On Multiresolution in Numerical Premixed Turbulent Combustion with VLES

A 3-D vessel case with the Level-Set formulation of the G-equation using General Motors CFD code (GMTEC)

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till Anna-Karin
för ditt tålamod
y en especial a Désirée
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Chapter 1

Introduction

Humans are social beings living in societies. Production and service are parts of any community. Power generation and transportation are fundamental services. Goods transportation add a cost to the original product without improvement its properties and therefore the importance of keeping it as low as possible. Any transportation system is compounded by several stages. Sometimes, different types of vehicles are needed from the source to the destination, where a simple or no infrastructure might be present at the final stage. Among the land transportation system available, road and rail road have been developed since late XIX century. Rail roads rely on expensive infrastructures depending on government tax incomes and therefore, sensitive to global and local economic fluctuations. Also, it can not complete the final transportation stage, i.e. "to-door". Hence, (off) road vehicles are a must in people and goods transportations.

A road vehicle should meet transportation requirements such as performance, power-\(\frac{\text{weight}}{\text{distance}}\) and re-fuelling time-\(\frac{\text{re-fuelling}}{\text{time}}\) ratios. Vehicles can be powered by steam plants, electric motors, fuel-cell and internal combustion engines (ICE). The last one are fossil- or tillage\(^1\)-fuelled engines and have shown to fulfill the above ever increasing demands.

In ICE, hot combustion products become the working substance and energy is transferred directly from them as work. Depending on fuel ignition, they can be compression-ignition or spark-ignition (SI) engines. The last type is the most used in road vehicles and its combustion is aboard in this work. In a SI-engine, combustion corresponds to about one-sixth of a crank rotation and is largely independent of engine speed. Therefore, turbulence is needed to accelerate the combustion and make the engine operable.

The power of a spark-ignition engine is limited by the airflow into the

\(^1\)Ethanol can be obtained from sugar cane.
engine. The fuel characteristics only influence how much of that air can be fully utilized, and have minimal effect on the amount of air available. The efficient of the engine, or its fuel consumption, is governed by the basic chemical energy content of the fuel, the extent to which the fuel is fully burned (almost completely, but not quite), and the compression or expansion ratio of the engine (Heywood (1993)). Thus, the importance of understanding the fluid dynamics and combustion process inside an ICE.

Numerical simulations of ICE are out of the reach of today (2004) computational capacity, but studies of simplified cases can be carried out. In this thesis, the combustion inside a 3D cylindrical vessel is analyzed.

1.1 Combustion and Turbulence

Combustion is a mass and energy conversion process of oxidation of molecules, usually carbon, hydrocarbons, during which chemical bond energy is transformed to thermal energy. It occurs readily at high temperature with the release of energy, i.e. an exothermic process. In addition, a mixing mechanism, e.g. turbulence, might favorite combustion. In turbulence flows, the fluid velocity field varies significantly and irregularly in both position $x$ and time $t$. Thus, turbulence has the ability to transport and mix fluid much more effectively than a comparable laminar flow. Turbulence mixing consists of two simultaneously process; one which increases interfacial surface area called stirring, and other which smoothes out interfaces called diffusion. The combination of heat release due to combustion with mixing process due to turbulence creates a symbiosis between combustion and turbulence:

- Combustion releases heat that generates flow instability by buoyancy\textsuperscript{2} and gas expansion, which enhances transition to turbulence.
- Turbulence increases the mixing process and thereby enhances combustion.

Thus, combustion usually occurs within turbulence flow field. On the other hand, there exist an optimal turbulence flow field from where an increase/decrease will deaccelerate combustion (c.f. Katoh et al. (1985). A similar analysis might apply for a certain heat release value. Although instabilities starts the transition to turbulence, this dynamics phenomena is not fully understood, which coincides with the same part in the orbit diagram of nonlinear dynamics.

\textsuperscript{2}no buoyancy effects are assumed in the numerical computations in this work.
1.2 On this thesis and Scientific Computing

There are several definitions on what scientific computing (SC) is. One of them is represented in Figure 1.1.

![Diagram of Scientific Computing](image)

Figure 1.1. A definition of Scientific Computing

Although SC can be defined as the intersection of numerical mathematics, computer science and modeling, it is difficult to predict how much modeling, in detriment of programming and numerical mathematics, will be needed when one take up a certain problem. Numerical turbulent combustion can be classified on the top of a hierarchical CFD scale since it may contains subjects such as chemistry, turbulence, combustion, fluid-structure interactions, SC, etc. Therefore, lot of theory has to cover before any code line is written. In the present thesis, it turns out that a very simple implementation was needed.
1.3 Why Multiresolution?

A system, whose evolution is based on repeating a certain structure, will probably dominate its environment faster than any other competitor using a different approach. A mother structure is copied, re-scaled, shifted and placed at several levels to create, describe a process. As Russian dolls, the mother contains re-scaled mothers. Nature has shown such successful. The idea of multiresolution starts with a mother function (table 4.1). Each level has different complexity and they should be numerically resolved using different schemes adaptively.

Turbulence has gone a transformation from a classical to a multiresolution approach during the last few years. In addition, combustion has been analyzed using a similar perspective as well. Thus, a unified study has been intended\(^3\), based on the author’s previous experience on multiresolution (Machado (2000)). Because of lack of time, only few aspects are touched in this direction while many propositions, ideas, open questions are left as further work.

1.4 Literature Research

An extensive-intensive literature research has been carried out. This is not an easy task in combustion. The spirit of let to publish works without many restrictions, in order to expose new ideas to the rest of the research community, has lead that fundamentals errors, misleading approaches, etc have gone through. Sometimes, not even publications from some well established researchers escape from criticisms.

\(^3\)The insertion of multiresolution analysis into these subjects is still an ongoing research. The author just points out some properties of such approach as open issues, because many proofs remain to be done. In addition, some models are more suitable for the multiresolution approach than others.
Chapter 2

Turbulence

The definition of turbulence has been updated since von Kármán (1937) p. 1109 and even far behind in time. Today, any specific definition is avoided; instead the nature of turbulence is defined as (Tennekes and Lumley (1972)):

- Irregularity (chaotic velocity fluctuation) and unpredictability
- Diffusivity
- Three dimensional and high Reynolds numbers.
- Continuum flow

The unpredictability comes from the intrinsic behavior of chaotic dynamical systems while the diffusivity increases rate of momentum heat and mass transfer rapid mixing. The physical understanding of isotropic (i.e. directional independent) turbulent relies on the Kolmogorov (1941) approach.

2.1 The Kolmorogov Approach

Kolmogorov (1941) idea is that (Figure 2.1)

- The fluid is filled by circulating eddies of all scales.
  Two mechanism act on the eddies: i) inertial effects (e.g. vortex stretching, instabilities), which are important for high $Re_T$ ii) viscous effects, which damp the motion and are important for low $Re_T$. The (turbulent) Reynolds number is defined as $Re_T \equiv \frac{\text{inertia effects}}{\text{viscous effects}} = \frac{u \ell}{\nu}$.

- Kinetic energy $k = \frac{1}{2}(\overline{w^2} + \overline{v^2} + \overline{w^2}) = \frac{1}{2} u_i u_i$ is introduced into a fluid on large scales with length $\ell$. Thus, the large eddies are the energy bearing
eddy with turnover velocity \( u \sim k^{1/2} \) and kinetic energy dissipation \( \varepsilon \sim \frac{u^3}{\ell} \). Because \( \ell \) is large, the \( \varepsilon \) at this scale is small. The large (integral) scales know their direction (i.e. anisotropic) and they dominate the turbulent transport.

- The kinetic is transferred by the motion of the fluid through a cascade-like sequence of eddies of decreasing size with (intermediate) Taylor micro-length scale \( \lambda \) and \( \varepsilon \sim \frac{\nu^2}{\lambda^2} = \frac{\nu}{3^{1/2}} u^4 = \frac{1}{Re_3} u^4 \) (even here, the \( \varepsilon \) can be considered small due to the existence of this inertia (sub)range region requires fully turbulent flow \( \Rightarrow \) high \( Re \)).

- until it reaches the small eddies at which dissipation occurs (90\% of the energy) in form of heat. The length scale at this level is the Kolmogorov microscales \( \eta \). These small scales do not know their directions (i.e. isotropic). Because of \( \approx 90\% \) of the kinetic energy is destroyed (= dissipated) at Kolmogorov microscales by viscous forces, it is natural to assume that viscosity \( \nu \) plays a part together with \( \varepsilon \) in determining the Kolmogorov velocity scale \( u_\eta \), length scale \( \eta \) and time scale \( t_\eta \). Using dimension analysis of \( u_\eta = \nu^a \varepsilon^b \), which is equivalent to \( [m/s] =

![Figure 2.1](image.png)

**Figure 2.1.** a) Energy spectrum representation of the Kolmogorov universality hypothesis (Ronney (2002) Lect. 10, p. 9). b) Log-Log scales of the energy spectrum for a turbulent flow (Wilcox (2000b) p. 11).
2.1. THE KOLMOGOROV APPROACH

\[ u_\eta = (\nu \varepsilon)^{1/4}, \quad \eta = (\frac{\nu^3}{\varepsilon})^{1/4}, \quad t_\eta = (\frac{\nu}{\varepsilon})^{1/2} \tag{2.1} \]

Solving \( \varepsilon \) from the first two equation gives \( \frac{u_\eta}{\nu} = 1 \) and \( \varepsilon = \frac{\nu u_\eta^2}{\eta} \).

The order of magnitude among these scales can be exemplified using the length scale of the planet earth’s boundary layer: integral scale \( \ell \sim \Lambda \gg \) intermediate Taylor scale (in the inertial range) \( \lambda \gg \) small (Kolmogorov) scale \( \eta \) (or below), where \( \ell \sim 1km, \lambda \sim 0,1m \) and \( \eta \sim 1mm \) (Atkinson (1981)). In cylinders of ICE, the cascade of turbulent length scales goes from the size of the bore diameter to length scales as small as \( 10^{-3} \) cm.

The energy inserted in the integral scale region is related with the dissipation region by \( \varepsilon \sim \frac{u_\eta^3}{\ell} \). Because of a wavenumber \( \kappa \) is mathematically related with an eddy size (= length) \( \ell_n \) by \( \kappa = \ell_n^{-1} \), at scale \( \ell_n \) the kinetic energy \( u_n^2 \sim (\varepsilon \ell)^{2/3} = \varepsilon^{2/3}k^{-2/3} \), which states that shear across eddies/structures scale with \( \frac{2}{3} \). The density of the kinetic energy per unit wavenumber \( \kappa \) is

\[ E(\kappa) = \frac{dv_n^2}{dk} \sim \varepsilon^{2/3}k^{-5/3} \tag{2.2} \]

where \( E \) stands for the energy spectrum and it includes the \( k^{-5/3} \) law (Figure 2.1).

The Kolmogorov (1941) idea implies that due to the fluid is filled by eddies of all scale, then the dissipation of energy as heat should occurs uniformly throughout the fluid. Mathematically, it can be expressed by \( \varepsilon(x) \) being the rate of dissipation per unit volume at the point \( x \). Thus, the heat generated in a small volume \( \delta V \) around the \( x \) in time \( \delta t \) is \( \varepsilon(x)\delta V\delta t \). The uniform dissipation assumption implies that \( \varepsilon(x) = \varepsilon \) for all \( x \in A \), where \( \varepsilon \) is the rate of input of energy into a fluid region \( A \), which is given in unit volume.

However, experiments by Batchelor and Townsend (1949) using hot-wire anemometer reveals that in turbulent fluid the rate of dissipation differs substantially in different parts of the fluid due to internal intermittency\(^1\). Also, wavelets calculations of the local and global energy spectra by Farge et al. (1990) using Direct Numerical Simulation (DNS) data have shown very large deviation of the local, from the mean energy spectrum due to internal intermittency. Thus, energy associated with the small scales of a turbulent flow is not distributed uniformly in space and the transfer of energy

\(^1\)Do not confuse the terms internal intermittency with intermittency. The last one is usually used to describe fluid motion that is sometimes turbulent and sometimes non-turbulent. The intermittency referred in this work is the internal intermittency.
CHAPTER 2. TURBULENCE

is spatially intermittent. The energy and the dissipation are concentrated on a small part of the fluid. The variation of $\varepsilon(x)$ can be quantified by (auto)correlation using a small vector $h$. The correlation of the dissipation rates between points separated a distance $h$ is given by $\varepsilon(x)\varepsilon(x+h)$, i.e. averaged $\forall A$. The experiments have shown

$$\varepsilon(x)\varepsilon(x+h) \simeq \varepsilon^2 |h|^{-d} \quad \text{for } d = 4 \sim 5$$

(2.3)

Therefore, in order to explain internal intermittency, the Kolmogorov approach should be modified from the idea of, eddies at each scale filling the space, to eddies filling a successively smaller proportion of space as their size decreases. The kinetic energy, originally introduced into the largest eddies, passes through a cascade of eddies which sizes are continuously decreasing.

The cascade (Figure 2.1) is a fission process and the energy transfer from larger to smaller scales is called forwardscattering. The energy cascade terminates, as the kinetic energy of the small eddies (at or below the Kolmogorov length scale) is dissipated by viscosity into thermal energy, i.e. molecular motions. Although in the mean, the kinetic energy is transferred from large scales to small scales, there exist locations in the flow where the energy cascade, actually operates from small to large scales locally. This phenomenon is called backscattering. The use of discrete wavelet transform in experimental data and DNS conducted by Meneveau(1990) has shown the presence of both forwardscattering and backscattering, when energy transfer among scales expressed in wavenumbers is calculated.

