (row 2) extracted at one integral time scale.

Both flames are positioned in the distributed reaction zone regime. Due to the much higher laminar flame speed as well as smaller laminar flame thickness for hydrogen flames compared with methane flames, its corresponding Karlovitz number as turbulence fields of similar magnitudes are used is very much lower (Ka=150 for H₂/air and Ka=9500 for CH₄/air). However, the large scale distortion shown in Fig. 4.3 is quite similar for the two flames. Pockets of unburned gases are able to penetrate into the burned gases where they are finally
consumed. Structures of the flame are dragged by turbulent eddies into the unburned gases where they are quenched due to severe heat losses. Difference due to fuel quality is discernable through the discrepancy between large scale convex and concave surfaces for the H₂/air flame. Differential diffusion cause focusing of hydrogen in convex surfaces and defocusing in concave surfaces, which affects the burning rate through locally raised or lowered equivalence ratio. As mentioned in chapter 2, this is a well known effect for laminar flames and turbulent flames in the flamelet regime. Here, it can also be seen in the distributed reaction zone regime a significant effect of differential diffusion. For methane flames, due to the overall $Le \approx 1$, a strong differential diffusion effect is not expected and a heat release layer of quite constant magnitude is observed in Fig. 4.3.

For investigation of differential diffusion effect local equivalence ratio for the H₂/air flame is plotted versus temperature in a joint probability density function (JPDF), Fig. 4.4. It can be seen that, for a flamelet case, quite unique correlation between temperature and local equivalence ratio is found. For increasing Karlovitz number broadening of the flamelet profile occurs, which is due to enhanced flame curvature induced differential diffusion. At the highest Karlovitz number studied, it can be seen that the flamelet core structure, Fig. 4.4. (a), has also decreased its amplitude. This is probably due to decreased influence of diffusion (relative to convection) acting in the flame normal direction. Convection has the same influence on temperature and species, independent of Lewis number, and therefore decreases the effect of differential diffusion. However, the rapid formation of heavily curved flame segments resulting in focusing and defocusing of hydrogen in convex and concave flame surfaces respectively making the differential diffusion due to higher dimension (≥2D) still important also in the distributed reaction zone regime.

Figure 4.4. JPDF of local equivalence ratio as function of temperature for (a) Ka = 1, (b) Ka = 50, (c) Ka = 100 and (d) Ka = 150 H₂/air flames.

The same type of analysis was performed for the CH₄/air cases, where JPDF of local equivalence ratio as function of temperature is displayed in Fig. 4.5 for the (a) Ka = 600, (b) Ka = 2000 and (c) Ka = 9500 cases respectively. Even though the fuel Lewis number is close to unity, as the flame is studied utilizing detailed chemistry differential diffusion of intermediate species is also accounted for. Both H and H₂ are important intermediates in CH₄/air flames, which appear through decreased local equivalence ratio in the preheat zone. In high Karlovitz number flames, similar trend as for the H₂/air flame can be seen. The unique 1D correlation between temperature and local equivalence ratio is spread due to curvature induced differential diffusion and the reduced local equivalence ratio in the preheat zone is raised towards a unity Lewis number profile. Therefore, differential diffusion that is mainly considered as a secondary effect and often neglected during modeling, may play an important role in methane/air flames similar to that in the H₂/air flames.
Scatter plots of mass fractions of $\text{HO}_2$, $\text{H}_2\text{O}_2$, $\text{OH}$, $\text{H}_2$, $\text{O}_2$ and $\text{H}_2\text{O}$ for $\phi = 0.6$, $\text{Ka} = 150$ $\text{H}_2$/air flame are visualized in Fig. 4.6. Compared with the flamelet case profiles in Fig. 4.2 extensive broadening of the profiles for all species can be seen. Due to the strong convection affecting the flame at small scales, OH is no longer limited to reaction zone and oxidation zone. This is a highly important species for chain branching and chain propagating reactions and this modification of local flame structure will heavily effect species reaction rates. It is clear however that the small turbulent scales are easily penetrating the preheat zone whereas reaction zone is less perturbed. $\text{HO}_2$ and $\text{H}_2\text{O}_2$ are characteristic species for preheat zone and strongly affected in this region, however, in reaction zone profiles similar to flamelet shape, Fig. 4.2, are maintained. The uncorrelated profiles in Fig. 4.6 make the difficulties of flame modeling in the distributed reaction zone regime evident.

Figure 4.6. Scatter plots of mass fractions of $\text{HO}_2$, $\text{H}_2\text{O}_2$, $\text{OH}$, $\text{H}_2$, $\text{O}_2$ and $\text{H}_2\text{O}$ as function of temperature for $\phi = 0.6$, $\text{Ka} = 150$ $\text{H}_2$/air flame presented in Figs. (a)-(f) respectively.

4.2 Lean methane/air low swirl stabilized combustion: LES study

An interesting case of applied flame/turbulence interaction is swirl stabilized premixed flames. In this project the low swirl burner developed by Robert Cheng [7] is used as test case and it has been the objective of an extensive experimental campaign at Lund University [60, 61, 62, 63] for providing modeling validation data. Similar setups of the burner have also been utilized in separate studies [64, 65, 66, 67, 68].

