On the Modeling of Premixed Combustion under Varying Equivalence Ratios

Karl-Johan Nogenmyr

May, 2008
Abstract

This thesis deals with numerical simulation of reactive flows. The numerical method is three dimensional and unsteady, which allows for spatial and temporal resolution of the fluid motion and reaction process. In the turbulent cases studied the spatial resolution goes down to the Taylor scale, hence, it is a large eddy simulation, LES. In the laminar cases studied, all fluidic motions are resolved. The reaction modeling is based on the flamelet concept, where the scale separation of the flow and chemistry is exploited. This gives the opportunity to use the computational resources to capture the fluidic motions in three dimension, instead of solving for the vast amount of species present in the flame.

The behaviour of swirling flows in confined geometries is complicated. In this thesis, a highly swirling, S=1.5, confined flame is studied in a model combustor. The combustor has a sudden contraction at the outlet, which alter the complete flow field structure. The influence of this contraction is investigated. In addition to this, the effect of heat release is studied. For all these cases the flow field structure is carefully examined and a mechanism describing the behaviour is put forward. The numerical computations are validated against experimental data.

The second flame studied is situated in low swirling unconfined flow. The flame is fully detached from the burner which allows for entrainment of surrounding air into the fuel/air mixture ahead of the reaction zone. This introduces several challenges for the modeling. A model is put forward in the thesis, and when validated, the model is used to study the dynamics and the stabilization mechanism of the low swirl flame. All computations and conclusions are backed up with experimental data.

The third flame studied in this thesis is an unsteady laminar jet flame. A rich methane/air mixture is issued into the surrounding air at a low velocity. The mixture is within the flammability limit and a conical, Bunsen flame similar, premixed flame front is found. The incompletely oxidized products from this flame is mixing with the surrounding air and are completely oxidized in a reaction layer surrounding the premixed flame. The structure and
the instability of this partially premixed flame is investigated. Also here, the numerical results are validated against experimental data.
# Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nomenclature</td>
<td>vii</td>
</tr>
<tr>
<td>1 Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2 Turbulent Flows</td>
<td>5</td>
</tr>
<tr>
<td>2.1 Phenomenological Description of Turbulence</td>
<td>6</td>
</tr>
<tr>
<td>2.2 Statistical Description</td>
<td>7</td>
</tr>
<tr>
<td>2.2.1 Probability</td>
<td>7</td>
</tr>
<tr>
<td>2.2.2 Averages</td>
<td>9</td>
</tr>
<tr>
<td>2.3 Scales in Turbulent Flows</td>
<td>9</td>
</tr>
<tr>
<td>2.4 Calculation of Turbulent Flows</td>
<td>11</td>
</tr>
<tr>
<td>2.4.1 Direct Numerical Solution</td>
<td>11</td>
</tr>
<tr>
<td>2.4.2 Reynolds Averaged Navier-Stokes</td>
<td>12</td>
</tr>
<tr>
<td>2.4.3 Large Eddy Simulation</td>
<td>12</td>
</tr>
<tr>
<td>3 Combustion</td>
<td>17</td>
</tr>
<tr>
<td>3.1 Chemistry</td>
<td>17</td>
</tr>
<tr>
<td>3.1.1 Reaction Rate</td>
<td>18</td>
</tr>
<tr>
<td>3.2 Premixed Combustion</td>
<td>19</td>
</tr>
<tr>
<td>3.2.1 Turbulent Premixed Flames</td>
<td>20</td>
</tr>
<tr>
<td>3.2.2 Premixed Flames with Varying Equivalence Ratio</td>
<td>23</td>
</tr>
<tr>
<td>3.3 Combustion in Gas Turbines</td>
<td>23</td>
</tr>
<tr>
<td>3.3.1 Swirl Stabilization</td>
<td>24</td>
</tr>
<tr>
<td>3.4 Modeling of Reacting Flows</td>
<td>25</td>
</tr>
<tr>
<td>3.4.1 Steady One Dimensional Flames</td>
<td>27</td>
</tr>
<tr>
<td>3.4.2 Unsteady Three Dimensional Flames</td>
<td>29</td>
</tr>
<tr>
<td>4 Numerical Methods</td>
<td>33</td>
</tr>
<tr>
<td>4.1 Discretization of the PDEs</td>
<td>33</td>
</tr>
<tr>
<td>5 Summary of Publications</td>
<td>35</td>
</tr>
</tbody>
</table>
Nomenclature

Latin Characters

\( a \) \quad \text{strain rate, [1/s]}

\( A_p \) \quad \text{pre-exponential factor, [m}^3/\text{kmol} \cdot \text{s]}

\( C_p \) \quad \text{specific heat, [J/kg \cdot K]}

\( C_{p,i} \) \quad \text{specific heat for species } i, \ [\text{J/kg \cdot K]}

\( D \) \quad \text{molecular diffusivity, [m}^2/\text{s]}

\( E \) \quad \text{turbulent kinetic energy per unit wavenumber and mass, [m}^3/\text{s}^2] \)

\( E_A \) \quad \text{activation energy, [J/kmol]}

\( F \) \quad \text{filter function, [1/m}^3] \)

\( F_i \) \quad \text{body force in direction } i, \ [\text{N/m}^3] \)

\( G \) \quad \text{flame coordinate [m]}

\( h \) \quad \text{specific enthalpy, [m}^2/\text{s}^2] \)

\( h_i \) \quad \text{specific enthalpy for species } i, \ [\text{m}^2/\text{s}^2] \)

\( h_{0,i} \) \quad \text{enthalpy of formation for species } i, \ [\text{m}^2/\text{s}^2] \)

\( k \) \quad \text{turbulent kinetic energy per unit mass, [m}^2/\text{s}^2] \)

\( k \) \quad \text{reaction rate coefficient, [m}^3/\text{kmol} \cdot \text{s]}

\( k_B \) \quad \text{Boltzmann constant, [1.380658 \cdot 10^{-23} J/K]}

\( k_t \) \quad \text{thermal conductivity, [J/m \cdot K \cdot s]}

\( L \) \quad \text{length scale, [m]}

\( l_0 \) \quad \text{integral length scale, [m]}

\( l_F \) \quad \text{flame thickness, [m]}

\( l_{\delta} \) \quad \text{inner layer flame thickness, [m]}

\( M \) \quad \text{number of time steps, [-]}

\( Mtoe \) \quad \text{million tonnes oil equivalent, [\sim 42 \cdot 10^{15} J]}

\( N \) \quad \text{number of nodes, [-]}

\( N_A \) \quad \text{Avogadro constant, [6.0221367 \cdot 10^{23} \text{ molecules/mol]}}

\( p \) \quad \text{pressure, [N/m}^2] \)

\( ppmv \) \quad \text{volume parts per million, [-]}

\( R_u \) \quad \text{molar gas constant, [8.31451 \cdot 10^3 J/kmol \cdot K]}

\( \pi \) \quad \text{dimensionless parameters, [\sim 1]}

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

\( u \) \quad \text{velocity, [m/s]}

\( V \) \quad \text{volume, [m}^3] \)

\( \bar{v} \) \quad \text{velocity, [m/s]}

\( \omega \) \quad \text{angular velocity, [rad/s]}

\( \psi \) \quad \text{velocity potential, [m]}

\( \theta \) \quad \text{temperature, [K]}

\( \epsilon \) \quad \text{turbulent kinetic energy dissipation rate, [m}^2/\text{s}^3] \)

\( \phi \) \quad \text{phi function, [-]}

\( \phi_{d} \) \quad \text{fuel species, [-]}

\( \phi_{g} \) \quad \text{gas species, [-]}

\( \phi_{s} \) \quad \text{solid species, [-]}

\( \phi_{i} \) \quad \text{species } i, \ [-]
NOMENCLATURE

\( \mathbf{r} \) position vector, [m]

\( S_L \) laminar flame speed, [m/s]

\( S_{LES} \) flame speed at LES resolved scale, [m/s]

\( S_R \) enthalpy source term, [J/m^3]

\( T \) temperature, [K]

\( T \) averaging time, [s]

\( t \) time, [s]

\( t_0 \) integral time scale, [s]

\( t_\eta \) Kolmogorov time scale, [s]

\( \bar{U} \) velocity scale, [m/s]

\( u' \) residual velocity, [m/s]

\( u'' \) rms velocity, [m/s]

\( u_\eta \) Kolmogorov velocity scale, [m/s]

\( U, V, W \) velocity components, [m/s]

\( u, v, w \) velocity components, [m/s]

\( V \) sample-space variable

\( V_{i,j} \) diffusion velocity of species \( i \) in \( j \)-direction, [m/s]

\( W_i \) molecular weight of species \( i \), [kg/kmol]

\( x, y, z \) space, [m]

\( Y_i \) mass fraction of species \( i \), [-]

\( Z \) mixture fraction, [-]

Greek Characters

\( \delta_{i,j} \) Kronecker delta [-]

\( \Delta \) LES filter width [m]

\( \Delta x \) LES node spacing [m]

\( \epsilon \) dissipation rate of turbulent kinetic energy per unit mass, [m^2/s^3]