In turbulence, the number of degrees of freedom increases algebraically as the analysis goes to smaller and smaller scales. Any intention to direct numeric simulate a fully developed turbulence would require a cascade of computers. Therefore, some turbulence modeling is a must with today computational capacity limitations when a non-academic related case is study. When it is studied, turbulence should be described the same in all inertial frames of references in order to be consistent with the basic physics, i.e. Galilean invariance turbulence\textsuperscript{2}.

In industrial applications, is not feasible to resolve not even the largest scales at this moment (2004). Therefore, only the very large scales can be simulated while the rest are modeled. The integral length scale $\ell$ is the length scale of those eddies containing the most of the energy. It can be defined using the normalization of two-point correlation function:

$$R(x, r) = \frac{w'(x, t)w'(x + r, t)}{\sqrt{w'^2(x, t)}\sqrt{w'^2(x + r, t)}}$$

(2.4)

\textsuperscript{2}A quantity that is the same in different inertial frames is said to be Galilean invariant.
2.1. THE KOLMOGOROV APPROACH

where $R$ measures the correlation of the velocity fluctuations $u'(x, t)$ and $u'(x + r, t)$. $R$ indicates the degree of influence of the turbulent properties located at two points separated a distance $r$. For $r = 0$, $R = 1$ while $r \to \infty$ is $R \to 0$. From (2.4), the integral length is defined as

$$\ell = \int_{0}^{\infty} R(x, r)dr \quad (2.5)$$

where the integral length ($\ell$) is located in the shaded equal areas of Figure 2.2, above and below the two-point velocity correlation function. Therefore, the integral length scale can be interpreted as the length scale from which point on the velocity fluctuations are predominantly uncorrelated. It will be seen in the multiscale/multiresolution section, the difficulty of extracting fluctuations from these very largest scales (downward completeness in table 4.1).

![Figure 2.2. Integral length scale and micro (Taylor) scale (Willems (1996) p. 12)](image)
Chapter 3

Combustion

Combustion involves exchanges and/or rearrangements of atoms between colliding molecules, i.e. chemical reactions. Chemical species/molecules react with each other to form other chemical species/molecules. Thus, the atoms/chemical elements are conserved but not chemical species/molecules. In chemical reactions the mass of the species changes while the mass of the elements is conserved. In order to characterize the composition of the mixture with $n$ different chemical species, the mole fraction of species $i$, i.e. $X_i$ and the mass fraction of species $i$, i.e. $Y_i$ are defined.

$$X_i = \frac{N_i}{N_1 + N_2 + \ldots} = \frac{N_i}{N_{\text{tot}}} \quad (3.1)$$

$$Y_i = \frac{m_i}{m_1 + m_2 + \ldots} = \frac{m_i}{m_{\text{tot}}} \quad (3.2)$$

for $i = 1, 2, \ldots, n$. These fractions are related with the mean molar mass of the mixture$^2$,

$$MW_{\text{mix}} = \sum_{i=1}^{n} X_i MW_i = \frac{1}{\sum_{i=1}^{n} Y_i / MW_i} \quad (3.3)$$

where $MW_{\text{mix}}$ denotes an average molar mass and $MW_i$ is the molar mass$^3$, i.e. the mass of 1 mol for this $i$ species.

$$Z_j = \frac{m_j}{m} = \sum_{i=1}^{n} \frac{a_{ij} MW_j}{MW_i} Y_i = \frac{MW_j}{MW_{\text{mix}}} \sum_{i=1}^{n} a_{ij} X_i, \quad i = 1, 2, \ldots, n \quad (3.4)$$

$^1$1 mol of a compound correspond to $6.023 \times 10^{23}$ particles (atoms, molecules, etc).

$^2$sometimes known as mixture molecular weight or mean molecular weight.

$^3$sometimes known as molecular weight.
Note that, by definition, the sum of all constituent fractions must be unity, i.e.,

\[ \sum_{i=1}^{n} X_i = 1, \sum_{i=1}^{n} Y_i = 1, \sum_{i=1}^{n} Z_i = 1 \] (3.5)

In combustion processes, fuel and oxidizer (typically air) are mixed and burned. In premixed processes, the mixing take place first and followed by combustion, while in non-premixed cases both occurs simultaneously. The equivalence ration\(^4\) \(\Phi\) is used to indicate quantitatively whether a fuel-oxidizer (e.g. propane-air) mixture is rich, lean or stoichometric

\[ \Phi = \frac{(m_{\text{air}}/m_{\text{fuel}})_{\text{stoic}}}{(m_{\text{air}}/m_{\text{fuel}})} \] (3.6)

where \(m_{\text{air}}\) and \(m_{\text{fuel}}\) are related to the \(MW_{\text{air}}\) and \(MW_{\text{fuel}}\) (Turns (2000) p. 19).

Fuel-rich mixtures corresponds to \(\Phi > 1\), fuel-lean mixtures to \(\Phi < 1\) while a stoichiometric mixture is \(\Phi = 1\), which is assumed in this work.

### 3.1 Eigenvalue Analysis I

In combustion engines maximum torque and avoidance of explosion is a result of eigenvalue analysis. The combustion in spark-ignition reciprocated engines is usually premixed and turbulent. In the study of premixed turbulent combustion, the knowledge of the dynamics of flame front is important. Flames are the results from the interaction of convection and molecular diffusion with many chemical reactions on small scales. Flamelets are thin reactive-diffusive layers embedded within an otherwise non-reacting turbulent flow field.

In the intrinsic properties of a flame front, hydrodynamic instabilities are one of the reason of the existence of flame fronts with curved shapes. Curved flames move faster than planar flames facilitating a fast combustion, which is desired in internal combustion engines. Because of curved flames have more surface area than the planar more fuel consumption is expected in the first one. The thinner the flame front the more unstable it is. The problem stability limits is formulated as an eigenvalue problem.

Normally, the governing equations for steady premixed flames are used as a starting point for the eigenvalue analysis in combustion with a planar flame front, i.e.

\(^4\)In continental Europe, \(\lambda^{-1}\) is used instead of \(\Phi\).
3.2. BASIC DEFINITIONS

Continuity:
\[
\frac{\partial (\rho u)}{\partial x} = 0
\]  
(3.7)

Species ([138] p. 626, [90] p. 69):
\[
\rho u \frac{\partial Y_i}{\partial x} = - \frac{\partial j_i}{\partial x} + w_i
\]  
(3.8)

\[
\rho u c_p \frac{\partial T_i}{\partial x} = \frac{\partial}{\partial x} (\lambda \frac{\partial T}{\partial x}) - \sum_{i=1}^{n} c_{p,i} \frac{\partial T}{\partial x} - \sum_{i=1}^{n} h_i w_i + q_R
\]  
(3.9)

The outcoming unburnt flow velocity \( v_u \) is split into a tangential and a normal component. Because of only the normal component \( u_n \) is increased as a result of thermal expansion within the flame front, the integration of the continuity equation gives
\[
(\rho u_n)_u = (\rho u_n)_b
\]  
(3.10)

where density variation is present. Hence, compressible equations are needed. Assuming stationary condition, leads to \( s_{L,u} = u_{n,u} \), where \( s_{L,u} \) is the laminar burning velocity and the (3.10) is now
\[
(\rho s_{L})_u = (\rho u_n)_b
\]  
(3.11)

which means that the mass flow rate through the flame (unburnt = burnt) is constant. The \( s_L \equiv s_{L,u} \) is an eigenvalue, as it will be exposed in section 3.3.

Before continuing with this analysis, some fundamental definitions are needed.

3.2 Basic Definitions

Combustion can occur in either a flame or nonflame mode. 

**Flames** are the results from the interaction of convection and molecular diffusion with many chemical reactions on small scales. Flames cannot propagate through an opening smaller than the quenching distance \( y_Q \), which is 2 mm for typical hydrocarbon fuels ([97] p. 331 and [100]).

CHAPTER 3. COMBUSTION

The Schmidt number \( Sc \equiv \frac{\text{momentum diffusivity}}{\text{mass diffusivity}} = \frac{\nu}{D_i} \) is a rough measure of the relative importance of momentum transfer and mass transfer, where \( \nu = \frac{\mu}{\rho} \).

The Lewis number \( Le \equiv \frac{\text{thermal diffusivity}}{\text{mass diffusivity}} = \frac{D}{D_i} \), where \( D = \frac{\lambda}{(\rho c_p)} \), \( \lambda \) is the thermal conductivity and \( c_p \) is the specific heat capacity.

The flame thickness \( \ell_F \equiv \frac{D}{s_L} = \frac{\lambda}{(\rho c_p) s_L} \). Because of \( s_L \) is included in the definition of \( \ell_F \), the flame thickness is an eigenvalue too.

The flame time \( t_F \equiv \frac{D}{s_L} \) is a time scale of the laminar flame.

The Damköhler (1940) number \( Da \equiv \frac{\text{integral (macroscopic) time scale}}{\text{chemical time scale}} t_i = \{ [90] \text{ p. 78, [97], p. 187} \} = s_L \ell_F \) is defined for the largest eddies, where \( \ell \) is the turbulent length scale, \( \nu' \) is the turbulent velocity fluctuation, \( t_i \) or sometimes denoted solely as \( t = k/\varepsilon \), \( k = 1/2(u'^2_i) \) is the turbulent kinetic energy and the rate at which \( k \) decay, i.e. \( \varepsilon = \nu [\nabla \nu' + \nabla (\nu')^T] : \nabla \nu' \) is the viscous dissipation rate ([90] p. 12, [130] p. 175, [132] p. 590). \( Da \) can be taken as a qualitative measure of flow reactivity, in the same way as the \( Re \) is a measure of flow turbulence.

The Reynolds number \( Re \equiv \frac{\text{inertial forces \( \nu' \ell \)}}{\text{viscous forces \( \nu \)}} = \{ \text{with} \ \nu = D \text{ and} \ \ell_F = D/s_L \} = \frac{\nu' \ell}{\nu s_L} \).

The Zeldovich number \( Ze \equiv \frac{T_b - T_u}{T_b} \left( \frac{\partial \ln w}{\partial \ln T} \right)_{T=T_b} \) measures temperature sensitivity of the overall reaction rate \( w \) (Williams (1985) p. 144, 155). Small temperature variation due to turbulent fluctuations to result in highly non-linear changes in \( w \) can be quantified by \( Ze \).

Ignition increases the temperature and thereby, the chemistry accelerates. Chemical time scale on the upper branch (Figure 3.1) is short compared to all turbulence time scales and they are concentrated in thin layers known as inner layer (Figure 3.2), due to molecular diffusion.

Markstein length \( L \) is a constant intended to describe influences of flame-structure modifications on the flame speed and it is of the order of the flame thickness \( \ell_F \).

Markstein number \( Ma \equiv \frac{L}{\ell_F} \).
Flamelets are thin reactive-diffusive layers embedded within an otherwise nonreacting turbulent flow field.

**Figure 3.1.** The S-shaped curve is a 2D cut of a saddle-node bifurcation written in parametric form (Strogatz (1994) p. 78). The lower branch corresponds to slowly reacting state prior to ignition point I. Lowering the flow velocity, the Da is increased until the point I, DaI from which a rapid unsteady transition to the upper close-to-equilibrium branch takes place. On the other hand, moving from the upper branch to the left (e.g. by increasing the flow velocity), the Q point is reached, where extinction occurs, i.e. flame quenching by turbulence.

**Figure 3.2.** Schematic representation of the structure of a stationary, laminar stochiometric (Φ = 1) methane-air (CH₄ - O₂) flame (Herman (2001), p. 9). Observe that \( \ell_F = \frac{\tau^p}{\partial T/\partial X} = \frac{\lambda e}{\rho v c} \). Kennel et al. (1990) gives the basic structure of propane-air (C₃H₈ - O₂) flame.
Laminar flamelet structure is assumed when the inner layer is thinner than the size of a Kolmogorov eddy, facilitating that the layer can be embedded within the quasi-laminar flow field of such an eddy. Accordingly, laminar flamelet structure is for larger values of $Da >> 1$ where chemical times scales are shorter than integral turbulence time. Thus, turbulence does not affect the inner flame structure which remains close to a laminar flame, wrinkled by turbulence motions. Therefore, laminar flamelet is a laminar flame whose chemistry is sufficiently fast and that locally and instantaneously can exist in a turbulent flow. Thus, at a particular location in a turbulent flow, at one instant of time a flamelet may exist, at an other instant of time at the same location a flamelet may, possibly, not exist. As a consequence of the turbulent velocity fluctuations, flamelets experience strain and develop curvature.

Laminar premixed flames propagate normal to themselves.

Laminar nonpremixed (diffusion) flames are attached to the local, instantaneous surface of stoichiometric mixture.

The flame surface is defined by the location of the inner layer.

Flamelet concept uses statistical considerations focus on the location of the flame surface and not on the reactive scalars themselves. That location is defined as an iso-surface of a nonreacting scalar $G$ for premixed combustion.\footnote{The nonreacting scalar $Z$ is used for nonpremixed combustion.}

Flamelet equations describe the reactive-diffusive structure in the vicinity of the flame surface as a function of $G$. These equations calculate the profiles of the reactive scalar normal to the surface, using the previous obtained solutions of the equations that describe the statistical distribution of $G$.

Flamelet library is a dataset containing a collection of numerical results exclusively obtained from the computation of a number of laminar flames and that it is assembled prior to any turbulent flame calculation. It contains, for instance, profiles of strained laminar diffusion flames as functions of mixture fraction variable or profiles of unstrained laminar premixed flames as functions of a physical distance scale.