This work has also been conducted in collaboration with experimental groups during new experimental campaigns. An instantaneous snapshot of oxygen mole fraction and simultaneous temperature is displayed in Fig. 4.7. This figure gives a quite good
understanding of the combustion case and modeling difficulties. Premixed CH₄/air is exiting the nozzle \( (u_{axial} \sim 10 \, m/s) \) resulting in a shear flow with surrounding air co-flow \( (u_{axial} \sim 0.35 \, m/s) \). A turbulent flame is stabilized in the center region above the nozzle, whereas flame segments at the trailing edge of the flame are convected downstream [63].

Figure 4.7. Instantaneous O₂ mole fraction (left) and temperature (right) in the axi-symmetric plane from LES. The vertical axis denotes the height above burner (HAB) in unit m. The vertical dashed line indicates the symmetry axis of the flame.

During an experimental campaign of rotational coherent anti-Stokes Raman spectroscopy (RCARS) temperature and relative oxygen mole fraction were evaluated along the center-axis of the burner as well as in the radial direction at several heights. The data is of central importance due to the quantification of (i) the turbulent flame fluctuation, (ii) ambient air entrainment rate into burned gases and (iii) flame width. LES with G-equation flame modeling has been applied for this flame, which is visualized in Fig. 4.8. Overall, the comparison shows reasonable agreement. However, even though the stabilization height is well captured, the turbulent flame fluctuation is under-predicted. Also the mean temperature does not reach the adiabatic flame temperature as the experiments suggest. This comes from a too rapid entrainment of ambient air as can be seen by the oxygen fraction, which also implies an under-predicted flame width. As previous validation has shown [62] the flame stabilization is sensitive to inflow boundary condition, which also for this validation is likely to be the most dominant parameter.

The flow field exiting the burner nozzle has also been shown to contribute to the flame stabilization in the high speed region of the flow through large scale coherent structures. As found in a previous study [63], strong frequencies were found to appear in the inner and outer shear layers of the flow. Through utilization of dynamic mode decomposition (DMD) [58, 59], frequency specific flow motions corresponding to the frequencies found in previous discrete Fourier transform (DFT) [63] was distinguished. The real part of the two dominating DMD modes are plotted in Fig. 4.9 corresponding to frequencies of 175 Hz and 211 Hz respectively. These structures are believed to play an important role in the “grabbing” of outer flow region flame segments, making the flame stabilized at a rather low lift off height in this part of the flow. Further analysis is required to quantitatively connect the coherent structure motion captured in the modes to the dynamics of the flame.
Figure 4.8. The upper panel shows mean and standard deviation (std) of temperature evaluated from 1000 individual RCARS single-shots, and a comparison with LES results along the vertical central axis, while the lower panel shows the corresponding data for relative O\textsubscript{2} concentration.

Figure 4.9. 3D DMD modes corresponding to frequencies 175 Hz (a) and 211 Hz (b) visualized through isosurfaces of tangential vorticity with orange and white corresponding to positive and negative vorticity respectively.

4.3 Publications


This paper utilizes 2D DNS to study the effect of Karlovitz number on flame structure and differential diffusion in lean premixed hydrogen/air flames propagating in decaying
turbulence fields. The flames investigated have starting Karlovitz number ranging from 1 to 150 covering all the theoretical combustion regimes. The simulations show that the unique correlation between temperature and local equivalence ratio observed in the laminar flamelet regime due to differential diffusion in the flame normal direction is heavily affected by the flame curvature induced differential diffusion and intense convection speed already in the thin reaction zone regime. It can be further seen that increased Karlovitz number causes further decoupling of local equivalence ratio to reaction progress as the core structure seen in PDFs of Fig. 4.4 becomes less prominent.

Simulations, analysis and post-processing were performed by the candidate. The paper was written by the candidate and Prof. Xue-Song Bai.

**Paper II** “Turbulent methane/air premixed flame structure at high Karlovitz numbers”. *Flow, Turbulence and Combustion, accepted for publication.*

In this paper 2D DNS is utilized to study the effect of Karlovitz number on flame structure in lean premixed methane/air flames. Flames with Karlovitz numbers ranging from 600 to 9500 where investigated and it was reported that the flames did not reach a distributed state for Karlovitz numbers below 2000. This observation was claimed to be due to the rapid dissipation of small scale turbulence as it penetrates the flame with corresponding viscosity increase. A modified Karlovitz number accounting for the density ratio of the observed flame was proposed, positioning solely the Ka=9500 case in the distributed reaction zone regime during the entire simulation. Flame broadening as well as species concentration correlations with progress variable along with corresponding reaction rates was reported, presenting effect of distributed burning on flame composition. Significant discrepancy from flamelet was observed.

Simulations were performed by Dr. Julien Savre. The candidate participated in analysis, post-processing and writing of the paper along with Dr. Julien Savre and Prof. Xue-Song Bai.