\( \eta \) Kolmogorov length scale, [m]

\( \phi \) generic variable

\( \lambda \) Taylor scale, [m]

\( \mu \) dynamic viscosity, [kg/m · s]

\( \nu \) kinematic viscosity, [m^2/s]

\( \rho \) density, [kg/m^3]

\( \tau_{ij} \) turbulent stress tensor, [m^2/s^2]

\( \tau^r_{ij} \) residual stress tensor, [m^2/s^2]

\( \dot{\omega}_i \) rate of formation of species \( i \) [kg/m^3 · s]
Non-dimensional Numbers

\[ Da = \frac{S_L}{u_0 l_p} \]  Damköhler number

\[ Ka = \frac{l_F^2}{\eta^2} \]  Karlovitz number

\[ Ka_\delta = \frac{l_\delta^2}{\eta} \]  Karlovitz number based on inner layer thickness

\[ Re = \frac{\mu C}{\nu} \]  Reynolds number

\[ Re_t = \frac{u_{0t}}{\nu} \]  turbulence Reynolds number

\[ Re_\lambda = \frac{u_\lambda}{\nu} \]  Taylor Reynolds number

Abbreviations

CDF  cumulative distribution function
CFD  computational fluid dynamics
DNS  direct numerical simulation
LES  large eddy simulation
LP   lean premixed
LPP  lean premixed prevaporized
PDF  probability density function
PVC  precessing vortex core
RANS Reynolds-averaged Navier-Stokes
SGS  subgrid scale
UHC  unburned hydrocarbons
**Chemical Compounds**

H  hydrogen radical  
H$_2$  hydrogen molecule  
HO$_2$  hydroperoxyl radical  
H$_2$O  water molecule  
CO  carbon monoxide molecule  
CO$_2$  carbon dioxide molecule  
CH$_4$  methane molecule  
CH  methylidyne radical  
M  third body  
NO  nitrogen oxide molecule  
NO$_2$  nitrogen dioxide molecule  
NO$_x$  oxides of nitrogen, NO$_2$ and NO  
O  oxygen radical  
O$_2$  oxygen molecule  
OH  hydroxyl radical
Chapter 1

Introduction

Combustion of fossil fuels has been one of the corner stones for the last centuries’ technical development. The supply of cheap and easy-to-use energy from coal, oil, and natural gas sources has dramatically changed the everyday life of humanity. In the dawn of human life, combustion of mainly wood was used for cooking, heating, and keeping wild animals away. Later in history, the human learned how to use combustion to treat and refine metal - a skill developed by blacksmiths. But it is not until the 18th century, in the beginning of the industrial revolution and with the invention and subsequent development of the steam engine, that the chemically bound energy is transformed into mechanical energy. It is not until this stage that the fuels can actually perform work. So far, the humans had to rely on themselves, animals or hydro- and wind-power. The following development is well-known: Soon to follow was the piston engine and its huge relevance for agriculture and road transport, and in the mid 20th century the gas turbine, important for mainly air transport and later electricity production.

This development has been a great blessing to the humanity, but severe problems have arisen. While burning fuels, directly harmful species may appear: Oxides of nitrogen, (NO\textsubscript{x}), carbon monoxide, (CO), and unburned hydrocarbons, (UHC). While this problem can be avoided by careful design of the machines, the next problem is harder to avoid while burning fossil fuels: There is no sustainability in the current system; fossil fuels are being consumed at a rate orders of magnitude larger than the recreation, which will eventually lead to depletion of the resources. Tightly coupled with this is the fact that the concentration of carbon dioxide in the earth’s atmosphere is continuously increasing as a result of the combusted fuels. Carbon dioxide is the single most important greenhouse gas that threatens to substantially change the climate on this planet. The earth is continuously radiating heat to the surrounding universe. This radiation has to pass through the atmosphere,
but as more species is present here, more energy will be absorbed and hence trapped on the earth. This may ultimately lead to an increase of the mean temperature, and may result in growth of deserts and melting of glaciers and the ice on the poles. A rising sea water level together with larger deserts may destroy areas with fertile soils.

In the World Energy Outlook, published by the International Energy Agency, IEA, long-term projections and market analyses are presented. In a recent issue (IEA, 2006) a reference scenario shows the predicted future energy demand and its share between fuels if no actions are taken to solve climate and supply issues, Fig. 1.1.

To avoid such a future, actions must be taken already now. This involves both refining the current as well as developing new technology. For both these tasks, there is a need for detailed understanding of the processes occurring in combustion devices. For engines, this involves turbulent reacting flows in complicated geometries, i.e. a gas turbine combustor. Unfortunately, insights in an operating combustor are limited due to lack of optical access. Here modeling of flows and reaction plays a large role. By modeling the flow and reaction, the operation of a current design can be understood, and new designs can be investigated and developed on the desk. This is both faster and cheaper than investigating each design in a laboratory.

**Research Objectives**

Fluid mechanics computations on reacting flows have been performed since the seventies. In the early days, the computations were mainly done with ensemble averaged equations in order to get a steady and less computer demanding solution. However, when averaging the equations, certain information about the inherently unsteady turbulent flow is lost. A great fraction of
this interesting information is not lost if some of the unsteadiness is retained in the solution. This is done in the technique named large eddy simulation, LES. In this thesis, LES is used as a tool to develop and investigate models for reacting flows related to gas turbine combustion.

The objectives for this thesis are:

- With experimental support, apply an existing validated LES-code to a swirling premixed flame to investigate flow dynamics in a combustor.
- Develop a new combustion model aimed at stratified premixed flames, and, together with experimentalists, investigate such a flame.
- Validate the results against experimental obtained in parallel.

**Thesis Outline**

To begin with, issues concerning the physics of turbulent flows and ways to compute such flows are addressed in Ch. 2. This is followed by a discussion concerning the combustion processes related to gas turbines and their modeling, Ch. 3. Chapter 4 concerns the implementation of the models discussed in the two preceding chapters. In the following chapter, selected results are presented, the results are mainly discussed in the papers. The thesis is concluded with a summary.
Chapter 2

Turbulent Flows

Most flows occurring in industrial processes are turbulent. In some, it is an unwanted feature; the turbulence is a just consequence of the high flow rates. In others, properties of the turbulence is exploited for various purposes, i.e. increased mixing, enhanced heat transfer, etc. In premixed reacting flows, turbulence enhances the mixing of reactants and products. Beside this, it also increases the area of the flame surface. These two effects can together greatly increase the fuel conversion rate. For non-premixed reacting flows, the reaction is sustained by continuous mixing of the fuel and the oxidizer on a molecular level. The mixing of these two reactants can be substantially improved by turbulence, which in turn enhances the reaction. Clearly for reacting flows, turbulence is a desired property.

Flows are often characterized by non-dimensional numbers. For viscous incompressible flows, the Reynolds number is the single most important parameter:

\[
Re = \frac{UL}{\nu}. \tag{2.1}
\]

\(U\) and \(L\) are typical velocity and length scales of the particular system and \(\nu\) is the molecular kinematic viscosity. The Reynolds number describes the ratio of convective forces and (molecular) diffusive forces. If the value is low enough, below a critical Reynolds number, small disturbances to the flow field are damped in time by viscous forces. Above this number, disturbances grow in time. A small disturbance to an initially laminar flow can now grow exponentially and develop to large unsteady structures. This critical number differs from system to system, but is well known for canonical flows, like for example pipe flows; \(Re_{cr} \sim 2300\).
2.1 Phenomenological Description of Turbulence

Giving a detailed and precise definition of turbulence is difficult. However, one can list a set of characteristic features for turbulence (Tennekes and Lumley, 1972):

- **Irregular.** By observing a turbulent flow with the naked eye, for instance the smoke plume from a chimney, one quickly realizes that the behavior of the flow field is highly random - seemingly chaotic.

- **Diffusive.** Turbulence enhances the molecular diffusion of both momentum, energy, and species. For example, in a mixing process of hot and cold air, the turbulent motions locally and momentarily set up sharp temperature gradients which causes strong diffusive fluxes of heat in the mixing layer.

- **Large Reynolds number.** For turbulence to occur, the Reynolds number has to be large. As a flow is dominated by convection, the diffusive forces are too weak to dissipate unsteady motions.

- **Three-dimensional.** Characteristic for turbulent flows are the unsteady rotating structures, eddies, present. They appear in various sizes and give a high level of unsteady vorticity. The vorticity of the flow field can be increased by stretching of the eddies, however, in systems with less than three dimensions this cannot occur.

- **Dissipative.** Turbulence needs a continuous feed of kinetic energy to be sustained. The eddies of various sizes present ranges from a large scale determined by the geometry of the system down to a scale uniquely determined by the dissipation of turbulent kinetic energy and the molecular viscosity. At the smallest scale, the kinetic energy is dissipated into heat.

- **Continuum.** The scales of turbulent motions may be small at high Reynolds numbers, however, they are still much larger than the mean free path. Hence, the continuum assumption is not violated, and the flow is still governed by the Navier-Stokes equations.