Flamelet models of turbulent combustion are models that describe turbulent flames using laminar flamelets as the basic elements of which the
3.2. BASIC DEFINITIONS

turbulent flame is composed. In many models the turbulence flame is viewed as an ensemble of small laminar flame elements (flamelets).

**Flamelet regimes** are diagrams of flamelet models of turbulent combustion, which are approximations to reality under certain conditions. These conditions can be expressed in terms of nondimensional parameters such as a Reynolds number, a Damköhler number and Karlovitz number. The premixed turbulent combustion regime diagram presented in this work (Figure 3.3) has been proposed by Peters (1986). It contains five zones and needs two definitions of the Karlovitz number.

The first **Karlovitz number** \( Ka \equiv \frac{t_F}{t_\eta} = \left\{ \begin{array}{l} \text{with } t_\eta = (\nu/\varepsilon)^{1/2}, \\
\eta = (\nu/\varepsilon)^{1/4}, \varepsilon \sim v'^3/\ell \text{ and } \nu = D ([90] p. 15, 16, 78) = \frac{\ell_F^2}{\eta^2} = \frac{\nu^2}{\varepsilon} \end{array} \right. \] 

The smallest eddies, i.e. Kolmogorov eddies\(^7\), which is used to measure the flame scales in terms of the Kolmogorov scales. For dimensions below \( \eta \), the flow is laminar (Peters (1986)).

The second \( Ka \) is in fact based on the first definition. Here, the thickness of the inner layer, which is a fraction \( \delta \) of the flame thickness \( \ell_F \) (Peters (2000) p. 28), is taken into consideration by using \( \ell_\delta = \delta \ell_F \). Hence the second **Karlovitz number** is \( Ka_\delta = \frac{\ell_F^2}{\eta^2} \).

The five zones are:

1. **Laminar Flames**: pure laminar flame front propagation.
2. **Wrinkled Flamelets**: laminar flame front propagation dominates.
3. **Corrugated Flamelets**: \( Re > 1 \) and \( Ka < 1 \Rightarrow \ell_F < \eta \). Quasi-steady flames due to the flame structure is not perturbed by turbulence fluctuations.
4. **Thin Reaction Zones**: \( Re > 1 \), \( Ka > 1 \) and \( Ka_\delta < 1 \Rightarrow \ell_F > \eta > \ell_\delta \). Therefore \( \eta \) penetrates the preheated zone and cause unsteady perturbations, but still can not go into the inner layer \( \delta \).
5. **Broken Reaction Zones**: \( Re > 1 \) and \( Ka_\delta > 1 \Rightarrow \eta < \ell_\delta \). Thus, \( \eta \) penetrates and perturbs the inner layer thickness \( \ell_\delta \), chemistry breaks down locally, the heat loss to the preheated zone increase, temperature decrease and the flame extincts.

\(^7\)The Kolmogorov length scale is denoted in the litterature as \( \eta \) or \( \ell_\eta \) or \( \ell_K \). On the other hand, the Kolmogorov time scale is denoted as \( \tau_K \) or as \( \tau_\eta \).
Figure 3.3. Regime diagram for premixed turbulent combustion. It is a diagram $\ell/\ell_F$ versus $v'/s_L$ with delimitations at $Re = 1$, $v'/s_L = 1$ from $\ell/\ell_F \geq 1$, $\eta = \ell_F$, $K\alpha = 1$ and $\eta = \ell_\delta$, $K\alpha_\delta = 1$ from $\ell/\ell_F \geq -0.1$. 
Beside the regime diagram (Figure 3.3), the regimes in turbulent combustion can be classified based on $Ka$, $Da$ (Table 3.1).

<table>
<thead>
<tr>
<th>$Ka &lt; 1$ ($Da &gt; 1$)</th>
<th>$Ka &gt; 1$ and $Da &gt; 1$</th>
<th>$Da \ll 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flamelets</td>
<td>Thickened flames</td>
<td>Well stirred reactor</td>
</tr>
<tr>
<td>(flame is thinner)</td>
<td>(Small turbulent scales may enter the flame front)</td>
<td>(All turbulent time scales are smaller than the chemical time scale)</td>
</tr>
</tbody>
</table>


Although the above definitions are helpful tools in combustion analysis it is important to have in mind that some of them are based on (sometimes simplistic) assumptions. Unfortunately, the complexity of the combustion problems makes it difficult to determine the main parts in which they are wrong. Numerical analysis can be the tool to ascertain where these errors are. Some criticisms are given by Ronney (1994) and Williams (1985).

3.3 Eigenvalue Analysis II

Most of the turbulent combustion models existing today take the geometry of a planar or almost planar flame as a basis. Based on literature research and Bychkov (2004), so far the eigenvalue problem has been solved for three cases:

1. for a planar flame front.
2. for small perturbations of a planar flame (the linear stage).
3. for small velocity increase of a slightly curved flame (the nonlinear stage).

The first case concerns a planar or locally quasi-planar flame only, where the stretch and curvature are very small (sometimes neglected). There is quasi-planar flame when the length scales $\ell$ characterizing variations of initial thermal parameters is much larger than the flame thickness, $\ell >> \ell_F$. In this case there are similar eigenvalue problems locally in all points of the flame front with some variations of the initial conditions, which play the role of boundary conditions for the eigenvalue problem. The eigenvectors represent the structure of the flame front. The eigenfunction varies on large length scales $\ell >> \ell_F$, but calculated in a similar way everywhere.

Using numerical calculations of planar steady state flame together with experimental data (Peters (1992) pp. 88-98 and Williams (1985) pp. 144,
171-172) gives that the laminar burning velocity $s_L = \left( \frac{\lambda_b}{\rho_u c_p \ell_c} \right)^{1/2}$, which defines a velocity scale, is an eigenvalue. Because of $s_L$ is hidden in the definition of flame thickness, $\ell_F$ is also an eigenvalue. The eigenvalues $s_L$ and $\ell_F$ can be described as follows (Peters (2003)):

The laminar burning velocity $s_L$ and the flame thickness $\ell_F$ constitute the eigenvalues of convective diffusive reactive flame structures, where $s_L$ and $\ell_F$ are independent of the fluid flow.

The second and third case take into account small flame stretch and curvature, where there are local variations of the flame velocity and thickness, which influence perturbation growth at the linear stage and the velocity of flame propagation at the nonlinear stage (cases 2 and 3, respectively). In these two cases the complete eigenvalue problem based on hydrodynamic equations is reduced to simplified eigenvalue problems for simplified linear (case 2) or nonlinear equations (case 3) for the position of a flame front. This simplification has been made assuming that the planar flame velocity and thickness remain almost the same all over the front, while the small corrections to $s_L$ and $\ell_F$ came to the simplified equation in the form of the second-order derivatives of the flame position, etc. For these two cases, the simplified equations for a flame front exclude the inner flame structure.

In the general case of a strongly curved flame the literature research shows no attempts to solve the eigenvalue problem.

The study of the above cases shows that for planar flame front the $s_L$ and $\ell_F$ are constants all over the front, while for small curved flame front the $s_L$ and $\ell_F$ are as for plane front + small corrections. Does this mean that for strongly curved flames the value of $s_L$ and $\ell_F$ change if we go along the flame front?

A laminar flame with a curved shape propagates faster than the laminar planar flame. Since turbulent flames are described from laminar flames and a faster flame propagation is desired in internal combustion engines (Zhang (1995)), the curved laminar flame front dynamics should be studied.

### 3.4 Flame Front Dynamics

Burning process present in closed chambers, as those in ICE, involve many different combustion phenomena simultaneously. For instance: instabilities, acoustic and shock waves (e.g. from the ignition), adiabatic compression and pre-heating of the fuel mixture, detonation triggering ("knock"), among others. The dynamics of curved laminar flames can be a result from an
3.4. FLAME FRONT DYNAMICS

external flow and from flames own properties. The influence of an external flow can be studied with Renormalization group theory, introduced by Yakhot (1986). Gostintsev et al. (1988) experiments have shown that a flame front, which is initially influenced by a strong external turbulence, can recover its self-similar propagation regime after some transitional time. Thus, the intrinsic properties of a flame front should not be neglected, but studied. This section reflects the literature available, where many of the studies on premixed flame front (dynamics) are done for stationary curved flames (e.g. the work of Bychkov, Liberman, Khanna (2001) and many others).

Curved flame shape is the result of hydrodynamic instabilities of a flame front. The Darrieus-Landau (D-L) instability is one of the important and studied instability in combustion (Figure 3.4).

![Figure 3.4. Darrieus-Landau (D-L) instability (Schreel (2001) p. 14).](image)

The thermal gas expansion degree/parameter\(^8\) \(\gamma = (\rho_u - \rho_b)/\rho_u\) and eigenvalue flame thickness \(\ell_F\) show their importance in the D-L instability analysis. A flame front of \(\ell_F = 0\) is inherently unstable due to thermal expansion in the flame. Even a slight distortion applied to a flat flame might be amplified, curving the front. The deformation is caused when some of the burnt gases move to areas previously occupied by unburnt gases, moving the front interface forward. The opposite happens for unburnt gases, as sketched in

\(^8\)In the literature, the term thermal expansion coefficient of a flame is sometimes defined as \(\rho_u/\rho_b\) instead of \((\rho_u - \rho_b)/\rho_b\).
Figure 3.4. This, because thermal expansion in the front causes that the flow velocity perpendicular to the front increases and the streamlines are bend towards the local normal vector on the front. Thus, the streamlines must diverge in front of the bulges, leading to a decreasing of local velocity ahead of the front. Consequently, the burning velocity will be larger than the gas velocity and the distorsion will grow.

Observations from the experiments by Gostintsev et al. (1988) show that further development of the D-L instability leads to a fractal flame structure. A flame structure of a flame front implies cascades of humps and cusps of different sizes imposed to one another (Bychkov et al. (1999)). Also, from the numerical simulation of nonlinear dynamics of a slow laminar flame front subject to the D-L instability conducted by Blinnikov and Sasorov (1996) is observed that the acceleration of a front, wrinkled by the D-L instability, can be ascribed to the development of a fractal structure along the front surface. The bending degree of the front is direct proportional to $\gamma$. Zaitsev and Bychkov (2002) has shown that the Darrieus-Landau instability influences the flamelet velocity considerably, when a nonlinear model proposed by Bychkov (2000) is implemented. In addition, a simplified model has been used by Ashurst (1997) to show the obtation of D-L instability and the flame acceleration by gas expansion.

However, the effects of gas expansion on the turbulent burning velocity using the $G$-equation has been studied by Peters et al. (2000) p. 243, concluding that the heat release effects do not strongly influence the turbulent burning velocity for $v'/s_L \gg 1$. The $G$-equation may not be the appropriated tool to analyze D-L instabilities for scales smaller than the integral scales (Peters (2000) p. 120); but possible useful for larger scales. Thus, the importance of VLES.

As it has been said earlier, the development of a curved front shape increases the surface area of a flame, so that the flame propagates faster, but also the flame consumes more fuel per unit time. Thus, there exists a wish of finding a compromise solution where the fastest flame propagation is reached at the lowest possible fuel consumption.

On the other hand, if a flame front is of $\ell_F \neq 0$ then stabilisation of the planar flame can occur. Here, flame front can be represented as a band thickness with two interfaces. The interface unburnt mixture-band and band-burnt gases. Inside this band, the concentration of unburnt species diminishes towards the interface band-burnt gases. This concentration deficit causes

\begin{footnote}
Remember that the burnt gases zone has lower density than the unburnt mixture zone. Also, that the second thermodynamic law implies movement from zone of high concentrations to lower concetrations zone.
\end{footnote}
a lateral diffusion from a point located inside the band, say $p$, towards the interface band-burnt gases. Thus, the reaction rate at $p$ is reduced, and hence the propagation rate, which can no longer compensate for the flow velocity and the concavity is increased as a result. But on the contrary, the diffusion of heat is directed from the burnt gases towards the band, smoothing the concavity. Stability tends to be reached when thermal diffusion $D$ predominates over mass diffusion (for disturbance with small wavelength).

In reality, the flame front has a certain thickness, where all the physical properties of the medium (e.g. temperature, pressure, composition) vary continuously through it (Figure 3.2). The stretching causes that the existence of stable laminar flames is possible. Both the stretch and curvature influence on the burning velocity, and can be expressed in term of the Lewis number and Marstein number. (e.g. Eichenberger and Roberts (1999), Chen and Im (2000), Kwon and Faeth (2001), Sung et al. (2002))

Not only the intrinsic hydrodynamic flame instability (the Darrieus-Landau instability) has a significant effect on the combustion dynamics but also the change of a spark advance angle. It influences directly the flame initiation phase which occurs on a large time-rate for an increasing spark advance. Summing to that the modeling of a spark in a CFD code is carried out unphysically, by setting few cells (e.g. 2) to burn, it is important to understand what it happens in reality in order to have an idea of what we are missing from the model.

### 3.4.1 Ignition and Hot Spot

The expansion during the first moments after ignition in a SI engine determines if the flame extinguishes or becomes self-sustainable. The ignition process can be considered in three phases (Stone (1992) p. 150)

1. Pre-breakdown.

2. Avalanche Breakdown, also known as Plama phase.

3. Initial combustion phase.

Before the spark, the mixture is an isolator. Once the potential is established, the electrons in the cathode, accelerate towards the anode. In their way, the electrons collide with mixture molecules, which becomes ionized. In turn, this produce more electrons, and so on.