This paper presents pure rotational coherent anti-Stokes Raman (RCARS) spectroscopy in a turbulent premixed low swirl stabilized flame. Temperature as well as relative concentration of O\(_2\) is measured, where the accuracy of the temperature measurement has been proven less than 3 % through extensive testing prior to this application of the technique. Measurements along the center axis of the burner is presented and compared to LES. Reasonable comparison between experiments and simulations is found. However, it can be seen that the central lift-off is slightly under-predicted in LES and also that the air entrainment rate to burned gases is over-predicted. This new set of accurate mean and rms temperature data is of central importance for validation and development of boundary conditions as well as combustion model, since the measured range is covering the two most essential regions of the low swirl flame; the turbulent flame fluctuation as well as the air entrainment into burned gases. Temperature as well as relative oxygen fraction comparison between LES and RCARS as function of height along the center-axis of the burner is shown in Fig. 4.8.
Experiments were performed by Alexis Bohlin and Emil Nordström. Simulations were performed by the candidate, who also participated in analysis, post-processing and writing of the paper along with the other authors.


In this paper 2D particle image velocimetry (PIV) is performed for flow field capturing along with simultaneous OH laser induced fluorescence (LIF) for capturing of the flame front. Both techniques are performed with high repetition frequency \( f \leq 4000 \text{ Hz} \). For analysis of the data, modal decomposition was performed enabling frequency specific flow motion structures to be analyzed. Through this type of analysis different regions of the flow could be characterized: (a) a central region with major influence from symmetric vortex pair likely springing from the inner shear layer of the burner and (b) an outer region where vortices follow diverging vortex streaks. From 3D simulations similar modal decomposition was performed where two very distinct modes were observed, visualized in Fig. 4.9. Neither of the modes show importance in the central region, instead they show clear coherent structures in the swirl direction and normal to the swirl direction respectively. They also have different rotational directions as well as different points of origin. These modes can therefore be said to characterize the experimentally observed outer region into two additional regions springing from the inner and outer shear layers respectively.

Experiments were performed by Per Petersson and Rikard Wellander. Simulations were performed by the candidate, who also participated in analysis, post-processing and writing of the paper along with Per Petersson, Christian Carlsson and Prof. Xue-Song Bai.
Chapter 5
Concluding remarks and future work

5.1. Concluding remarks

In this thesis flame/turbulence interaction at moderate and high Karlovitz numbers has been investigated using direct numerical and large eddy simulations. The direct numerical simulations have been primarily focused on premixed flames in the distributed reaction zone regime whereas the large eddy simulation has been utilized for swirl stabilized flames in the flamelet and thin-reaction zone regimes.

DNS studies of H\textsubscript{2}/air and CH\textsubscript{4}/air flames in the distributed reaction zone regime have shown large overall similarities between the flames. Intense large scale structures have been shown to penetrate the flames, forming pockets of unburned fuel/air mixture within the burned gases as well as straining of flame segments into the unburned side until quenching. Flame broadening at very high Karlovitz numbers has been shown, which implies interaction of scales smaller than the inner reaction zone thickness within the flame. This has however not been explicitly shown. Significant effect of both flame normal as well as flame curvature induced differential diffusion can be concluded. The flame normal differential diffusion effect has shown to decrease for increasing Karlovitz number, but it is also proven significant well above the Ka = 100 limit of the distributed reaction zone regime. Flame curvature induced differential diffusion has on the contrary been shown to increase for flames in the distributed reaction zone regime compared to flamelets. Rapid formation of highly curved flame segments is believed to be the cause of this.

LES studies of the low swirl burner have been conducted. Quantitative comparisons with temperature and relative oxygen concentration RCARS measurements have shown reasonable agreement, but also addressed room for improvement. Under prediction of the turbulent flame fluctuation suggests the use of a model providing more dynamic movement of the flame. The entrainment rate of ambient air to the burned gases downstream of peak temperature is shown to be over-predicted. This observation can origin from several different issues; under prediction of flame width, over prediction of inflow fluctuations, far-field boundary conditions or lack of reignition in the model. Distinguishing the different causes as well as improving them requires additional consideration.

Coherent structures formed in the swirling burner have been investigated using modal decomposition. Frequency specific flow motion organized in coherent structures was characterized in 3D where the two dominating modes previously have been considered relevant in the stabilization process of the outer regions of the flame. Through dynamic mode decomposition, it has here been shown that the frequency specific flow motion origins from the inner and outer shear layers of the burner corresponding to the vortex streaks observed in planar PIV experiments.

5.2. Future work

The next step to achieve convincing DNS data is of course to perform 3D simulations. Sufficient computational power was not available during the start of this project, however, now it is feasible. For further investigation of the differential diffusion effect, fuel with Lewis number larger than unity can also be interesting to investigate. Also the current simulations have been restricted to quite short simulated time due to the use of decaying turbulence fields.
and limited computational resources. If inflow/outflow configuration is employed and flame/turbulence is simulated across several integral time scales, quenching and re-ignition processes can be possible to study.

In the LES studies, a dynamic determination of the SGS wrinkling factor needs to be employed. The current prediction of the low swirl flame is too static, whereas for well capturing of ambient air entrainment into burned gases, a detailed validation of inflow boundary condition needs to be conducted.
Bibliography