- **Flow quantity.** Turbulence is a property of the flow, not the particular fluid. Fluid properties influence the flow field only by viscosity and density (if the velocity is much smaller than the sound speed; low Mach numbers).
2.2. Statistical Description

As stated above, the continuum assumption holds and then the time evolution of an incompressible Newtonian fluid with uniform density is governed by the Navier-Stokes equations:

\[ \frac{\partial \hat{U}_j}{\partial \hat{x}_j} = 0, \]  
\[ \frac{\partial \hat{U}_i}{\partial \hat{t}} + \hat{U}_j \frac{\partial \hat{U}_i}{\partial \hat{x}_j} = -\frac{\partial \hat{p}}{\partial \hat{x}_i} + \frac{1}{\text{Re}} \frac{\partial^2 \hat{U}_i}{\partial \hat{x}_j^2}, \]

where \( \hat{x} = x/L, \hat{t} = tU/L, \hat{U}_i = U_i/U, \hat{p} = p/(\rho U^2). \)

Here, the variables have been non-dimensionalized to explicitly show the dependence of the Reynolds number. As mentioned in the first paragraph in this chapter, the Reynolds number determines whether the solution is laminar or turbulent. For flows with Reynolds numbers below the critical, the solution to these equations is stable. When the Reynolds number is above the critical, the solutions is in general unstable, and suffers from severe sensitivity to initial and boundary conditions. This makes an approach of directly solving the equations, hoping to predict an exact time evolution, impossible. For high Reynolds numbers we have to abandon the idea of calculating the exact value of \( U_i \) and retreat to statistical tools.

2.2 Statistical Description

Due to this urgent sensitivity, only a small variation of the experimental or computational setup will, after enough time, completely change the resulting instantaneous flow field. Therefore, snapshots of a flow field lack scientific value in the sense that they cannot be reproduced by other researchers (Popper, 1934). However, what can be reproduced are statistically converged quantities, for example the ensemble average of a velocity component. A typical behavior of a quantity in a turbulent flow field can be seen in Fig. 2.1.

2.2.1 Probability

The probability \( p \) that the velocity component \( U \) is less than some value \( V \) is given by the cumulative distribution function, CDF (Pope, 2000):

\[ \text{CDF}(V) \equiv p(U < V) \]  

(2.4)
Some trivial properties of the CDF are immediately realized:

\[ \text{CDF}(\infty) = 0, \quad \text{CDF}(\infty) = 1, \quad \text{CDF}(V + \epsilon) \geq \text{CDF}(V), \quad (2.5) \]

since \( U \) can not be less than \(-\infty\). Also \( U \) is certain to be smaller than \(+\infty\).

The last inequality in Eqs. 2.5 states that the CDF increases monotonically.

When the cumulative distribution function is obtained, the *probability density function*, PDF, can be computed:

\[ \text{PDF}(V) \equiv \frac{d\text{CDF}(V)}{dV}. \quad (2.6) \]

As the name implies, the PDF determines the probability of finding \( U \) in some small region \( V \leq U \leq V + dV \):

\[ p(V \leq U \leq V + dV) = \text{CDF}(V + dV) - \text{CDF}(V) = \text{PDF}(V)dV. \quad (2.7) \]

For a random variable, like a velocity component in a turbulent flow field, the PDF (or the CDF) fully characterizes the behavior. Random variables with the same PDF are *statistically identical*. 

---

Figure 2.1: Random variable \( U \) in a turbulent flow field fluctuating around its average, \( \overline{U} \).
2.2.2 Averages

When the PDF has been determined, several statistical properties can be computed. First of all the mean value of $u$ is:

$$\overline{U} = \int_{-\infty}^{\infty} V \cdot \text{PDF}(V) dV.$$  \hfill (2.8)

From the fluctuation of $U$, $u \equiv U - \overline{U}$, the variance (also known as the mean-square fluctuation), can be obtained from the PDF:

$$\overline{u^2} = \int_{-\infty}^{\infty} (V - \overline{U})^2 \cdot \text{PDF}(V) dV.$$  \hfill (2.9)

All flows considered in this thesis are statistically stationary, i.e. the PDF has no time dependence. Given that, according to the ergodic hypothesis, the ensemble average equals time average. Hence, for time resolved calculations of statistically stationary flows, time averages are used:

$$\overline{\overline{U}} = \frac{1}{T} \int_{t_0}^{t_0+T} U(t) \, dt,$$  \hfill (2.10)

$$\overline{\overline{u^2}} = \frac{1}{T} \int_{t_0}^{t_0+T} (U(t) - \overline{U})^2 \, dt.$$  \hfill (2.11)

2.3 Scales in Turbulent Flows

As mentioned earlier in this chapter, turbulent flows contain unsteady structures, eddies, of various sizes. The largest are created by strong mean shear flow, and their size is limited by the geometry of the system wherein the flow is taking place. At this large scale, viscosity has negligible influence on the dissipation of the kinetic energy of these structures, and therefore their motion is not damped. Instead the large eddies break up into smaller eddies by stretching. The fate of these smaller eddies depends on their size - if they are large enough they will break up again into even smaller eddies. However, sooner or later the turbulent kinetic energy will be transferred to such small eddies that viscosity comes into play. At that scale the turbulent kinetic energy is dissipated into heat. If the Reynolds number is sufficiently large, the scale at which this happens is independent of the geometry of the system and size of the large eddies. Its only dependence is the fluid viscosity $\nu$ and the rate at which the turbulent kinetic energy is transferred from the large scales, $\epsilon$. Knowing these two quantities, three scales can be formed:
\[ \eta \equiv \left( \frac{\nu^3}{\epsilon} \right)^{\frac{1}{4}}, \quad t_\eta \equiv \left( \frac{\nu}{\epsilon} \right)^{\frac{1}{2}}, \quad u_\eta \equiv \eta / t_\eta = (\nu \epsilon)^{\frac{1}{4}}. \] (2.12)

These scales are known as the Kolmogorov length-, time-, and velocity scales respectively, and apply to the smallest eddies present. A Reynolds number based on these scales is identically unity, since at this scale, the convective forces are balanced by dissipative forces. Other useful scales in turbulent flows are:

- **Integral scales**: These are the scales relevant to the largest eddies in the flow field; length, \( l_0 \), time, \( t_0 \), and velocity, \( u_0 = l_0/t_0 \). The Reynolds number characterizing the turbulence is based on these scales: \( \text{Re}_t = u_0 l_0/\nu \).

- **Taylor length scale**, \( \lambda \): This scale applies to eddies shorter than \( l_0 \) and larger than \( \eta \). There is no clear physical interpretation of this scale, however, it has a some modeling relevance and a strict definition exists (not shown here). The Reynolds number for this scale is: \( \text{Re}_\lambda = u_0 \lambda/\nu \).

Using the relation between the large eddies and the dissipation, \( \epsilon \sim u_0^3/l_0 \), the Kolmogorov scales can be related to the integral scales:

\[ \eta/l_0 \sim \text{Re}_t^{-3/4}, \quad t_\eta/t_0 \sim \text{Re}_t^{-1/2}, \quad u_\eta/u_0 \sim \text{Re}_t^{-1/4}. \] (2.13)

**The Energy Spectrum**

In a flow field with isotropic turbulence, i.e. a flow field where statistical quantities are invariant under rotations and reflections of coordinate axes, the spectrum of the turbulent kinetic energy, \( k \), has a universal form. A sketch of this is shown in Fig. 2.2. The spectrum shows the energy per unit wavenumber, hence it is an energy density. The size of a scale is inversely proportional to its wavenumber, and the Kolmogorov scale is found to the right in Fig. 2.2. The largest fraction of energy is found in the integral scales, \( l_0 \), at which the turbulence is fed with kinetic energy. As energy is transferred to smaller scales, the energy content per unit wavenumber is decreasing and as the energy reaches the Kolmogorov scale, all kinetic energy is eventually dissipated. There is, however, at sufficiently high Reynolds number, a range in-between \( l_0 \) and \( \eta \), where turbulent kinetic energy is neither produced, nor destroyed, and the statistics of the motions are universal and only dependent on \( \epsilon \). In this range, the spectrum is decaying with \( k^{-5/3} \), as can be derived from Kolmogorov’s theory of turbulence.
2.4 Calculation of Turbulent Flows

The calculation of turbulent flows is a part of the art of Computational Fluid Dynamics, CFD. Here the three major branches in this topic will be briefly discussed.

2.4.1 Direct Numerical Solution

The conceptually simplest way of calculating turbulent flows is just brute force direct numerical solution, DNS, of Eqs. 2.2 and 2.3 (or their equivalents in wave-space). However, solving these equations requires a numerical mesh with a node spacing $\Delta x$, at least, in the order of $\eta$. For flows relevant to industry, the Reynolds number can be very high, and as implied by Eqs. 2.13, the Kolmogorov length scale is quite short in comparison. The node requirement for a DNS calculation can be estimated to:

$$N^3 \sim \left( \frac{l_0}{\Delta x} \right)^3 \approx \left( \frac{l_0}{\eta} \right)^3 \approx Re_t^{9/4}. \quad (2.14)$$

Hence, the number of nodes increases rapidly with the Reynolds number. Besides this, the numerical scheme usually requires that the time-step scales with the node spacing. If the required number of time-steps is $M$, the computational demand depends on $Re$ as $MN^3 \sim Re_t^3$. Due to this, DNS for industry related flows is today out of reach with current computers. Still, this approach is feasible for academic study of turbulence and development.
and validation of turbulence models, since no, potentially erroneous, modeling is introduced.