The avalanche breakdown phase starts when an increase of the number of electrons can make the discharge self-sustainable creating a very small conductive path or channel across the plug gap with temperature of about 60
000K and pressure of 20 MPa. The high pressure and temperature difference between the very small path and the surrounding mixture causes expansion of the channel at supersonic speed by a shock wave initially, and later by heat conduction. In a very small path with high temperature, expansion is dominated by thermal conduction and the combustion reactions can be neglected. As the channel expands the potential energy is converted to thermal energy and thereby the plasma (i.e. ionized gas) is cooled. The decrement of the temperature implies that the combustion reactions becomes more predominant. The end of this phase shows by a transition from the plasma kernel to flame kernel. Willems and Sierens (1999) have proposed a mathematical model for the first two phase.

In the initial combustion phase, the combustion reactions dominates the expansion of the flame kernel (Figure 3.5). Willems and Sierens (2003) have proposed another mathematical model that distinguishes the three phases and has been validated using measurements of the expansion in a propane-air mixture from Pischinger (1989) claiming good agreement.

![Figure 3.5. Thermodynamic model of the flame kernel during the initial combustion phase (Willems and Sierens (2003) p. 480).](image)

Also, models and experiments from Ishii et al. (1990) show that the flame kernel configuration is governed by the gas flow pattern near the spark gap and that the flow pattern is affected by the the spark gap width, spark gap duration and spark electrode diameter. Their study of the temperature distribution of a flame kernel in a propane-air mixture show a ellipsoid form, which agrees with the Schlieren measurements [59]. Unfortunately, researchers have not reached an agreement about an optimum park type.
3.4. FLAME FRONT DYNAMICS

The CFD modeling of a spark in today (2004) state of art is based on setting some cells to burn (Figure 3.6). This creates a hot spot. The flame dynamics behaves differently when it develops from a hot spot. Shock wave fronts are the results of the spark and not of hot spots. Hence, the flame tends to develop slower in CFD than in reality. A way to overcome this problem is to increase the flow velocity around the hot spot. However, experiments with propane-air mixtures by Borghese et al. (1990) have shown that a fast release of electrical energy between two electrodes leads both to the heating and to establishment of not so well understood peculiar flow-field in the gas medium. It is believed that the ignition spark triggers complex phenomena consisting of heating, recirculation, turbulent mixing and combustion chemistry. Therefore, the numerical ad-hoc of increasing the flow velocity around the hot spot in CFD is not the right procedure, which sometimes leads to results away from the experiments after expensive computations.

Figure 3.6. Two cells are set to burn with level-set coded in GMTEC.

The insertion of ignition spark models (e.g. Willems (2000)) in a CFD code should be considered when more reliable results are feasible in the future.
CHAPTER 3. COMBUSTION
Chapter 4

Turbulence Modeling

The behavior of a (viscous) fluid is believed to be predicted by the Navier-Stokes (N-S) equation:

\[ \frac{\partial \mathbf{u}}{\partial t} = -(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f} \]  

(4.1)

or represented using Einstein notation:

\[ \frac{\partial (u_i)}{\partial t} = -\frac{\partial (u_i u_j)}{\partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} + f \]  

(4.2)

where \( u \) is the velocity, \( p \) is the pressure, \( \nu \) is the kinematic viscosity, \( f \) is the applied force density and \( NS_i \) is the Navier-Stokes operator. Its derivation is out of the scope of this work and can be found in the literature.

The modeling procedure needs certain mathematical tools, which link them with the physics of turbulence. A glimpse of some of these means is given before going into more finished equations.

4.1 Multifractals

The presence of (all) the initial kinetic energy and dissipation concentrated on very small scales has lead to numerous studies. The entire energy cascade, excluding the molecular motion zone, is assumed viscosity free and no dissipation is present (in fact, neglected). From this analysis two issues emerge: i) viscosity is ignored (\( \Rightarrow \) N-S is scale invariance) and ii) the cascade idea by eddies (a recurrent mechanism) (Figure 4.1 a)). Both can be supported by the multifractal theory (Mathieu (1995)).
Since the largest eddy contains the smaller eddies, the recurrent mechanism can be represented as in Figure 4.1 b) which can be mathematically described as an attractor for contractions (= smaller eddies) that maps the largest eddy (Falconer (2003) p. 127).

![Eddy cascade representation](image)

**Figure 4.1.** Eddy cascade representation.
4.1. MULTIFRACTALS

In addition, the cascade idea can be linked with turbulence mixing: *stirring* and *diffusion*. The stirring increases the interface surface areas, and thus the eddy-cube\(^1\) is divided into 8 (Figure 4.2); while diffusion smoothes out the interfaces, and thus the eddy-cube form is conserved.

![Figure 4.2](image.png)

**Figure 4.2.** The first \((N = 1)\) *eddy turnover time* (from \(a\) \(\rightarrow\) \(b\)), the eddy-cube of edge length \(\ell\) is subdivided into eight cubes of edge length \(\ell/2^N\). This implies that the surface area is increased from \(6\ell^2\) to \(2^N 6\ell^2\). For the second \((N = 2)\) *eddy turnover time* (from \(b\) \(\rightarrow\) \(c\)), only one eddy-cube is represented (Warnatz et al. (2001) p. 185).

The Figure 4.1 and 4.2 reveals some of the following characteristics:

- The cascade is obtained by a recursive procedure.
- The small are geometrically similar to the larger eddies, scaled by a factor. Thus, self-similar.
- The continuation of the subdivision leads to arbitrarily small scales.
- The size of the smallest scales can not be quantified by the usual measures such as length.

These and other properties (Falconer (2003) p. xviii) imply that turbulent flows can be analyzed from the fractal approach. The importance of understanding (and the use of) multifractal turbulence approach lies that flamelets combustion is embedded on the turbulent flow field. Because of modern ICE require fast combustion; fast combustion implies strongly curved flame fronts; curved flame shape is the result of hydrodynamic instabilities of a flame front (D-L instability); further development of the D-L instability can lead to a fractal flame structure; then, a fractal approach of the turbulent flow field as well as the combustion will give the 'sandwich' turbulent-combustion a unified approach. In addition, there exist flame-acoustic interactions: flames can produce noise and acoustics wave might lead to a resonance. When combustion and acoustics get strongly coupled combustion instabilities show up (Schuller (2003)). Confined flames, like those enclosed in chambers, can

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\(^1\)The eddy-cube is only an easier representation of a more likely eddy-sphere present in reality.
exhibit strong combustion instabilities (e.g. oscillating regimes). Ho and Huerre (1984) have already shown that hydrodynamics and acoustics can get coupled. The work of Lyamshev (1996), Zosimov (1996) and others on fractal acoustics might be used to extend the ‘sandwich’. A consequence might be an easier way of modeling, with the possibility of decreasing computational complexity.

Many models have been showed up in order to take the advantage of hierarchical scales. Scotti and Meneveau (1999) has developed a fractal model based on fractal interpolation technique (FIT) (c.f. Barnsley, M.F. (1986)). FIT facilitates the interpolation of the resolved velocity with fields that have fluctuations down to much smaller scales and to compute the required stresses explicitly. The work of Schertzer (1997) et al. and Schmitt (2000) explore some fundamentals issues on multifractal turbulence. Because of the wavelet transform is the ideal tool for analyzing multifractal structures, Farge (1990) and his collaborators have used wavelets as a turbulence analysis tool. The fractal approach of (turbulent) combustion is tackled in chapter 5.

The construction of a self-similar fractal as Figure 4.1 b) for a large number of i-stages (= levels) gives a relation similar to (2.3), with dissipation concentrated on a fractal dimension value consistent with the experiments. Although it is not an easy task, it is possible to determine from N-S equations that some ‘intense activity’ is concentrated on sets of very small dimensions.

Fractal process can be studied using multiresolution approximation (e.g. Falconer and Fernández (2004)).

### 4.2 Multiscale/Multilevel/Multiresolution Approach

The hierarchical representation in Figure 4.1 a) of multiscaled eddies in a multilevel organization reduced into smaller (multi)resolutions induce its study from a multiscale/multilevel/multiresolution approach (MSA/MLA/MRA). It is also coupled with the schematic representation of the turbulent kinetic spectrum as a function of the wavenumber (Figure 2.1). The analysis starts with the classical Reynolds decomposition of the velocity field \( u_i(x, t) = \mathbf{u} \) = mean velocity \( U_i(x) = \langle u_i(x, t) \rangle = \mathbf{U} \) + turbulent fluctuation \( u'_i(x, t) = \mathbf{u}' \). Theoretical studies of the N-S equations (Foias et al. (1988)) shown that

- \( ||\mathbf{u}'|| \ll ||\mathbf{U}|| \), i.e. the energy of the smaller scales is much smaller than of the large scales.
4.2. MULTISCALE/MULTILEVEL/MULTIRESOLUTION APPROACH

- \( t(u') \ll t(\overline{u}) \), i.e. eddy turnover time of the smaller scales is much smaller than of the large scales.

which are consistent with the Kolmogorov theory. Thus, the mean and the velocity fluctuation have different temporal and spatial behaviors. These properties give a mathematical justification of treating the small and large scales of the flow differently.

Separating the largest eddies from the smaller means filtering (Figure 4.4) and the filter itself is the grid. The velocities, as well as other related parameters/states, are functions and can be measured using grids, as it is done in most of the computational fluid dynamics (CFD) codes. Every eddy has a certain velocity and a length \( \ell \). Measuring the velocity value of an eddy is equivalent to detect the intersection of this eddy with the grid of distance \( \Delta \approx \ell \) (Figure 4.3). Hopefully, when large distance \( \Delta \) are used, only large eddies are detected while for a small \( \Delta \) only small eddies. In reality, a small eddy can intersect grids with large \( \Delta \) (Figure 4.3) and vice versa. Therefore test grids are implemented. Normally, a test filter is twice the size of the grid filter (Davidsson (2002) p. 46). Unfortunately, these test filters or double filtered fields can significantly contaminates the large scales and necessitate the inversion of filtered quantities, which is equivalent to solving a Fredholm\(^2\) integral equation of the first kind: an ill-posed problem.

The eddies of the eddy cascade (Figure 4.1) can be detected separately using spatial definition of the problem with the possibility of reducing the computational costs (Figure 4.4); but also by a series of filters i.e. filter bank (Figure 4.5). In addition, the above two properties justify the treatment of

\(^{2}\)Fredholm was professor in mathematics at the Royal Institute of Technology (KTH).
the small and large scales of the flow by different numerical schemes (Dubois et al. p. 140). Therefore, Terracol (2001) has proposed a generalized full approximation scheme (FAS), which deals with the use of an arbitrary number of nested resolution levels (Figure 4.4). Based on the grid, the time-cycling is self-adapted decreasing the computational time.

Figure 4.4. Representation of the filter multilevels (Terracol (2001) p 69).

Figure 4.5. Representation attributed to Harten (1996).
4.2. MULTISCALE/MULTILEVEL/MULTIRESOLUTION APPROACH

The filter banks (Figure 4.5) can be used to obtain the Reynolds decomposition $(u = \overline{u} + u')$ at each level. The analysis starts with a certain turbulent flow state denoted here by the function $f \in L^2(\mathbb{R})$. At a certain level $0$, a piece of the state $f$ lives in a subspace $V_0$ as $f_0$. $f_0 \in V_0$ is then filtered and thereby decomposed into its high- and low-frequency part. The low-frequency or smooth parts are mathematically described by the (orthogonal) projection $P_1f_0$ onto a smaller space $V_1$, which contains the smooth functions in $V_1$. The (orthogonal) complement of $V_0$ in $V_2$ is denoted by $W_1$, a space, which due to its construction, contains the high-frequency or rough elements of $f_0$. Denoting the projection of $f_0$ onto $W_1$ being $Q_1f_0$, then

$$f_0 \in V_0 = P_1f_0 + Q_1f_0 = af_0 + df_0 = f_1 + df_0$$

$$= f_2 + df_1 + df_0 = f_2 + \sum_{j=1}^{0} df_j$$

$$= f_j + \sum_{j}^{0} df_{j-1} \quad \text{for } j > 0 \quad (4.3)$$

$$f_i = f_j + \sum_{j}^{i} df_{j-1} \quad \text{for } j > i$$

$$\left( V_0 = V_1 \oplus W_1 = V_2 \oplus W_2 \oplus W_1 = V_2 \oplus \sum_{j=2}^{1} W_j \right)$$

$$V_i = V_j \oplus \sum_{j}^{i+1} W_j$$

where the addition in (4.3) indicates that the summands reconstruct $f_0$, $a$ stands for approximation, average, $d$ for details, fluctuations, while $\oplus$ means that the subspaces $V_0$ and $W_0$ cross each other only in the zero function. Any particular function in $V$ (or in $W$) can be represented as a linear combination of functions that span those subspaces and the smallest set of these functions is the basis of $V$ (or $W$). The basis can be chosen conveniently, for instance, hierarchical basis that order the function in terms of scales. Examples of basis are Fourier, Karhunnen-Loéven expansion, polynomials and wavelets (Figure 4.6). Assuming that the state $f$ is now the velocity $u$, it can be noticed that from the averages $u_1$ on $V_1$ and $u_2$ on $V_2$, the fluctuation $u'_1$ on $W_2$ can be obtained (= reconstructed) due to $u'_1 = du_1 = u_1 - u_2$. Equation (4.3) shows that any velocity $u_i$ at level $i$ can be theoretically reconstructed using
an average velocity $\mathbf{u}_j$ on $V_j$ (at a lower level $j > i$) + all the fluctuations up to level $i$. The grid at level $n$ in figure 4.4 can resolve a function with a certain smoothness while the other grids at its right are better suitable to read fluctuations.

**Figure 4.6.** Decomposition of $f_0 = a f_0 + df_0$ (above) and $f_1 = a f_1 + df_1$ (below) using wavelets (Machado (2000) p. 14).

Notice that Figure 4.6 exemplify that what it is considered averaged velocity at level $j$, i.e. $\overline{u}_j$, in fact, contains fluctuations at level $j+1$, i.e. $u_{j+1}$. In addition, going downward in Figure 4.5 is equivalent to going leftward in Figure 4.4 and equivalent to going downward in Figure 4.6 where more smoother functions are obtained. As we go downward in Figure 4.5, the filtered low-passed functions in Figure 4.6 get smoother and more difficult to extract fluctuation from them. The fluctuation $df_1$ is flatter than $df_0$ in Figure 4.6. Finally, the level $j$ at which the very largest eddies are located, will contain almost zero fluctuations due to it is getting closer to downward completeness (table 4.1). The present analysis agrees from the explanation related to Figure 2.2: the fluctuations are predominantly uncorrelated with the very large scales. This is very important when it comes to the initial conditions. When the entire field is simulated directly (i.e. Direct Numerical Simulation (DNS)), the creation of eddies of all size (parameterized by $\kappa = \frac{2\pi}{\lambda}$) is a must, before any computation is carried out (Appendix A). Similarly initial conditions are needed when the large eddies are resolved down to a certain size $\kappa$ located in the inertial range $-5/3$ (Figure 4.7). Afterwards, a cut-off
4.2. MULTISCALE/MULTILEVEL/MULTIRESOLUTION APPROACH

Frequency is done separating the resolved part from the modeled one. This, because of any \( \mathbf{u} \) at a level \( n \) (Figure 4.4) has 'extractable fluctuations' (Figure 4.6). On the other hand, when only the very large eddies are simulated, very flat-small-amplitude signals (Figure 4.8 b)), functions on subspaces \( W \) show up and the use of the classification 'fluctuations' can be questioned. In principle, Unsteady RANS (URANS) and VLES are the same. The use of Very Large Eddy Simulations (VLES) are justified for turbulence generating flows. Examples of these cases are shear flows and swirls flows (section 4.4).

The use of VLES in straight cannels using an initiated flow field has shown that all turbulence die after a while (Dick (2003)), which can be seen as the meaningless of VLES applications in non-turbulence generation flows. In addition, the energy spectrum generators available, such as Pao (1965), do not create the slope = 2 (Pope (2000), figure 6.15, p. 236), where the cut-off is normally carried out in VLES (Figure 4.7). They overestimate \( E(\kappa) \) for low values of \( \kappa \). Some researchers (Dick (2003), Sagaut (2004)) consider the initialization of the flow field in VLES/URANS, while others (Davidson (2004)) do not normally do it. In cases of highly sheared flows, as swirls, any primary instability will (re)build fluctuations very quickly. In the 3-D cylindrical vessel application, a pulse-like tangential velocity is created in the initial conditions, to mirror the experiments in Hamamoto et al. figure 3, p. 141. Thus, any equilibrium between fluid inertia and internal stress of pressure is broken down and a primary instability shows up (Drazin and Raid (1981)). The generation of turbulence by shears is guaranteed in this work.

![Figure 4.7](image.png)

**Figure 4.7.** Schematic cut-off frequency representation in Direct Numerical Simulations (DNS), Large Eddy Simulations (LES) and Very Large Eddy Simulation (VLES) in the space spectrum. The entire field is modeled in Reynolds Averaged Numerical Simulations (RANS).
Figure 4.7 can be represented as Figure 4.8 a) when it comes to terms of computational efforts and modeling complexity.

![Figure 4.8. a) Modeling complexity and computational efforts (Williams (1996) p. 2). b) Time evolutions of a local quantity computed with DNS, LES, VLES and RANS.](image)

From Figure 4.8 it is observed that filter width $\Delta_f$, which says how fine or coarse the grid is, is fine in both DNS and LES and fluctuations can be extracted from them, while $\Delta_f$ is coarse for VLES and RANS.

![Figure 4.9. Reconstruction procedure. Because $u_1 \in V_1 = u_2 \in V_2 + d\text{u}_1 \in W_2$, the details in $W_2$ is the difference $u_1 - u_2$. The subspaces $V_1$ and $V_2$ are obtained in a similar procedure fulfilling $V_1 = V_2 \oplus W_2$.](image)

The multiresolution has some important properties that relates the $V_j$ subspaces (Table 4.1).
4.2. Multiscale/Multilevel/MultiResolution Approach

1. **Containment**: \( \cdots \subset V_1 \subset V_0 \subset \cdots \subset V_{j+2} \subset V_{j+1} \subset V_j \subset \cdots \)

2. **Upward Completeness**: \( f_j \to f \) as \( j \to -\infty \).

3. **Downward Completeness**: All the details of \( f \) are lost as \( j \to \infty \).

4. **Shift invariance**: \( V_0 \) is invariance by any translation \( m \) proportional to the scale \( s = 2^{-j} ( = 2^{-n} \) in Figure 4.1 and 4.2 \), i.e. \( f(t) \in V_0 \iff f(t - ms) \in V_0 \).

5. **Scale invariance** (Dilation): \( V_{j-1} \) consists of all rescaled functions in \( V_j \), i.e. \( f(t) \in V_j \iff f(2t) \in V_{j-1} \).

6. **Shift-invariance basis**: There exist a \( \theta(t) \in V_0 \) such that its translation \( \theta(t - s) \) forms the basis of \( V_0 \). The basis can be either orthogonal or not.

| Table 4.1. | The subspaces \( V_j \) are related with each other by six (6) properties from the multiresolution approach (Machado (2000) p. 15 or any other reference on multiresolution or wavelets). |

Since the MRA helps to decompose, separate scales and reconstruct them, wavelets has been by Farge and Schneider (2000) as an alternative to LES. This reconstruction procedure (Figure 4.5, Figure 4.9) can be used to create multilevel, multiresolution RANS/LES algorithms, as the one by Labourasse (2002), whose implementation resembles part of the work by Terracol (2001) and Quéméré (2001). Labourasse’s algorithm one-way couples LES with RANS: Feedback from RANS to LES but not the opposite due to large computational costs.

Indeed, Eddy Simulations (either DNS, LES or VLES) goes the same path as Finite Element Method (FEM): initiated by engineers using *ad-hoc* and continued by applied mathematicians rigorously. Under the name of Variational Multiscale (VMS) (Hughes *et al.*), the explanation from Figure 4.5 is used to scale separate *a priori*, instead of spatial filtering. In VMS, the analysis starts with the weak or variational form of the N-S. Based on Hughes *et al.*, Collis (2002) p. 29 has recommended an improvement. Terracol (2001) multilevel algorithm seems to be a more general approach. A comparison is given by Sagaut (2003) p. 225.

Some multiresolution properties, such as scale invariance, have encountered certain problems in turbulent combustion. It is model dependent and further work is under way. That is why no discussion is included in this work about such unanswered issues. The importance of scale invariance relies on
the validity of a relation independently of the length of the scale range. Scale invariance is covariance by integration in scale space. The resolution can be changed by spatial dilation or spatial contraction. The insertion of MRA has shaken some well established models or how we see them.

4.3 RANS and (V)LES

Many of the implemented equations in this work and coded in GMTEC can be and/or has been derived from the MRA. The practical way to split the scales is by filtering (e.g. Figure 4.6), while the smooth flow states (e.g. $U(x)$ and $P$) can be obtained directly by averaging them. Because of the filtered and the averaged of the time dependent N-S equations, i.e.

$$\frac{\partial (u_i)}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \Rightarrow \frac{\partial u_i}{\partial t} = NS_i(u_j),$$

look similar, they are analyzed simultaneously helping to connect them.

**Filtered-NS eq.**

- velocity decomposition = filtered (= resolved) velocity + residual (= subgrid scale) field NOT filtered, i.e. $u_i(x, t) = \hat{u}_i(x, t) + u^{SGS}_i(x, t)$, where $u^{SGS}_i(x, t) \equiv u_i(x, t) - \hat{u}_i(x, t)$

- together with $p = \hat{p} + p^{SGS}$ and knowing that:

  1. filtering some residual
     \[ \Rightarrow \phi^{SGS} \neq 0. \]
  2. filtering some derivate \( \Rightarrow \frac{\partial \phi}{\partial I} = \frac{\partial \hat{\phi}}{\partial I} \) (+ commutation error) for $I$ being time, space (for uniform steady grid)
  3. doble filtering
     \[ \Rightarrow \tilde{\phi} \neq \hat{\phi}. \]

**Averaged-NS eq.**

- Reynolds decomposition = mean velocity + turbulence fluctuations, i.e. $u_i(x, t) = U_i(x) + u'_i(x, t)$, where $u'_i(x, t) \equiv u_i(x, t) - U_i(x)$

- together with $p = P + p'$ and knowing that:

  1. averaging some fluctuation \( \Rightarrow \overline{\phi} = 0. \)
  2. averaging some derivate \( \Rightarrow \frac{\partial \overline{\phi}}{\partial I} = \frac{\partial \phi}{\partial I}, \) for $I$ being time, space
  3. doble averaging
     \[ \Rightarrow \overline{\phi} = \phi. \]
4.3. RANS AND (V)LES

Filtered-NS eq. (cont.)

- then, the filtered NS eqs., i.e.,
  \[ \frac{\partial u_i}{\partial t} = \hat{NS}_i(u_j) \]

- that is, an additional term is added to the original NS where
  \[ \tau_{SGS}^{ij} = L_{ij} + C_{ij} + R_{ij} \]

Leonard stresses: \( L_{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \)
subgrid-scale cross stresses: \( C_{ij} = \hat{u}_i \hat{u}_j' - \hat{u}_i \hat{u}_j \)
Reynolds stresses: \( R_{ij} = u_i' u_j' \)

- simplification gives
  \[ \tau_{SGS}^{ij} = \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \]

- which is analogous to \( \Rightarrow \)

Averaged-NS eq. (cont.)

- then, the RANS eqs., i.e.
  \[ \frac{\partial u_i}{\partial t} = NS_i(U_j) \]

- that is, an additional term is added to the original NS where
  \( \tau_{RST}^{ij} = \hat{u}_i \hat{u}_j \) is the specific Reynolds stress tensor.

\( \tau_{RST}^{ij} \) is solved with modeled transport equations for turbulent kinetic energy \( k \) and dissipation rate \( \varepsilon \), i.e., the \( k - \varepsilon \) turbulence model.

- since \( \hat{u}_i \hat{u}_j = U_i U_j + \hat{u}_i \hat{u}_j \) due to Reynolds decomp. Hence

- \( \tau_{RST}^{ij} = \hat{u}_i \hat{u}_j - U_i U_j \)

Multiresolution has been used to obtain N-S equations for each \( \ell \)-level in subspaces \( V \) and their corresponding evolutions equations for the details in subspaces \( W \) (Sagaut (2003)). This approach helps to interconnect RANS with (V)LES. Thus, on the basis of operational decomposition, the subgrid-scale stress tensor \( \tau_{SGS}^{ij} \) and the specific Reynolds stress tensor \( \tau_{RST}^{ij} \) must be related. Assuming \( (\ldots) = (\ldots) \) yields (Germano (1999) p 34)

\[
\begin{align*}
\tau_{RST}^{ij} &= \hat{u}_i \hat{u}_j - U_i U_j \\
&= \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j + (\hat{u}_i \hat{u}_j) - (\hat{u}_i \hat{u}_j), \quad \text{i.e.}
\end{align*}
\]

\[ \tau_{RST}^{ij} = \tau_{SGS}^{ij} + T_{ij} \]  

where \( T_{ij} \) are resolved stresses. The equation (4.4) relates DNS, (V)LES and RANS models. It suggests the possibility of constructing a dynamic identity, where those models can be interconnected. For that purpose, a dynamic
function \( f(r) \) is obtained from (4.4), i.e.
\[
\tau_{ij}^{SGS} = f(r)\tau_{ij}^{RST}
\] (4.5)
Inserting (4.4) in (4.5) gives
\[
\tau_{ij}^{SGS} = f(r)\tau_{ij}^{RST} + T_{ij} + Q_{ij}
\] (4.6)
where \( Q_{ij} \) is a residual that is minimized using least square (Germano (1999)) giving:
\[
f(r) = 1 - \frac{\tau_{ij}^{SGS}T_{ij}}{\tau_{ij}^{RST}}
\] (4.7)
Worth to notice is that when \( T_{ij} \to 0 \), \( f(r) = 1 \) and \( \tau_{ij}^{SGS} \) becomes \( \tau_{ij}^{RST} \) from equation (4.5), i.e. the RANS limits. On the other hand, when \( T_{ij} \to \tau_{ij}^{RST} \), \( f(r) = 0 \) and \( \tau_{ij}^{SGS} = 0 \) from equation (4.5), the DNS limits.