### 2.4.2 Reynolds Averaged Navier-Stokes

One way to handle the complexity of the solution of the Navier-Stokes equations is to ensemble-average the equations \textit{a priori}:

\begin{equation}
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{U}_j}{\partial x_j} = 0, \tag{2.15}
\end{equation}

\begin{equation}
\frac{\partial \bar{\rho} \bar{U}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{U}_j \bar{U}_i}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{U}_i}{\partial x_j} \mu \frac{\partial \bar{U}_i}{\partial x_j} - \frac{\partial \bar{\rho} u''_i u''_j}{\partial x_j}. \tag{2.16}
\end{equation}

\begin{equation}
U_i = \bar{U}_i + u''_i, \quad \bar{U}_i = \frac{\bar{\rho} \bar{U}_i}{\rho}. \tag{2.17}
\end{equation}

These are the Reynolds averaged Navier-Stokes, \textit{rans}, equations. Since this thesis concerns reacting flows with non-uniform density, a density weighted average is considered, so-called \textit{Favre-averaging}. The velocity has been decomposed into an averaged and fluctuating part, Eq. 2.17. As can be seen, the averaging does not change the principal form of the continuity equation, Eq. 2.15. However, comparing Eq. 2.16 with Eq. 2.3 one extra term has emerged out due to the averaging, the Reynolds stress tensor:

\begin{equation}
\tau_{ij} = -u''_i u''_j. \tag{2.18}
\end{equation}

This term is unclosed and needs modeling. Typically this term is modeled as a shear stress, based on the turbulent-viscosity hypothesis introduced by Boussinesq (1877). A general conclusion is that these models fail for flows with strong curvature of the mean streamline, for instance swirling flows, and flows with strong pressure gradients.

\textit{RANS} has been used since the early days of turbulent flow computation, and several turbulence models dedicated to \textit{RANS} are implemented in commercial \textit{cfd}-codes. It is today widely used in industry, and will be used for many years to come owing to its low computational requirements and robustness.

### 2.4.3 Large Eddy Simulation

Large eddy simulation, \textit{LES}, can be seen as compromise between \textit{RANS} and \textit{DNS}. In \textit{LES}, the governing equations, Eqs. 2.2 and 2.3, are low-pass filtered
in wave-space a priori. If the cut-off scale of the filter, $\Delta$, is chosen to be well in the inertial subrange, the motion of the large scales are explicitly calculated with the filtered equations, and the effects of residual motion has to be modeled. However, as predicted by Kolmogorov theory (Sec. 2.3), these small scales are more likely to have a universal behavior and as a consequence of this, the modeling problem becomes significantly easier. Generally, the filter is chosen to be comparable to the Taylor scale, $\Delta \sim \lambda$.

**Filtering**

The filtering of the flow field is performed with a filter, $F$:

$$\bar{\rho}\tilde{U}_i(r_0, t) = \iiint_V F(r - r_0)\rho U_i(r, t) \, dr.$$  \hfill (2.19)

Now, the residual motions can be expressed:

$$u'_i(r, t) = U_i(r, t) - \tilde{U}_i(r, t).$$  \hfill (2.20)

The filter $F$ can have different forms, for example top-hat or Gaussian. In general the filter function may be dependent on position, i.e. different filters are applied in different parts of the flow. However, if the filter is homogeneous, the filtering operation and space derivative commute, and the filtered Navier-Stokes equations are:

$$\frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{p}\tilde{U}_j}{\partial x_j} = 0,$$  \hfill (2.21)

$$\frac{\partial \bar{p}\tilde{U}_i}{\partial t} + \frac{\partial \bar{p}\tilde{U}_j\tilde{U}_i}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \mu \frac{\partial \tilde{U}_i}{\partial x_j} - \partial \tau_{ij}^r.$$  \hfill (2.22)

Like when obtaining the rans equations, Eqs. 2.15 and 2.16, an unclosed term appears here as well, the residual stress tensor:

$$\tau_{ij}^r = \bar{p}\tilde{U}_i\tilde{U}_j - \bar{p}\tilde{U}_i\tilde{U}_j.$$  \hfill (2.24)

This term describes the influence of the small unresolved motions on the resolved motions. However, contrary to rans, this term is less dominant. This term is also known as the sub-grid scale, sgs, stress, since a common filtering technique is to let the numerical grid, upon which Eqs. 2.21 and 2.22 are solved, act as an implicit filter. To close this term, several models have been proposed during the years.
CHAPTER 2. TURBULENT FLOWS

Models for the residual stress term

Returning to the turbulence spectrum, Fig. 2.2, we saw that the main part of the turbulence kinetic energy was dissipated at the smallest scales. This is the main impact of the small scales on the larger scale; to drain kinetic energy. In a LES these scales are typically below the filter cut-off length scale, hence, there is a need for a model which can drain the kinetic energy from the resolved scales.

The simplest model was proposed by Smagorinsky (1963), in which, similar to RANS-models, an increased viscosity amplify the dissipation:

\[
\tau_{ij}^r = -2\nu_r \tilde{S}_{ij} \quad (2.25)
\]

\[
\nu_r = (C_s\Delta)^2 \mathcal{S} \quad (2.26)
\]

\[
\mathcal{S} \equiv \sqrt{2 \tilde{S}_{ij} \tilde{S}_{ij}} \quad (2.27)
\]

where \(\tilde{S}_{ij}\) is the filtered rate of strain. In this thesis, a conceptually more difficult, but computationally simpler model is used. It may be observed, that if the convective term in the momentum equations are discretized by a mid-ordered odd scheme (see Sec. 4.1) the numerically approximated system has a dissipative nature, hence, energy can be drained from the resolved scales.

This technique has been explored in several papers (Jessica Fureby), and is generally acceptable if fine grids are used. Mid-ordered should be interpreted as; not too low, like 1st order, since that will generally be too dissipative, and not too high order, since that may provide insufficient numerical viscosity. In this thesis a 3rd order upwind scheme is used.

Boundary conditions

The momentum equations are very general, they describe flows in small blood vessels up to exploding supernovas; the solution obtained is totally dependent on the boundary conditions posed to the equations. For unsteady approaches like DNS and LES this causes some trouble if the flow is turbulent at the boundary. Basically, this can be handled in two ways; put steady boundary conditions sufficiently far away from the domain of interest, or, explicitly prescribe the turbulence at the boundary. The first alternative is attractive as steady profiles are easy to set, but the domain may become unreasonably large, demanding huge computational resources. This may however be resolved by doing a separate computation, simulating the flow between the steady inlet and the domain of interest, and then sample the flow. This is
done for some of the computations in this thesis. However, mainly the second approach is applied by reconstructing turbulence at the boundary by the method described below.

The idea is based on creating turbulence with prescribed properties in a three dimensional domain. Then, by Taylors hypothesis of frozen turbulence, this is convected into the domain where the momentum equations are solved.

Consider the series of random data, \( r_m \), with \( r_m = 0 \) and \( r_m r_n = \delta_{m,n} \). Given a digital filter with coefficients \( b_n \), a signal, \( u_m \), with two-point correlation can be obtained:

\[
 u_m = \sum_{n=-N}^{N} b_n r_{n+m} \tag{2.28}
\]

\[
 R_{uu} = \frac{u_m u_{m+k}}{u_m u_m} = \frac{\sum_{j=-N+k}^{N} b_j b_{j-k}}{\sum_{j=-N}^{N} b_j^2} \tag{2.29}
\]

Hence, the autocorrelation, \( R_{uu} \), can be related to the filter coefficients. If 2.29 can be inverted, and the autocorrelation is prescribed, the signal \( u_m \) can be retrieved. In Klein et al. (2003) it is shown how the method may be applied to three dimensions, and how Eq. 2.29 can be approximately inverted. The autocorrelation is assumed to be an exponentially decaying function where the desired length scale of the flow determines the exponent. When the filter coefficients of the three dimensional digital filter are computed, a random three dimensional field is filtered, and a resulting velocity field is obtained. For each point, this field is scaled to fit the Reynolds stress tensor, and a mean component is added.

Input to this method is the desired mean velocity, Reynolds stress tensor, and the integral length scale. All these quantities can be obtained experimentally or, at least, estimated intuitively.

At the outflow of the computational domain it is desired to have a boundary condition that disturb the upstream flow as little as possible. Akselovoll and Moin (1996) performed LES on two confined coannular jets, where the outflow of the domain was determined by,

\[
 \frac{\partial U_i}{\partial t} + U_{con} \frac{\partial U_i}{\partial x} = 0, \tag{2.30}
\]

where \( U_{con} \) is the spatially averaged outflow velocity. This allows for flow structures to be convected out of the domain without being reflected. It was shown that this boundary condition gives influence of statistics only close to the boundary, and is therefore used throughout this thesis.
Chapter 3

Combustion

Combustion is an interdisciplinary science that involves:

- **Chemical kinetics** - The study of the rates of the fundamental reactions.
- **Fluid dynamics** - The study of flow and turbulence phenomena.
- **Thermodynamics** - The study of energy.
- **Heat and mass transfer** - The study of the transport of heat and mass.