### 4.3.1 Speziale Model

Based on the above analysis, Speziale (1998) has obtained (using least squares minimization)
\[
\tau_{ij}^{SGS} = \left[ 1 - \exp\left( -\beta r \right) \right]^n \tau_{ij}^{RST} / f(r)
\] (4.8)
where \( \beta \) and \( n \) are constant while \( r = \text{computational mesh size} / \text{Kolmogorov length scale} = \Delta / \eta \) and \( \eta \equiv \nu^{3/4} / \varepsilon^{1/4} \).
The \( \eta \) is estimated\(^3\) by the modelled transport equation for \( \varepsilon \). Notice that
\begin{itemize}
  \item when \( r = \Delta / \eta \to 0 \) \( \Rightarrow \tau_{ij}^{SGS} \to 0 \) \( \Rightarrow \) DNS
  \item when \( r = \Delta / \eta \to \infty \) \( \Rightarrow \tau_{ij}^{SGS} \to \tau_{ij}^{RST} \) \( \Rightarrow \) RANS
\end{itemize}
and that
\[
0 \leq f(r) \leq 1
\] (4.9)
The relation between lhs and first rhs term of \( \frac{\partial \hat{u}_i}{\partial t} = \text{NS}_i(\hat{u}_j) - \frac{\partial}{\partial x_j}(\tau_{ij}^{(SGS)}) \) and \( \frac{\partial \bar{U}_i}{\partial t} = \text{NS}_i(U_j) - \frac{\partial}{\partial x_j}(\tau_{ij}^{RST}) \) comes from the fact that \( \hat{u}_i \to U_i \) as the grid get coarser which is regulated by \( r = \Delta / \eta \to \infty \)

\(^3\)crucial part in this approach!!
4.3.2 Willems Model

Before the paper from Speziale (1998) came to light, Willems (1996) published a VLES turbulent model in his PhD (In German), which is also a rescaling method. Unlike Speziale (1998), \( \eta \) is not used here, but the integral turbulent length \( \ell (= \ell_t) \). As a literature curiosity, Magnient (2001) arrived the same model as William’s five years latter, based on the work from Peltier et al. (2001).

The Willem (1996) model can be seen as a part of Speziale (1998) more general approach. It is a \( k - \varepsilon \) that resolves turbulent structures of sizes smaller than \( \ell \) but larger than filter scale \( \Delta_f \). For DNS: \( \Delta_f < \eta \), for LES: \( \eta < \Delta_f < \ell \), for VLES: \( \eta \ll \Delta_f \leq \ell \) while for RANS: \( \Delta_f = \ell \) (Figure 4.8). The grid size must be \( \Delta \leq \Delta_f \) (Figure 4.10).

![Figure 4.10. Filter width/scale/size \( \Delta_f \) and integral length scale \( \ell \) (Willems (1996) p. 26).](image)

The two grids \( \ell \) and \( \Delta_f \) are connected by down-scaling and up-scaling:
• integral length scale $\ell$

Transport equations for $\overline{k} - \overline{\varepsilon}$

↓ down-scaling up-scaling ↑

• filter scale $\Delta_f$

Transport equations for $\hat{\rho}, \hat{\mathbf{v}}, \hat{\text{Energy}}$ and $\hat{Y_i}$

The turbulent kinetic and dissipation at the filter scale $\Delta_f$ are $\hat{k}$ and $\hat{\varepsilon}$, and obtained by down-scaling their corresponding integral scales values $\overline{k}$ and $\overline{\varepsilon}$ using

$$\hat{k} = \overline{k}(1 - f(r)) \quad (4.10)$$

$$\hat{\varepsilon} = \overline{\varepsilon} \quad (4.11)$$

(equation (4.11) is due to in the inertial range there is no dissipation, i.e. they are the same.)

where

$$f(r) = \begin{cases} 
1 - r^\frac{4}{3} & \text{for } r \leq 1 \Rightarrow \text{from DNS (at } r=0) \text{ to RANS (at } r=1) \\
0 & \text{for } r > 1 \Rightarrow \text{not physical according to (4.9)} 
\end{cases} \quad (4.12)$$

![Figure 4.11. Approximation of the correlation function equation (4.12) (Willems (1996) p. 28)](image-url)
Willems’ simplifications gives:

\[ \ell = \left( \frac{4}{3C_K} \right)^{3/2} \frac{k^{3/2}}{\varepsilon} \]  

(4.13)

Hence,

\[ r = \frac{\Delta f}{\ell} \rightarrow \begin{cases} 0 & \Rightarrow \text{DNS (Upward Completeness)} \\ \infty & \Rightarrow \text{RANS (Downward Completeness)} \end{cases} \]  

(4.14)

Equations (4.14) and (4.12) are implemented in the GMTEC code as:

\[ \nu_{\text{SGS}} = \left( \frac{\Delta f}{\ell} \right)^{4/3} \cdot \nu_{\text{RANS}} \]  

(4.15)

The algorithm starts at the \( \ell \)-level with initial estimated values (or from the previous time-step) for \( \overline{k} \) and \( \overline{\varepsilon} \) from which \( \tau_{ij}^{\text{RST}} \) is calculated.

- **at \( \ell \)-level:**
  1. \( \tau_{ij}^{SGS} = f(r)\tau_{ij}^{RST} \) are calculated (using Willems’ (4.11),(4.10) together with Boussinesq, etc) +
  2. transport equations for \( \widehat{\rho} \), \( \widehat{u}_j(j = 1,2,3) \), Energy and \( \widehat{Y}_i \), scalar species and the filtered NS eqs. i.e. \( \frac{\partial \overline{u}_i}{\partial t} = \overline{\nu}_i(\widehat{u}_j) - \frac{\partial}{\partial x_j}(\tau_{ij}^{SGS}) \) are solved
  3. **Up-scaling:** taking up values of \( \rho, p, u_j \), energy and scalars (Nothing in the implementation).
  4. transport equations for \( \overline{k} \) and \( \overline{\varepsilon} \) are solved, and
- **at \( \Delta f \)-level:**
  5. **Down-scaling:** taking down \( \tau_{ij}^{RST} \) and back to 1.

It is an open question to know how this simplifications influence in the results. Another issue is that a (2nd order) central difference is implemented in GMTEC and not the 4th-order recommended by Speziale.
In the RANS part, the standard \( k - \varepsilon \) model consists of the following transport equations:

\[
\frac{\bar{\rho}}{\partial t} \left( \tilde{k} \right) + \bar{\rho} \cdot \nabla \left( \tilde{k} \right) = \nabla \cdot \left( \frac{\bar{\rho} \nu_t}{\sigma_k} \nabla \tilde{k} \right) - \bar{\rho} \nu_t \frac{\partial \tilde{v}_a}{\partial x} - \bar{\rho} \tilde{\varepsilon} \quad (4.16)
\]

\[
\frac{\partial \tilde{\varepsilon}}{\partial t} + \bar{\rho} \cdot \nabla \tilde{\varepsilon} = \nabla \cdot \left( \frac{\bar{\rho} \nu_t}{\sigma_\varepsilon} \nabla \tilde{\varepsilon} \right) - \frac{c_{\varepsilon 1} \tilde{\varepsilon}}{k} \tilde{v}_a \frac{\partial \tilde{v}_a}{\partial x} - c_{\varepsilon 2} \tilde{\varepsilon}^2 \quad (4.17)
\]

where the first term on the r.h.s. represent turbulent transport, the second one turbulent production while the third one turbulent dissipation.

### 4.4 Swirl Flows

Any numerical turbulent combustion study demands a minimization of the computational complexity to have at least, some solution. Thus, only the main parts will be considered our efforts while the rest is left. However, it is important to have in mind the untreated part, since it can influence the final solution. In the present work, the turbulent combustion is numerical studied in a swirl flow, which can affect the combustion process in different ways (Zhang (1995), Park et al. (2002), Jakirlić et al. (2001), Hamamoto and his collaborators, and others). Among them, in :

i) **turbulence generation**: Swirl generates turbulence near the wall due to tangential shear and to shed vortices around a blunt body. Results form measurements show that the top dead centre (TDC) turbulence intensity with swirl can be as much as double the value with no swirl.

ii) **heat transfer**: Increased swirl leads to increased heat transfer coefficient, but to which extent that the turbulence intensity can affect the total heat loss is not clear. Its understanding can avoid the effect of excessive heat loss on thermal efficiency.

iii) **flame propagation due to swirl induced buoyancy**: Swirl-induced buoyancy can affect the flame propagation and change the configuration of the burning zone, which could in turn affect the global combustion rate and heat transfer rate. Relations among the swirl intensity, turbulence intensity, physical and chemical properties of reactants and products, and the flame propagation are not clear.
iv) **burning rate:** Most experimental results show that increased swirl lead to increased combustion rate, but the reverse had also been observed in few cases. The swirl influences combustion rate in a broad range of swirl levels. A set up criterion can be used to classify the swirl intensity, with which one can apply swirl in a proper range to enhance combustion and avoid negative effect of swirl on combustion. Considering the different effects of swirl on the combustion process, it is expected that there should be a optimum range of swirl level with which the shortest combustion duration can be achieved. Also, it is important to know how swirl affects the initial combustion duration (defined as the time period of 0 - 10 % mass burned) and main combustion duration (10 - 90 % mass burned).

No optimum swirl has been investigated in this work, nor heat release or turbulent generation. The buoyancy effects have not been considered in the computations. Thus, any improvement in the results should include such issues.

### 4.5 Wall Treatment

Because of boundary layers are usually too thin to be resolved, near wall models are implemented. Confined areas, such as channels and vessels, demand the use of Low Reynolds turbulent models. It implies some of the following grid characteristics near the wall:

- $\Delta y^+ = \frac{\Delta y u_\tau}{\nu} \rho / \rho = \frac{\Delta y u_\tau}{\nu} \sim +1$, where $\Delta y$ is the height of the cells closest to the wall, $u_\tau = \sqrt{\tau_w/\rho}$ is the friction velocity, $\tau_w = C_f q$ is the wall shear, $q = \frac{1}{2} \rho_\infty u_\infty^2$, and $C_f$ comes from the experiments (Wilcox (2000 b)). In numerical computations, $C_f$ is usually estimated first. From the results, $\Delta y^+$ is computed until it gives +1 in a procedure represented by Figure 6.1.

- As we move away from the wall, the height of a cell should not the increase larger than 10 % compared to its predecessor cell.

The above explanation reveals an increased number of small cells to compute. Those models are too costly. Therefore, the law-of-wall is applied in numerical combustion to have, at least, feasible solutions. A detailed discussion of this alternative approach is given by Poinsot and Veynante (2001) p. 345-354.
It is important to remember, from the fluid mechanics point of view, that if the computations on cells near the wall are wrong, the rest is wrong. This gives an idea about how desperate numerical combustion really is to get solutions. If outputs from CFD are considered qualitative results, those from CFD-combustion should be placed in a lower qualitative level.

At least, no near wall agreements with the measurements are expected from the numerical results.

### 4.6 On Renormalization Group Theory

In turbulence, 90% of all energy production is dissipated in the molecular zone, where a renormalization procedure is sometimes implemented. Few lines are dedicated to this modeling tool for the sake of completeness.

Renormalization is a tool initially introduced to remove divergences in quantum mechanics. Later, it has been used for the study of nonlinear systems, whose essential form is repeated at infinitely many scales. The interaction of \( f \) can be renormalized or rescaled to yield new dynamical systems of the same general shape as the original map \( f \) (c.f. McMullen (1994)). This can be achieved using a scaling law function type \( f(x) = Cx^a \), where \( C \) is a constant and \( a \) is the exponent. Such power laws have the property of scaling or self-similarity because given a constant \( b \) we have \( f'(x) = f(bx) = C(bx)^a = C'b^a \). Thus, the properties look the same at different scales. Renormalization can be done to functions that present all self-similar properties.

On the other hand renormalization group (RG) theory has been introduced by Gell-Mann and Low (1954) to improve perturbation theory by exploiting the non-uniqueness in the renormalization procedure. Here, the renormalization group is used as a systematic procedure for isolating phenomena, which exhibit despair scales and self-similarity. The focus of study when RG is used is on the small scales (i.e. high wavenumbers \( \kappa \)), where dissipation occurs. It is in this zone where molecular mechanisms occur and fractal approach does not apply due to viscosity. Remember that the initial kinetic energy, inserted in the largest scales by production mechanisms, is then transported through the inertial range with neglected dissipation down to the molecular zone. Thus, the exact amount of produced energy \( \approx \) dissipated energy, and one can obtain a relationship between large scale production and small scale dissipation. The production mechanisms such as compressibility, rotation, buoyancy, etc can be modeled by Gaussian random stirring force function \( f_i \) inserted in the N-S equations. The \( f_i \) force is homogeneous in space and time and isotropic in space. It also respects the \(-5/3\)
decay law in the inertial range. This is the idea behind Yakhot and Orszag (1986) work.

\[
\frac{\partial u_i}{\partial t} + \lambda u_j \frac{\partial u_i}{\partial x_j} = f_i + \frac{\partial P}{\partial x_i} + \nu \kappa_c \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{4.18}
\]

where \(f_i\) is white noise in time and soleniodal, \(\lambda\) is introduce for the perturbation analysis sake and \(\kappa_c\) is the wavenumber cut-off.

The RG theory is then used as a mode elimination procedure which starts from the scales where the initially inserted energy is dissipated into thermal energy, i.e. from the small scales. The modes above \(\kappa_c\) are eliminated while modes below are kept. Since the elimination procedure is based on wavenumbers, the N-S eqns have to be Fourier expanded both with respect to space and time, which requires that the velocity field has to be statistically stationary. This implies that the RG theory cannot handle freely-decaying turbulence, and it is one of the limitations of the theory.

Although this theory is already established still there exist questions about its main part, namely the \(\epsilon\)-expansion. Eyink (1994) goes further and states that the Yakhot and Orszag (1986) approach is a not true renormalization group.
Chapter 5

Combustion Modeling

Combustion Modeling has not escaped from the multiresolution attack. In turbulent combustion, local quantities at different multiscales has been defined and coupled to a (multi)resolution problem by Pocheau (1994). Based on it, Bychkov (2003) has shown that the behavior of a strongly corrugated flame front, influenced both by the external turbulence and by the D-L instability, can be studied from self-similar multiscale approach.