The scope of this text is not to give a complete survey of the vast area of combustion; rather, assuming that the reader is somewhat familiar with the three last fields listed above, this should give an introduction to the branch of turbulent premixed combustion.

### 3.1 Chemistry

In the later half of the 18th century, Lavoisier discovered that combustion is a chemical reaction between oxygen and a combustible material. This was an important result which disproved the prevailing idea of phlogiston. In the following century, it was discovered that the combustion of CO was greatly enhanced by adding small amounts of, obviously incombustible, water. This did not get a proper explanation until the 20th century with the discover of the free radicals. Nowadays, we know that combustion involves many more chemicals than the fuel, oxidizer, and the formed products. For instance, consider the reaction between hydrogen and oxygen. It is very unlikely that an oxygen molecule would collide with a hydrogen molecule to directly form water. This would require that several bonds should break and new one be formed at one time. Instead, what happens is that several intermediate
species are formed. For the conversion of hydrogen and oxygen into water, several reactions take place, some of them important, others less important. Since a complete list would include more than 20 species, only the most important are listed here:

\begin{align*}
    \text{H}_2 + \text{O}_2 & \rightarrow \text{HO}_2 + \text{H}, \\
    \text{H} + \text{O}_2 & \rightarrow \text{OH} + \text{O}, \\
    \text{H} + \text{O}_2 + \text{M} & \rightarrow \text{HO}_2 + \text{M}, \\
    \text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H},
\end{align*}

where M represents a third body, which could be any atom or molecule. As can be seen in these reactions, only one bond is broken and only one new is formed. Since these reactions describe what actually happens in detail they are named \textit{elementary reactions}. In the first reaction above, 3.1, the hydrogen molecule reacts with the oxygen molecule to form one of the important intermediate species, the \textit{free radicals}, in this case atomic hydrogen. The free radicals are highly reactive since they have an unpaired electron and together with their high mobility they attack and break down other species. In this system, three different radicals exist; H, OH, and O. The second reaction, 3.2, is important due to the fact that it consumes one radical, but form two new ones. For that reason it is called \textit{chain branching} reaction (Williams, 1985). This reaction is competing with the third reaction, 3.3, which consumes one free radical. Hence the name \textit{chain terminating} reaction. As long as the chain branching overcomes the chain terminating reaction, the combustion is sustained. The last reaction above, 3.4, is one of the reactions that eventually forms the final result; water. This system also illustrates the role of the hydrogen atom in a reacting system, as it is involved in two of the radicals. This explains the influence of water on combustion of CO; the water is a source of hydrogen.

### 3.1.1 Reaction Rate

An open question is still at which rate the individual reactions proceed. For a reaction to happen, two molecules have to collide, and enough kinetic energy has to be available in that collision in order to break the bonds. This energy threshold is called \textit{activation energy}. Let us consider a general reaction:

\[ A + B \rightarrow C + D, \]

under which the \textit{reactants} A and B forms the \textit{products} C and D. The rate under which this reaction proceeds is directly proportional to the concent
3.2. PREMIXED COMBUSTION

Chemical reactions can occur in a spatially large extent, like in a city when pollutants form smog. However, here we restrict the discussion to chemical reactions concerning combustion in technical devices. Here, in general, the reactions are concentrated in thin layers: flames. Such flames can mainly be divided into two regimes; premixed or non-premixed. The mixing refers to the fuel and oxidizer: If they are mixed prior to the reaction, the flame is said to be premixed. If they are apart prior to the reaction, and mix while they burn, we call the flame non-premixed. A good example of a non-premixed flame is a candle-light where the fuel is continuously evaporating from the wick, and oxidizer is the surrounding air. An example of a premixed flame could be the Otto engine, where fuel and air are mixed in the cylinder in the intake stroke. During the compression stroke, the fuel has time to diffuse to form a uniform mixture at ignition. Then, from the spark plug a premixed flame front propagates throughout the chamber. An intrinsic property of a mixture of fuel and air is the speed at which this front is propagating, a quantity called the laminar flame speed, $S_L$. In an inertial system traveling at this speed with the flame front in a quiescent medium, the detailed structure of the flame can be examined.

In Fig. 3.1, some of the species and the temperature profiles across a lean premixed methane flame is schematically plotted versus the flame coordinate,
Figure 3.1: The structure of a freely propagating planar premixed flame.

$G$. The flame can be divided in four layers, the \textit{preheat zone}, \textit{inner layer}, \textit{oxidation layer}, and \textit{postflame zone} (Seshadri et al., 1998; Pitsch and Peters, 1998). In the first zone, none, or few, chemical reactions happen. The deviation from the inlet values here is mainly owing to diffusion (of heat and mass) to and from the inner layer. In the thin inner layer most of the chemical reactions are happening, and most of the heat is released here. Not shown here is the profiles of all the intermediate species (except CO), which peak in this layer. This layer is followed by the oxidation layer zone, where oxidation the intermediate species, like CO, is completed, and the product species are approaching steady state. In the high temperature part of the flame, e.g. the postflame zone, NO is formed.

An important quantity for classifying premixed flames is the flame thickness. Several methods for estimating this exist in the literature. Here we will use an expression based on the thermal diffusivity and the laminar flame speed. These quantities can also be used to form a time scale for the flame:

$$l_F = \frac{D}{S_L}, \quad t_F = \frac{l_F}{S_L} = \frac{D}{S_L^2} \quad (3.8)$$

3.2.1 Turbulent Premixed Flames

As the flows considered in this thesis are turbulent, we need to extend the analysis of premixed flames beyond the laminar flow regime. Turbulent premixed flames are usually discussed with support from the Borghi dia-
3.2. PREMIXED COMBUSTION

Figure 3.2: The Borghi diagram for premixed combustion (Peters, 2000).

gram, Fig. 3.2, (Peters, 2000). The diagram describes five different regimes for a premixed flame front interacting with turbulent eddies. The abscissa is the turbulence length scale, Sec. 2.3, normalized with the flame front thickness and the ordinate is the turbulence intensity normalized with the laminar flame speed. Assuming equal diffusivity of mass and momentum, $Sc = \nu / D = 1$, a few non-dimensional numbers will support our discussion; the turbulence Reynolds number, the turbulence Damköhler number and the turbulence Karlovitz number:

$$
Re_t = \frac{u_0 l_0}{S_L l_F}, \quad Da = \frac{S_L l}{u_0 l_F}, \quad Ka = \frac{t_F}{t_\eta} = \frac{l_F^2}{\eta^2} = \frac{u_\eta^2}{S_L^2} \quad (3.9)
$$

Using the flame thickness as in Eq. 3.8, this is the same Reynolds number as in Sec. 2.3. The Damköhler number relates the turbulence integral time scale to the flame time scale. The last number, $Ka$, relates the flame time scale to the Kolmogorov time scale. A second Karlovitz number can also be defined, based on the thickness of the inner layer of the flame, $l_\delta$. Typically, this thickness is one tenth of the flame thickness:

$$
Ka_\delta = \frac{l_\delta^2}{\eta^2} = \frac{1}{100} Ka \quad (3.10)
$$

Using these numbers, three lines can be drawn to divide the regimes in the diagram; $Re_t = 1$, $Ka = 1$, $Ka_\delta = 1$. In regime I, the flow is laminar,
and the discussion concerning the flame structure in the previous section is valid. In regime II, the turbulence intensity is still less than the laminar flame speed, hence turbulence cannot compete with the flame propagation - the flame is essentially laminar. This region has also minor relevance for industry and no details are given here. In regime III, the Kolmogorov scale is still larger than the flame thickness, hence at the scale of the flame, the flow is quasi-laminar and the turbulence cannot interfere with the local structure of the flame. Still, certain curvature of the flame front may locally alter the detailed flame structure and propagation speed. Further increase of the Karlovitz number brings us to the fourth regime. Here, the Kolmogorov eddies are smaller than the flame thickness, but still larger than the inner layer thickness, hence turbulence may interfere with the preheat layer and the oxidation layer, but the inner layer, which is responsible for the most important reactions, remains unaffected. Such an event is illustrated in Fig. 3.3, where a Kolmogorov eddy smears out the preheat layer. This process increases the reaction rate by enhanced heat transfer from the flame. Most industrial burners operate in this regime. As Karlovitz number is further increased, the turbulence can affect the inner layer, and local quenching of the flame may happen. This is usually unwanted, as it is believed to cause emissions of CO and UHC.
3.3. COMBUSTION IN GAS TURBINES

In today's stationary gas turbine combustors, premixed combustion is preferred, since it gives a possibility to control the flame temperature by adding excessive air (or in rare cases fuel) to the mixture. The unreacted oxygen acts as an inert gas, a heat absorber. A similar result can be achieved for non-premixed flames by adding an inert gas to the fuel, but a remaining problem is the soot particles formed in the rich part of the non-premixed flame. Low peak temperature in the combustors is aimed at, since the production of NO\textsubscript{x} is strongly dependent on the temperature. However, going too lean results in, additional to the risk for flame flow off, increased levels of CO- and UHC-emissions. Both these trends gives a window, where operation with overall low emissions is possible, Fig. 3.4. Techniques built on this idea are called, lean premixed prevaporized combustion, LPP, or in the case of gaseous fuel, LP. To complete the burn-out of CO and UHC, long residence time is used (Lefebvre, 1999). This is possible as NO\textsubscript{x} weakly increases with residence time for temperatures below 1900 K. A challenge with this design is to obtain a homogeneous mixture before combustion without problems with flashback or acoustic resonance.