The presence of strongly curved flame fronts can lead to fractal properties of the propagation interface. In the fractal analysis, the turbulent burning velocity is estimated considering that the flamelets (section 5.1) can be described as a fractal surface (Gouldin (1987)). The fractal nature of the combustion has been confirmed by several experiments (Gouldin et al. (1988); Murayama and Takeno (1988); Mantzaras et al. (1989); Shepherd et al. (1990); Das (1993)). This is still studied (Giacomazzi (1999)), sometimes coupled with LES (Knikker (2002)). The existence of such fractal surfaces in ICE has lead to a considerable number of works in this direction (Chin et al. (1990); Santavicca et al. (1990); Matthews et al. (1992); Chin et al. (1992); Hall et al. (1992); Wu et al. (1994); Zhu et al. (1995); Matthews et al. (1996); Yoshiyama et al. (2003); Suzuki et al. (2003)).

5.1 Flamelet Approach

A turbulent premixed reacting flow is under flamelet regime when a line connecting any point \( x_u \in \textit{unburnt} \) to another point \( x_b \in \textit{burnt} \) crosses at least one active flame front (Poinsot and Veynante (2001) p. 192). Competitor approaches: \( i \) \( G \)-equation and \( ii \) flame surface density concept (FSDC). The last one has its origins on the work of Marble and Broadwell (1977) for non-premixed combustion and later extended to premixed cases (Pope
(1988), Candel and Poinsot (1990), Cant et al. (1990)). FSDC has been popular since the early 1990’s and describes the mean reaction rate as the product of the flame surface density $\sum$ by the local consumption rate per unit of flame area. On the other hand, there exist two flamelets models for the $G$-equation based on:

<table>
<thead>
<tr>
<th>Propagation Variable</th>
<th>Level Set Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>• assumes that instantaneous flame is a discontinuity in the flow field.</td>
<td>• assumes that laminar flamelet equations use finite rate chemistry to reduce the inner structure of the flame.</td>
</tr>
<tr>
<td>• no turbulence effects on the inner structure.</td>
<td>• turbulence effects on the inner structure of the instantaneous flame is taken into account.</td>
</tr>
<tr>
<td>• hence, not useful for thin reaction zone regimes but still can be applied in corrugated regimes.</td>
<td>• hence, the level set method applies also in the thin reaction zone regimes as well as in corrugated regimes.</td>
</tr>
<tr>
<td>• exhibit an unphysical increase of combustion at the wall.</td>
<td>• does NOT exhibit an unphysical increase of combustion at the wall because the turbulent dissipative time scale $k/\varepsilon \to 0$ at the wall. This decreases the turbulent flame speed at the wall.</td>
</tr>
</tbody>
</table>

Therefore, the level-set formulation is the best approach for the $G$-equation. A comparison between flamelet models using FSDC and $G$-equation based on the level-set formulation is not available in the literature (2004). The work of Duclos et al. (1993) was prior the actual $G$-equation based on level-set proposed by Peters (1999). The FSDC defenders point out the difficulty of estimating heat release when the $G$-equation is implemented. Many researchers still couple the $G$-equation directly to the progress variable and forget its level-set formulation. The level-set is a mathematical method, which adds dynamics to the unburnt-burnt interface surface in an externally generated velocity field. The $G$-equation based on the level-set is the chosen flamelet model for this thesis due to its mathematical approach and potential.
5.2 Level Set and Fast Marching Methods

The (curved) surface flame propagates in a direction normal to itself with a velocity \( \frac{dx_f}{dt} \), which describes the displacement of a point at the position \( x \) on the flame front surface, when it deforms. The derivation of an equation that represent the flame front as an iso-scalar surface \( G(x, t) = G_0 \) is an applied mathematical problem (Figure 5.1) while to model the speed function \( \frac{dx_f}{dt} \) is a turbulent combustion problem (subsection 5.2.1). Depending on how the front is assumed to move, two options representing surface movements implicitly arise (Sethian (1999), Whitaker (2002), Osher and Fedkiw (2003)):

### Boundary value Problem (BVP)
- The front moves either outward \( \left( \frac{dx_f}{dt} > 0 \right) \) or inward \( \left( \frac{dx_f}{dt} < 0 \right) \).
- \( G(x(t)) \) is a single-valued due to it passes over a point \( x \) only one time.
- The static single-valued arrival function \( G(x(t)) \) of the front crosses monotonically each point \( x \) and contains a family of \( k \) level sets corresponding to surfaces at different times \( t \). Hence, \( G(x(t)) = k(t) \).
- The behavior of \( G \) is analyzed by derivation, i.e. \( \nabla G \cdot \frac{dx_f}{dt} = \frac{dk(t)}{dt} \).
- The behavior of \( G \) is analyzed by derivation, i.e. \( \frac{\partial G}{\partial t} + \nabla G \cdot \frac{dx_f}{dt} = 0 \).
- This problem is solved using the Fast Marching Method.
- This problem is solved using the Level-Set Method.
- This is a limited representation by definition.
- This is a more general representation.
- Less computational cost.

### Initial value Problem (IVP)
- The front can move both outward \( \left( \frac{dx_f}{dt} > 0 \right) \) and inward \( \left( \frac{dx_f}{dt} < 0 \right) \).
- \( G(x(t), t) \) is NOT a single-valued due to it can pass over a point \( x \) several times.
- The dynamic function \( G(x(t), t) \) is a one-parameter family of embeddings which changes over time. The \( x \) remains on the constant \( k \) level set of \( G \) as it moves. Hence, \( G(x(t), t) = k \).
- The behavior of \( G \) is analyzed by derivation, i.e. \( \frac{\partial G}{\partial t} + \nabla G \cdot \frac{dx_f}{dt} = 0 \).
- This problem is solved using the Level-Set Method.
- This is a more general representation.
- Large computational cost.

The \( k \) value associated with the iso-surface that passes through the point \( x \) is \( G(x) \). The \( G(x(t)) \) can be seen as an arrival time function \( T(x(t)) \) for the
CHAPTER 5. COMBUSTION MODELING

BVP and the behavior of the front can be described by the Eikonal equation

$$|\nabla T| \cdot \frac{dx_f}{dt} = 1.$$  

In Figure 5.1 the scalar $G$ represents the instantaneous level, $G_0=0$ level is the flame surface, while $G < G_0$ is unburnt and $G > G_0$ is burnt.

![Figure 5.1](image)

Figure 5.1. Schematic representation of the flame front as an iso-scalar surface $G(x,t) = G_0$.

In the kinematic balance for the unsteady\textsuperscript{1} case, ignoring initial flame development and effects of flame curvature, the propagation velocity field $\frac{dx_f}{dt}$ of the flame front is a consequence of an imbalance between the flow velocity $\mathbf{v}_f$ at the front and the burning velocity $s_L$ in the normal direction

$$\frac{dx_f}{dt} = \mathbf{v}_f + \mathbf{n} s_L \quad (5.1)$$

where $\mathbf{n}$ is the vector normal to the front in the direction of the unburnt gas (Figure 5.1)

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|} \quad (5.2)$$

Inserting (5.1) and (5.2) in the $G$-equation of the level-set formulation gives the field equation

$$\frac{\partial G}{\partial t} + \mathbf{v}_f \cdot \nabla G = s_L |\nabla G| \quad (5.3)$$

Although the value of $G$ outside $G_0$ (i.e. $G \neq G_0$) can be chosen arbitrarily, it is found useful to define $G$ as a distance function to the flame front. The advantage of this idea relies in the ability of direct coupling the $G$-equation with the temperature of the gas and thereby decreasing the computational cost. However, significant errors in the position of the flame front show up

---

\textsuperscript{1}The stationary case is covered in section 3.1.
after some time steps $\Delta t$. Sussman et al. (1994) has attacked this problem by solving
\[
\frac{\partial G}{\partial t} = S_s(G(x, t = 0) - G_0)(1 - |\nabla G|) \tag{5.4}
\]
until a steady state is reached, starting with the initial condition $G(x, t = 0) = G_0^0$. The $S_s(G^0) = \frac{G^0}{\sqrt{G^0^2 + \epsilon^2}}$ is a smoothed sign function. The time step to solve (5.4) can be $\Delta t = \frac{\epsilon}{10}$ while $\epsilon$ is determined by relating it with the grid spacing e.g. $\epsilon = \max(\max(\Delta x), \max(\Delta y), \max(\Delta z))$. The use of (5.4) implies that $G$ remains unchanged at the interface $G_0$, while away from $G_0$, the $G$ will converge to $|\nabla G| = 1$, which is equivalent to $G$ being a distance function. The distance from the flame front at a certain point $x$ is now easily determined from $G(x) - G_0$. The procedure of keeping $G$ as a distance function is known as reinitialization of $G$, which is carried out after every time step in the numerical solution (Figure 5.2). Thus, after integrating (5.3) over a certain time interval $\Delta t$, the hyperbolic differential equation $|\nabla G| = 1$ is solved outside the flame surface with boundary conditions at the surface.

\[\text{Figure 5.2. Flow diagram of the reinitialization proposed by Sussman et al. (1994).}\]

The Level Set Formulation of the $G$-equation is then
\[
\frac{\partial G}{\partial t} + \nabla f \cdot \nabla G = s_L|\nabla G|, \quad G = G_0 \tag{5.5}
\]
\[
|\nabla G| = 1, \quad G \neq G_0 \tag{5.6}
\]

Physical-mathematical interpretation:
- $G = G_0$ describes location and geometry of the flame front.
- $G \neq G_0$ describes the normal distance to the flame front.
• The iso-surface $G_0$ is introduced as a marker for the geometrical flame location.

• The $G$-equation (5.5) has only a physical meaning at the flame front $G_0$.

• Outside of the iso-surface $G_0$, the $G$ is not defined in (5.5).

• Any level set different from $G_0$ has no influence on the propagation of the iso-surface of $G_0$.

• The $G$-equation (5.5) is independent of the underlying equations of the fluid motion.

• The classical Reynolds averaging concept does not lead to a unique result for the mean $G$-field due to the value of $G$ is physically irrelevant and can be changed without altering the the actual position of the flame front (Oberlack et al. (2001)).

• The turbulent burning velocity $s_T$ is only defined at the flame front ($G = G_0$) and has no physical meaning outside ($G \neq G_0$). The $s_T$ is related to $s_L$ by the flame surface area ratio $A_T/A = s_T/s_L$.

• The modification of $s_L$ due to curvature, flame stretch or heat release does not break any symmetry except for scaling (Oberlack et al. (2001)).

Any overlook of the physical meaning of the level set formulation lead to result misinterpretation (e.g. Zimont and Lipatnikov (1995), Zimont et al. (1998)).

Although (5.5) does not depend on any value of $G$ away from $G_0$, the distance $x_n$ from the flame surface in normal direction (Figure 5.1) can be uniquely defined as

$$dx_n = -\mathbf{n} \cdot d\mathbf{r} = \{\text{inserting (5.2)}\} = \frac{\nabla G}{|\nabla G|} \cdot d\mathbf{r} \quad (5.7)$$

At a certain frozen $G$-field time, the differential increase of the $G$-level along $d\mathbf{r}$ is

$$dG = |\nabla G| \cdot d\mathbf{r} \quad (5.8)$$

Inserting (5.9) in (5.7) gives

$$dx_n = \frac{dG}{|\nabla G|} = \{\text{inserting (5.10)}\} = \frac{dG}{\sigma} \quad (5.9)$$
where absolute value of the gradient of $G$ at $G(x,t) = G_0$ is sometimes denoted in the literature as

$$\sigma = |\nabla G|_{G(x,t)=G_0} = \{\text{or simply}\} = |\nabla G| \quad (5.10)$$

## 5.2.1 On the Corrugated Flamelets Regime and the Thin Reaction Zone Regime

The $G$-equation (5.5) describes the propagation of thin flame structures and assumes that $\ell_F < \eta$. The entire flame structure is embedded within a locally quasi-laminar flow field. Thus, (5.5) can be used to describe premixed turbulent combustion problems on the corrugate zone. However, (5.5) demands a well-defined burning velocity $s_L$, which is modified due to curvature, stretch and heat release. Because of the variation of the normal vector (5.2) reveals front deformation, the flame front curvature $\kappa$ can be described as

$$\kappa = \nabla \cdot n \quad (5.11)$$

The insertion of the parameters that change $s_L$ lead to a final $G$-equation (Peters (2000) pp. 94-97) for the corrugate zone:

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s^0_L |\nabla G| - DL\kappa |\nabla G| - LS |\nabla G| \quad (5.12)$$

In addition, the (5.5) can be used to describe the thin reaction zone (Peters (2000) pp. 104-106): The location of the thin reaction zone is identified by the inner layer (Figure 3.2), whose position is described by a iso-scalar surface of the temperature $T(x,t) = T_0$. A temperature equation can be obtained. It contains a propagation velocity $\frac{dx}{dt}|_{T=T_0}$, which is related to a displacement speed similar to (5.1). This displacement speed replaces the $s_L$ in (5.5). Remember the coupling between the temperature and $G$-equation previously mentioned. Thus, a $G$-equation for the thin reaction zone is obtained:

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L \kappa |\nabla G| - D\kappa |\nabla G| \quad (5.13)$$

The two equations, each representing these two neighbor regimes, have some important component:
Corrugated Flamelets Regime

- propagation term $s_L^0 |\nabla G|$ is dominant. $s_L^0$ is the burning velocity of the unstretched planar flame.
- only eddies with turnover velocity $u'_n = s_L |\nabla G|$ interact with the flame front.
- $(\eta>)L \sim \ell_F \Rightarrow$ not important.

Thin Reaction Zone Regime

- curvature term $\kappa |\nabla G|$ is dominant.
- flame front advancement depends on mixing within the preheated zone.
- $L$ not defined due to not quasi-steady laminar flame structure.