Figure 3.4: Emission dependence on temperature for typical gas turbine combustion (Lefebvre, 1999).

3.2.2 Premixed Flames with Varying Equivalence Ratio

3.3 Combustion in Gas Turbines
3.3.1 Swirl Stabilization

In order to keep the flame fixed within the combustor, a velocity field that gives a region in space where the local flame speed can be balanced with flow velocity must be obtained. A simple solution is to introduce a bluff body in the flow, where the reversed flow will assure an area with low speed. This approach has, however, several drawbacks, where material sustainability is only one of them, and the most common technique applied for gas turbine combustors today is swirl stabilization. By introducing a swirl component on the inflowing mixture, a recirculation zone can be achieved by aerodynamic means, Fig. 3.5. The pressure is low in the center of the swirl vortex, but as the flow expands radially into the combustion chamber, the pressure in the center increases. This results in a pressure gradient along the centerline, adverse to the flow. If the swirl is high enough the gradient will overcome the axial momentum and reverse flow results. The reversed flow also continuously brings back hot combustion products to the fresh mixture, and by this way the flame is stable. There exists also so called low swirl burners, where no or minor recirculation appears (Cheng, 1995). These burners simply rely on the fact that the flow expands (similar to a diffusor) and at some point the flame speed balances the flow velocity. Some of these burners have however recirculation, but it appears far downstream and cannot contribute to stability.

The Reynolds number for a gas turbine combustor in operation is typically very large as a consequence of the high mass flows through the engine. The Reynolds number is far beyond its critical value, and the flow is highly turbulent. This has both advantages and disadvantages. The turbulence en-
hances the mixing of fuel and air by orders of magnitude, which gives high reaction rates for both non-premixed and premixed flames. Disadvantages are high pressure drops and heat transfer to combustor walls and turbine blades and guiding vanes.

In this thesis a strongly swirling lean premixed flame in a confined combustor is studied. Certain flow physics related to the swirling motion is investigated; such as the influence of downstream contraction on the flow field far upstream, existence of PVC motion, and the effect of heat release in a swirling flow.

An unconfined low swirl burner, similar to (Cheng, 1995) was also studied in this thesis. The low swirl, which results in a detached flame, together with the unconfinement gives rise to several interesting phenomenas, such as local quenching due to air leakage. The stabilization mechanism is found to be very similar to the stabilization mechanism of a lifted jet diffusion flame, where the leading edge is a premixed flame subjected to a shear layer with strong turbulence.

3.4 Modeling of Reacting Flows

As an exothermic chemical reaction is introduced into a gaseous flow, the viscosity and density are no longer constant. Allowing these fluid properties to vary, the conservation of mass and momentum is given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_j} = 0,$$  \hspace{1cm} (3.11)

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + F_i.$$  \hspace{1cm} (3.12)

$F_i$ denotes body forces, which may be significant for systems with large density gradients. When the fluid is a gas, as common for reacting systems, Newtons viscosity law is a good approximation to the viscous stress tensor:

$$\tau_{ij} = \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial U_k}{\partial x_k} \delta_{ij}$$  \hspace{1cm} (3.13)

Further, conservation of energy is given by, neglecting work done by viscous and pressure forces, as may be done for semi-compressible flows:

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho U_j h_j}{\partial x_j} - \frac{\partial p}{\partial t} = \frac{\partial}{\partial x_j} \left[ k_i \frac{\partial h}{\partial x_j} + \left( \rho D - \frac{k_i}{C_p} \right) \sum_i h_i \frac{\partial Y_i}{\partial x_j} \right] + S_R.$$  \hspace{1cm} (3.14)
Where \( k_t \) and \( D \) is the molecular heat conductivity and mass diffusivity respectively. \( C_p \) is the specific heat of the gas mixture, and given by:

\[
C_p = \sum_i C_{p,i} \tilde{Y}_i
\]  

(3.15)

Finally, \( S_R \) is the source term due to electromagnetic radiation and \( h \) is the mixture enthalpy, defined by:

\[
h = \sum_i h_i \tilde{Y}_i, \quad \text{where} \quad h_i = h_i^0 + \int_{T_0}^{T} C_{p,i} dT.
\]  

(3.16)

And \( h_i^0 \) is the heat of formation of species \( i \) at a reference temperature, \( T_0 \).

The enthalpy transport equation may be avoided in systems with constant pressure and a uniform enthalpy at inlet if differential diffusion and radiative source terms are neglected. Alternatively to the enthalpy transport equation, a transport equation for temperature may be used:

\[
C_p \rho \frac{\partial T}{\partial t} + C_p \rho \frac{\partial U_j T}{\partial x_j} = \frac{\partial}{\partial x_j} \left( k_t \frac{\partial T}{\partial x_j} \right) - \sum_i h_i \dot{\omega}_i - \frac{\partial T}{\partial x_j} \sum_i h_i C_{p,i} \tilde{Y}_i V_{i,j} - S_R
\]  

(3.17)

The conservation of the mass fraction of individual species, \( \tilde{Y}_i \), is given by:

\[
\frac{\partial \tilde{Y}_i}{\partial t} + \frac{\partial \rho U_j \tilde{Y}_i}{\partial x_j} = \frac{\partial}{\partial x_j} (\rho \tilde{Y}_i V_{i,j}) + \dot{\tilde{w}}_i.
\]  

(3.18)

The formation and destruction term, \( \dot{\tilde{w}}_i \), was discussed above and is given by Eq. 3.6. \( V_{i,j} \) denotes the diffusion velocity of species \( i \) in the \( j \)-direction. This term may be treated with different level of accuracy, however, neglecting diffusion due to pressure and temperature gradients, Ficks law may be used, assuming a constant Schmidt number:

\[
V_{i,j} = D \frac{\partial \tilde{Y}_i}{\partial x_j}
\]  

(3.19)

Finally, density, temperature, and pressure are linked via the equation of state,

\[
p = R_a \rho T \sum_i \frac{Y_i}{W_i}
\]  

(3.20)

where \( W_i \) is the molecular weight of species \( i \).
3.4. MODELING OF REACTING FLOWS

3.4.1 Steady One Dimensional Flames

Solving for the time evolution of a reacting turbulent fluid according to Eqs. 3.11, 3.12, 3.14, and 3.18 is prohibitive due to the large computational cost\(^1\). However, they may be solved for simplified cases at low Reynolds numbers, that, despite the simplicity, can provide significant insights into flames dynamics. In the literature a common setup, both numerically and experimentally, for studying flames is two opposed jets; a counter-flow configuration, (Smooke, 1991; Rogg, 1988). Classically, one jet is fuel, while the other is oxidizer, and a reaction can be sustained in the stagnant flow where they meet.

Consider the steady flow (low Reynolds number) near the stagnation plane in Fig. 3.6. In this area, the governing equations may be simplified by applying a Moore-Stewartson transformation (Bai et al., 2000; Rogg, 1988):

\[
\xi = x, \quad \eta = \sqrt{\frac{a}{\mu_\infty \rho_\infty}} \int_0^y \rho dy
\]

\[
\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi}, \quad \frac{\partial}{\partial y} = \sqrt{\frac{a}{\mu_\infty \rho_\infty}} \frac{\partial}{\partial \eta}
\]

\(^1\)Recall the number of species present for a typical fuel like natural gas, Sec. 3.1.1, and the fine meshing needed for the flow, Sec. 2.4.1.
CHAPTER 3. COMBUSTION

\[ U = a \xi \frac{\partial f}{\partial \eta}, \quad \rho V = -\sqrt{a \mu \rho \phi} \]  
\[ p = p_0 - \frac{1}{2} \left( a^2 \rho \xi^2 - a \mu \phi \right) \]  
\[ \frac{\partial^2 f}{\partial \eta^2} = -\frac{\rho \phi}{\rho} - \left( \frac{\partial f}{\partial \eta} \right)^2 \]  
\[ + \frac{\partial \left( \frac{\mu \phi}{\mu \rho \phi} \frac{\partial^2 f}{\partial \eta^2} \right)}{\partial \eta} \]  
\[ \frac{\partial T}{\partial \eta} = -\frac{\partial}{\partial \eta} \left( \frac{\rho k}{\mu \rho \phi} \frac{\partial T}{\partial \eta} \right) + \sum_i h_i \frac{\dot{\omega}_i}{\rho a} + \frac{\partial T}{\partial \eta} \sum_i \frac{C_{p,i} \rho Y_i V_{y}}{\sqrt{a \mu \rho \phi}} \]  
\[ \frac{\partial Y_i}{\partial \eta} = \sqrt{\frac{1}{a \mu \rho \phi}} \frac{\partial Y_i V_y}{\rho a} - \frac{\dot{\omega}_i}{\rho a} \]  

Where \( a \) is the strain rate, \( f(\eta) \) a non-dimensional stream function, \( \phi \) is taken at a reference point, and \( p_0 \) is the stagnation pressure. Transforming and simplifying the momentum equation (Eq. 3.12) yields:

The transformed temperature transport equation (Eq. 3.17):

The resulting equations, Eqs. 3.25 - 3.27, are one dimensional and may be solved in just a few minutes on a desktop computer even when applying a detailed mechanism. The two opposed jets may have any inlet species composition, and several different flame types can be studied by altering the boundary conditions. In this thesis two setups have been used:

- Two premixed methane and air jets resulting in two premixed reaction zones, each of them similar to the flame in Fig. 3.1. The flame may be subjected to various levels of strain by varying the parameter \( a \). In the limit \( a \to 0 \) a free premixed flame is obtained.

- A rich premixed methane jet counter to an air jet. Under low levels of strain, two separate reaction zones are found, one premixed flame and, closer to the air jet, a diffusion flame. However, increasing the strain rate pushes the two reaction zones together and finally they merge and form a flame structure similar to a diffusion flame.

This one dimensional setup is a very valuable tool for studying flame structures, flame speeds, and extinction limits. However, the setup is generally too simplified to describe a flame in an industrial device. Hence, there is a need for tools to handle more complex flames.
3.4.2 Unsteady Three Dimensional Flames

As was discussed in Sec. 3.2.1 the structure of a premixed flame may in several cases be rather unaffected by the local flow situation. Based on that observation the equation system, Eqs. 3.11, 3.12, 3.14, and 3.18, can be significantly reduced\footnote{The method described here relies on a constant enthalpy problem where the energy equation (Eq. 3.14) can be avoided. For other problems, for instance Otto-engines, the approach may be used with some modifications.} by just solving the momentum and continuity equations and then assume the local flame structure to be similar to a one dimensional flame. The evolution of this flame front may then be described by a front tracking technique. Hence, the flow and chemistry are decoupled, and the flame structure may be calculated separately, by the method described above (Sec. 3.4.1). A common way to track propagating surfaces is to introduce a levelset scalar, $G$, an approach where an isosurface (in three dimensions, isocontour in two dimensions) of the scalar, is selected to represent the front. The time evolution of the scalar is then given by the $G$-equation (Peters, 2000):

$$\frac{\partial G}{\partial t} + U_j \frac{\partial G}{\partial x_j} = S_L (1 + L_c \kappa) \left| \frac{\partial G}{\partial x_j} \right|$$  \hspace{1cm} (3.28)

This equation describes a surface propagating in space with a velocity, $S_L (1 + L_c \kappa)$, relative to the local flow speed, $U_j$. $\kappa = |\kappa|$ is the local curvature of the flame front, and is given by the divergence of the surface normal vector, $n$:

$$\kappa = \frac{\partial n_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\partial G/\partial x_j}{\partial G/\partial x_j} \right)$$  \hspace{1cm} (3.29)

The influence of the curvature is given by the Markstein length (Williams, 1985), $L_c$, which may be obtained by experimental means or by flame computations employing detailed chemistry. In the limit $L_c \kappa \rightarrow 0$, i.e. a planar flame or zero Markstein length, the propagation velocity is the laminar flame speed, $S_L$. To map the structure of a laminar flame onto the propagating surface, it is convenient to let the scalar $G$ be defined as a signed distance function, i.e in every point of the flow field, the scalar represents the closest distance to the flame front. By the sign of $G$ the unburned zone (negative $G$) is distinguished from the burned (positive $G$). Fulfilling this, the flame structure as in Fig. 3.1 may be readily mapped onto the domain, as the $G$ function now can be interpreted as a flame coordinate. However, the $G$-equation (Eq. 3.28) only describes the motion of the front and does not preserve the distance property during time evolution. To remedy this, a second equation is also solved:
 CHAPTER 3. COMBUSTION

\[ \left| \frac{\partial G}{\partial x_j} \right| = 1 \quad (3.30) \]

The boundary condition for this equation is the isosurface that represents the flame front. This step in the solution procedure is denoted re-normalization step.

The model shown this far is applicable to regime I-III in Fig. 3.2 where the entire flame structure is embedded in a quasi laminar flow. However, the approach may be extended to the thin reactions zone (regime IV) by observing the fact that the inner layer of the flame, which is responsible for keeping the flame alive, is still unaffected by the eddies. The main effect of the turbulent eddies entering the pre-heat zone is the increase heat and mass transfer and thereby the flame speed. Hence, a modification of the flame speed to the \( G \)-equation (Eq. 3.28) will allow us to extend its validity.

A similar method may be used for purely non-premixed flames, where the reaction is controlled by the mixing of fuel and oxidizer. Bilger (1977) proposed that the whole flame structure of a diffusion flame may be conditioned on one single nonreacting scalar; the mixture fraction, \( Z \). This is applicable for flames where the flow time scale is much larger than the chemical time scale, i.e. at small Ka numbers. The mixture fraction describes the mixing of fluid stemming from the fuel nozzle with the oxidizer stream:

\[ \frac{\partial \rho Z}{\partial t} + \frac{\partial \rho U_j Z}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D \frac{\partial Z}{\partial x_j} \right) \quad (3.31) \]

As seen, \( Z \) is a conserved scalar, and totally dependent on boundary conditions; typically \( Z = 1 \) in the fuel stream, and \( Z = 0 \) in the oxidizer stream. Further, all species are assumed to have equal diffusivities, \( D \). These two methods to decouple the flow and chemistry are denoted flamelet library models. In this thesis it is shown how these two approaches may be used in conjunction to describe stratified and partially premixed flames under certain conditions; for the low swirl burner and for a rich unconfined jet flame respectively.

The Propagation of the Filtered Flame Front

When the \( G \)-equation is used in a filtered context, as in LES, it should describe the time evolution of the filtered flame front. Under such conditions, certain small scale wrinkling of the flame is unresolved. As discussed in Sec. 3.2.1, this wrinkling is important for the flame front propagation, mainly due to increased flame surface area. The reactant consumption rate of a flame surface propagating with the speed, \( S_L \), can be expressed as
where $A_F$ is the flame surface area, and $\rho_u$ the density of the unburned mixture. Now, consider a filtered flame surface, as in Fig. 3.7 and let the filtered flame surface area be denoted $\tilde{A}_F$. In LES, we prefer certain properties to be conserved under the filtering process. In Sec. 2.4.3 it was seen that mass and momentum are conserved ??, while here, we prefer the reactant consumption rate to conserve:

$$\dot{m} = \rho_u A_F S_L,$$

(3.32)

Denoting the propagation velocity of the filtered flame surface $S_{LES}$, we may write the filtered $G$-equation:

$$\frac{\partial \tilde{G}}{\partial t} + \tilde{U}_j \frac{\partial \tilde{G}}{\partial x_j} = S_{LES} \left| \frac{\partial \tilde{G}}{\partial x_j} \right|$$

(3.34)

As when filtering the momentum equations, an unknown term shows up; the speed of the filtered flame front, $S_{LES}$. This quantity can, however, be provided by a model and several models can be found in the literature. Typically, they are based on estimations of the subfilter kinetic energy $k'$, similar to the Damköhler model:

$$S_{LES} = S_L + \sqrt{\frac{2}{3} k'}, \quad k' = \sqrt{\sum_i u_i'^2},$$

(3.35)

where $u_i'$ is the unresolved velocity fluctuations (Eq. 2.20), and can be estimated by the LES-filter length scale and the subfilter viscosity 2.26. When the filtered flame front is found, the re-normalization step is performed, to assure that the $\tilde{G}$-field represents flame normal distance. For this, the same equation as for the unfiltered $G$-field is used. Now, if the equations are solved on a numerical grid, the quantity $\tilde{\phi}_{cc}$, defined at cell centers, represent each cells average value of $\phi$. Consider the magnified cell in Fig. 3.7. If $\phi$ is two-valued;

$$\phi = \begin{cases} 
\phi_u & \forall \quad G < 0 \\
\phi_b & \forall \quad G > 0 
\end{cases},$$

(3.36)

$\phi$ at cell center is given by (for a cell with volume $V$):

$$\phi_{cc} = \frac{1}{V} \iiint_V \phi(G) dV = \frac{\phi_u V_{G<0} + \phi_b V_{G>0}}{V},$$

(3.37)
where \( V_{G<0} (V_{G>0}) \) represents the volume of the cell with negative (positive) \( G \). In a typical LES these volumes are, at least globally, conserved during filtering, hence, for a two valued scalar like \( \phi \) its filtered counterpart is easily determined from the filtered \( G \)-field (Wang, 2005); \( \bar{\phi}_{cc}(G) = \phi_{cc}(\bar{G}) \). On an LES scale, the major species, temperature, and density are approximately two-valued functions, and may be treated as such. However, scalars which cannot be approximated as two-valued functions, i.e. intermediate species like CO, needs further modeling to be determined. If just the fluid and flame dynamics is of interest this may be omitted, since only temperature (via viscosity) and density are coupled to the flow solver. However, in a finite volume, as a computational cell, the total mass of an intermediate species is proportional to the flame surface area. Since the filtering process smooths this surface, \( \bar{A}_F \leq A_F \), it is clear that the total mass is not conserved if the species is determined from the filtered \( G \)-field soley. This may be resolved by integrating over \( G \) with a Gaussian PDF, \( p(G, \sigma) \);

\[
\bar{\phi}(\bar{G}) = \int_{-\infty}^{+\infty} \rho(G) \phi(G)p(G - \bar{G}, \sigma)dG \int_{-\infty}^{+\infty} \rho(G)p(G - \bar{G}, \sigma)dG,
\]

(3.38)

where the width of the PDF, \( \sigma \), is determined by an estimation of the flame surface area ‘lost’ during the filtering. Then \( \bar{\phi}_{cc} \) is given by the cell volume average of \( \bar{\phi}(\bar{G}) \), similar to Eq. 3.37.

Figure 3.7: A wrinkled flame front and its filtered counterpart on a computational grid.
Chapter 4

Numerical Methods

The equations shown in the preceding chapters lacks analytical solution except for very simplified problems. This has led to the development of alternative techniques to study problems in fluid mechanics, which are mainly divided into:

- Theoretical analysis
- Experimental methods, i.e. hot wire anemometry, various laser techniques etc.
- Computational Fluid Dynamics, CFD

Many engineering problems can be handled by theoretical means, but, however, when detailed description of the flow is desired, they are generally too limited. Experimental methods may provide such detailed information, but they are expensive and access to the flow field may be limited. Since the birth of the digital computers and their extreme evolution since the 1950’ies computational fluid dynamics has grown dramatically, and occupies today a large fraction of the fluid mechanics community. In this chapter it is shown how the governing equations may be approximated numerically and solved by a computer.

4.1 Discretization of the PDEs

Three criterion should be fulfilled when solving difference equations numerically (Lax’s theorem), (Ferziger and Peric, 1999):

1. The problem should be well posed.
Figure 4.1: The cell structure in a staggered grid.

2. The equations are discretized using a finite difference approximation which is consistent, i.e. the truncation error goes to zero when infinitely fine grids are used.

3. The numerical solution should be stable, i.e. appearing errors should not be magnified.

Gullbrand et al. (2001)

\[
\frac{\partial^2 \phi}{\partial x^2} = \frac{-\phi_{i-2} + 16\phi_{i-1} - 30\phi_i + 16\phi_{i+1} - \phi_{i+2}}{12(\Delta x)^2} + O((\Delta x)^4) \quad (4.1)
\]

\[
u_i \frac{\partial \phi}{\partial x} = \frac{u_i}{12\Delta x} \left[ 8(\phi_{i+1} - \phi_{i-1}) - (\phi_{i+2} - \phi_{i-2}) \right] + |u_i| \frac{6\phi_i - 4(\phi_{i+1} - \phi_{i-1}) + (\phi_{i+2} - \phi_{i-2})}{12\Delta x} + O((\Delta x)^3) \quad (4.2)
\]

momentum and scalars
levelset re-normal
Chapter 5

Summary of Publications

**Paper I  Swirling Turbulent Flows in a Model Combustion Chamber with and without Heat Release**

This paper concerns numerical simulations, LES, and experimental velocity measurements using Particle Image Velocimetry, PIV, and Laser Doppler Velocimetry, LDV, of strong swirling flows in a confined model combustor. The behaviour of swirling flow in a confined geometry is complicated, and downstream conditions affects the flow far upstream. In this case there is a sudden contraction at the end of the combustion chamber, which totally alter the entire flow structure. This is shown by a LES where the contraction is removed. A mechanism to explain the observed behaviour is put forward. Further, the difference between reacting and non-reacting flows is examined. It is found that.... The results from the LES is compared with the obtained velocity statistics with a very satisfying agreement. The candidate performed all numerical computations and wrote parts related to those and the analysis of the results.

**Paper II  Large Eddy Simulation and Experiments of Stratified Lean Premixed Methane/Air Turbulent Flames**

This paper concerns a proposed model for stratified premixed combustion. The model is applied to a lifted weakly swirling flame. The stratification is induced by the unconfinement, which allow for air entrainment into the premixed fuel and air stream ahead of the reaction zone. The model is validated against experiments obtained in parallel, and reasonable quantitative and qualitative prediction is found. The candidate performed all numerical computations and wrote parts related to those and the analysis of the results.

**Paper III  Two Independent Large Eddy Simulation Studies on a Low Swirl Stratified Premixed Flame**

35
Figure 5.1: The three cases studied. From top: Isothermal, reacting, and isothermal without the contraction.
Figure 5.2: Time sequence of the velocity field on top of the temperature field. Eddies are approaching the flame tip and drag it upstream. This is believed to be the stabilization mechanism for the low swirl flame.

Figure 5.3: The low swirl burner. The flow passes through two perforated plates ahead of the swirler, then, at the swirler, about 60% passes through the swirler wanes, while the remaining part bypasses the swirler through a perforated plate in the centre (not seen in the figure).
This paper deals with the modeling aspects of stratified premixed flames. The candidate performed the computations related to the $G$-equation, while Prof. Fureby, at the Swedish Defense Research Agency, contributed with the computations related to the finite rate chemistry LES. The paper aims at using two different, separately validated, LES-codes. The paper is written by the candidate, Prof. Fureby, Per Petersson, and Prof. Xue-Song Bai.

**Paper IV** *A Comparative Study of LES Turbulent Combustion Models Applied to a Low Swirl Lean Premixed Burner*

This paper aims solely at investigating the performance of different combustion models when applied to the low swirl burner. It is found that all applied models can qualitatively capture the behaviour of the flame, however, certain differences in the quantitative results are found. The candidate performed the calculations related to the $G$-equation, while Prof. Fureby performed the other computations. The paper is written by the candidate and Prof. Fureby.

**Paper V** *Structure and Stabilization of a Low Swirl Turbulent Lean Premixed Flame*

This paper concerns the stabilization mechanism of the low swirl burner.
flame. New calculations with different boundary conditions and newly obtained measurement are used to get a relatively complete understanding of the stabilization. It is found that the flow structures formed inside the burner is important for the dynamics of the flame. Large eddies, found both in experiments and simulations, interact with the leading edge of the flame, and continuously drags the flame upstream. The paper is written by Prof. Xue-Song Bai and the candidate.

**Paper VI Numerical Computations and Optical Diagnostics of Unsteady Partially Premixed Methane/Air Flames**

In this paper an unsteady rich premixed jet flame at low Reynolds number is investigated by both numerical and experimental means. The flame has a very interesting 'double-flame' structure. The premixing lies within the flammability limit of methane, and a premixed reaction front forms a conical inner flame. Products from this flame, containg significant amounts of H$_2$ and CO mixes with the surrounding air, and is completely oxidized in a second reaction front outside the premixed flame front. The flame structure is investigated by analysing the spatial distribution of CH and OH, which is determined in both the numerical computation and in the experiments by Planar Laser Induced Fluorescence, PLIF. The influence of body forces is
Figure 5.6: The time evolution of the streamlines and the OH field. Large toroidal vorticies are formed continuously due to bodyforces.

also assessed, and the body force induced flickering of the flame is quantified from both experiments, using a high speed video camera, and the numerics. Similar trends for the flickering frequency are found, yet certain disagreement exists. All computations and analyses are performed by the candidate. The paper is written by the candidate, Zhongshan Li, and Johannes Kiefer.
Acknowledgements

This work was carried out at the Division of Fluid Mechanics, Lund University/Lund Institute of Technology, Sweden. The work was financially supported by the Center for Combustion Science and Technology, CeCOST, and partly supported by the Swedish Research Council, VR, and Swedish Foundation for Strategic Research, SSF. Computational resources were provided by the Center for Scientific and Technical Computing at Lund University (LUNARC).

I would like specially thank my supervisor Xue-Song Bai for giving me the opportunity to join his group, all the patient explanations, and valuable input to my work. I would never have reached this far without his support.

I would also like say a big thank you to all colleagues and ex-colleagues at the department of Energy Sciences, especially; Gunilla Andrée, Philip Evegren, Raik Orbay, Lisa Prahl, and Rixin Yu. I am very happy for meeting all of you, I have learned a lot about fluid mechanics, combustion and not least life in general. At the division of Combustion Physics, I would like to thank Per Petersson for all valuable discussions and the very fruitful cooperation on the low swirl burner.

I would also like to thank my family, all my old friend friends, and all new friends, which have made my time in Lund a pure pleasure, for all support and love during the years.
CHAPTER 5. SUMMARY OF PUBLICATIONS
Bibliography