Taking the dominants part from each regime and neglecting the strain term $\mathcal{L} \mathcal{S}$ yields:

$$
\rho \frac{\partial G}{\partial t} + \rho \mathbf{u} \cdot \nabla G = \left( \rho s_L^0 \right) \frac{\sigma - (\rho D)}{\rho} \kappa \sigma
$$

(5.14)

where each terms is multiplied by $\rho$ for consistency with other field equations and $\sigma = |\nabla G|$.

5.3 Premixed Turbulent Combustion Modeling with Level Set

In the modeling procedure, the mean position of the flame front $\bar{G}$ and its variance $\overline{G^2}$ are needed when flame fluctuations, deformations are considered. The location of the mean flame front $x_f$ is defined as $\bar{G}(x_f) = G_0$ while its variance $\overline{G^2}$ is defined by the shape of the (Gaussian) probability density function (pdf) axis symmetric at $\bar{G}(x_f) = G_0$. Thus, $\overline{G^2}$ is conditioned by $\bar{G} = G_0$ and writes $\overline{G^2}\big|_{\bar{G}=G_0}$, which measures the fluctuations of the instantaneous flame front about the mean $\bar{G} = G_0$. To compute the $\bar{G}$ and $\overline{G^2}$, a probability density function (pdf) $P(G;\mathbf{x},t)$ for the scalar $G$ at point($\mathbf{x},t$) have to be defined. In addition, $P(G;\mathbf{x},t)$ can be used to define the pdf of finding the flame surface $G(\mathbf{x},t) = G_0$. However, the pdf definition is possible when the $G$-equation have properties similar to those equations used in fluid dynamics and scalar mixing. Therefore, its
5.3. PREMIXED TURBULENT COMBUSTION MODELING WITH LEVEL SET

nonuniqueness outside the surface \( G(\mathbf{x}, t) = G_0 \) are overlooked.

\[
\bar{G} = \int_{-\infty}^{+\infty} GP(G; \mathbf{x}, t)dG
\]  
(5.15)

\[
\overline{G^2} = \int_{-\infty}^{+\infty} (G - \bar{G})^2 P(G; \mathbf{x}, t)dG
\]  
(5.16)

\[
P(G_0; \mathbf{x}, t) = \int_{-\infty}^{+\infty} \delta(G - G_0)P(G; \mathbf{x}, t)dG = P(\mathbf{x}, t)
\]  
(5.17)

where \( P(G; \mathbf{x}, t) \), (5.15) and (5.16) are nonunique outside the flame surface \( G(\mathbf{x}, t) = G_0 \) due to \( G \) is only defined at the flame front. The (5.17) is the number of flame crossings in a small volume \( \Delta V \) at \( \mathbf{x} \) over a small \( \Delta t \). Neglecting any perturbation, the pdf of \( G \) has a Gaussian pdf (Figure 5.3).

\[\text{Figure 5.3. Gaussian pdf. Definition of } \bar{G}, \overline{G^2} \text{ and } \ell_{F,t}. \text{ Burnt for } x_f < 0 \text{ and unburnt for } x_f > 0 \text{ (Herman (2000) p. 34).}\]

The equation (5.7), \( P(G; \mathbf{x}, t) \) and the standard deviation \( (\overline{G^2})^{1/2} \) can be used to define the turbulent flame brush thickness\(^2\)

\[
\ell_{F,t} = \left( \overline{G^2} \right)^{1/2} \left| \nabla \bar{G} \right| \bigg| \bar{G}=G_0
\]  
(5.18)

which can be used to measure the flame front fluctuations in front normal direction.

\(^2\text{see Peters (2000) pp. 111-112 for a 1D definition of } \ell_{F,t}.\)
In reality, the Gaussian shape is skewed due to heat release. Thus, the heat release can theoretically be estimated in the level set formulation of the $G$-equation from skewed-Gaussian shape - Gaussian shape.

The modeling procedure continues with the formulation for the mean, the (V)LES of $G$ and their variance.

### 5.3.1 Formulations for the Mean of $G$ and its Variance

A state function $f$ can be split into its mean function $\bar{f}$ and its fluctuation function $f'$, on the subspaces $\bar{f} \in V$ and $f' \in W$ when seen from the multiresolution perspective (Figure 4.5). Because of a combustion process shows large density $\rho$ variations crossing the flame front (Figure 5.1), the density should be included in the splitting to get more compact formulations. This is when Favre averaging is needed. The Favre average is a density-weighted average for an arbitrary $f$. It is defined by $\tilde{f} = \frac{\rho f}{\rho}$ and denotes the departure of $f$ from $\bar{f}$ as $f'' = f - \tilde{f}$. Thus, the average $\bar{f''} \neq 0$ but $\bar{\rho f''} = 0$ by the definition of Favre fluctuation. On the other hand, the Favre filtering is denoted as $\tilde{\hat{f}} = \frac{\hat{\rho f}}{\hat{\rho}}$. From equations (5.14), (5.10), (5.11) and (5.2) the Favre split of $G$ and $\upsilon$ are needed. For derivation purpose, unconditional averages $\tilde{\overline{G}}$ and $\tilde{\overline{\upsilon}}$ are assumed to exist temporarily.

$$G = \tilde{G} + G'' \quad \upsilon = \tilde{\upsilon} + \upsilon'' \quad (5.19)$$

The iso-surface $G(x, t) = G_0$ and the iso-temperature surface $T(x, t) = T_0$ are placed immediately ahead of the thin flame structure, where $\rho = \rho_u \approx$ constant along the $G_0$ iso-surface (Figure 5.1). Thus, $\tilde{G} = \frac{\rho G}{\rho} \approx \overline{G}$ for both corrugate flamelets and thin reaction zone flamelets regimes (Figure 3.3). Nevertheless, Favre average should be used to be consistent with standard turbulent modeling for variable-density flows. Contrary to $\tilde{G}$, the Favre mean velocity $\tilde{\upsilon}$ remains an unconditional average. Thus, a conditional counterpart is needed (Peters (2000) p. 115).

The derivation of an equation for the mean of $\tilde{G}$ starts with the average of (5.14):
5.3. PREMIXED TURBULENT COMBUSTION MODELING WITH LEVEL SET

\[
\frac{\partial G}{\partial t} + \rho \mathbf{u} \cdot \nabla G = (\rho s_0^L) |\nabla G| - (\rho D) \kappa |\nabla G| \n
= \{ \text{inserting (5.19) (see example in [130] p. 170)} \} = \\
\rho \frac{\partial (\tilde{G} + G'')}{\partial t} + \rho (\tilde{\mathbf{u}} + \mathbf{u}') \cdot \nabla (\tilde{G} + G'') = (\rho s_0^L) |\nabla (\tilde{G} + G'')| - (\rho D) \kappa |\nabla (\tilde{G} + G'')| \\
= \{ \text{use (5.11), that } \rho = \rho_u \approx \text{constant and } \rho f'' = 0. \}
\]

More details in [90] pp. 115-118

\[
\rho \frac{\partial \tilde{G}}{\partial t} + \rho \tilde{\mathbf{u}} \cdot \nabla \tilde{G} = (\rho s_0^L) |\nabla \tilde{G}| - \rho D_t \kappa |\nabla \tilde{G}| \quad (5.20)
\]

where \( s_0^L \) is the laminar burning velocity for a steady planar turbulent flame assumed to be solely depended on \( \text{mean} (= \text{averaged}) \) quantities. \( D_t \) is the molecular diffusivity. The equation for the variance of \( G \), i.e. \( \tilde{G}'' \), is derived by substracting the equation for \( \tilde{G} \) from (5.14) (Peters (2000) pp. 115-118):

\[
\rho \frac{\partial \tilde{G}''}{\partial t} + \rho \tilde{\mathbf{u}} \cdot \nabla \tilde{G}'' = 2 \rho D_t (\nabla \tilde{G})^2 - c_s \rho \tilde{\kappa} \tilde{G}'' + \nabla \parallel \cdot (\rho D_t \nabla \parallel \tilde{G}'' \parallel) \quad (5.21)
\]

where \( c_s = 2.0 \) is a modeling constant, \( \tilde{\kappa}/\tilde{\varepsilon} \) is the integral time scale and \( \nabla \parallel \) means that only gradients in the mean flame front \( \text{tangential} \) direction are calculated. The equation (5.20) and (5.21) shares the same mathematical properties, for instance:

\begin{itemize}
  \item \( \tilde{G}(\mathbf{x}, t) = G_0 \) describes the location of the mean flame front.
  \item \( |\nabla \tilde{G}| = 1 \) in \( \tilde{G}(\mathbf{x}, t) \neq G_0. \)
  \item Reinitialization (|\nabla \tilde{G}| = 1) of the \( \tilde{G} \)-field makes that normal diffusion vanishes.
\end{itemize}

but also

\begin{itemize}
  \item \( \tilde{G}'' \) represents the turbulent flame brush thickness.
\end{itemize}
5.3.2 Formulations for the Filtering of $G$ and its Variance

Up to this point, nothing has been said on any connection between multiresolution and level-set. Thus, is the level set method a multiresolution approach? In the level set method, the interface $G = G_0$ is defined as the zero level set of a function. For example, in 2D, it would be the zero level set of $G(x, y)$, where $(x, y)$ are on a discrete grid of $N \times M$ pixels. The values of $G(x, y)$ is then altered using a partial differential equation (PDE) to move the zero level set. Since the number of pixels, $N \times M$, doesn’t change during evolution, the approach is not multiresolution. It is worth noticing in Figure 4.4 how the number of pixels changes during the evolution in the turbulent filter representation. However, it is possible to execute the level set method in a multiresolution fashion. Consider a family of functions $G^j = G(2^j x, 2^j y)$ where $j$ is an integer $0, 1, 2, \cdots$ (Figure 4.5). These functions are multiresolution samples of $G(x, y)$. Each successive function has a lower resolution. For example, $G^0 = G(x, y)$ has $N \times M$ pixels, $G^1$ has $(N/2) \times (N/2)$ pixels, $G^2$ has $(N/4) \times (M/4)$ pixels, and so on. If desired, PDE can be solved at a coarser resolution, say $G_2$, until convergence. Then, that result can be projected into a higher resolution, say $G^1$, and the PDE is solved at the higher resolution. One can continue operating like this until the PDE is solved at the highest resolution $G^0$ (Figure 5.4). Observe that our friend, the scaling factor $2^j$ from Table 4.1, Figure 4.1 and Figure 4.2, has shown up again.

$G^j_0 \in V_j$

$G^{j+1}_0 \in V_{j+1}$

$\in W_{j+1}$

Figure 5.4. Decomposition of the interface $G^j = G((2^j x, 2^j y), t)$ in $V_j$ into its smooth component $G^{j+1} = G((2^{j+1} x, 2^{j+1} y), t)$ in $V_{j+1}$ and its rough component $G' = G((2^j x, 2^j y), t) - G((2^{j+1} x, 2^{j+1} y), t)$ in $W_{j+1}$. $G(2^j = 0 x, t) = G(2^{j+1} x, t) + \sum_{k=j}^{j-1} G'(2^k x, t)$.
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Such decomposition has been successfully achieved in image processing by Slabaugh (2002) et al. and can be extended to the scope of this work. The implementation here starts with the already explained idea that the actual combustion model is embedded on a turbulent flow. The turbulent flow can be decomposed by slices, organized in levels (Figure 4.4). Then, on each \( j \)-level slice, a level set combustion model \( G(2^j x, 2^j y) \) can be applied. The extension can continue based on Figure 4.4, where \( G \) at the interface is split into its rough component in \( V_j \) and its smooth component in \( W_j \). The combustion model is exposed to an equivalent analysis. The view to analyze the filtered \( G \) equation assuming multiresolution of the level set has been tackled (in Sweden) by the author, which welcomes any comment. Actually, a literature research (2004) does not give any hit where the multiresolution is applied in the \( G \)-equation using level-set. The word multiresolution is not even alluded in the works of Peters (2000), Pitsch and de Lageneste (2002) and Pitsch (2002) when the \( G \)-equation is formulated and/or used. The last paper is in fact an intention to derive the filtered \( G \)-equation reaching a result, which disagrees with the filtered \( G \)-equation used by the author in his previous work together with Lageneste. Some steps followed by Pitsch (2002) are not quite convincing; an opinion shared at ITM, RWTH-Aachen during the spring of 2003.

The multiresolution perspective may help to clarify how to attack some problems. For instance, in dynamic zonal multi-domain RANS/LES. Another example can be on small instabilities that may show up as small perturbations, distortions of the interface. Assume that the study of these perturbations at a certain frequency \( \kappa_j \) (Figure 4.4) is desired. The distortions can be read from the projection of the interface \( G = G_0 \) onto the subspace \( W_j \) (Figure 4.6). Also, a "Gibson resolution" can be helpful to study the only eddies interacting with the flame front, etc. However, any multiresolution decomposition/reconstruction procedure is filtering dependent and the presence of leakage, due to overlapping among frequency bands, can make difficult the extraction of a particular frequency (Machado (2000)). A mathematical analysis to proof whether or not the existence of a unique \( G^j \)-equation in \( V_j \) and in \( W_j \) is left as further work. The advantage of the MRA may not stop in the manipulation of the \( G \)-equation. It may add the opportunity of constructing fast (parallel) algorithms, well needed in numerical combustion. A closer look at these aspects are left as further work. A starting point can be Terracol’s FAS (2001), Slabaugh (2002) and Cai and Samuelsson (2000). Indeed, a parallel (adaptive) algebraic multigrid (AMG) algorithm, such as BoomerAMG (Henson and Yang (2002)), is a strong candidate to implement in codes with unstructured grids (e.g. GMTeC). To obtain good results in AMG, large positive off-diagonal elements must be
present in the matrix (Machado (2004)). Whether or not the AMG can be successfully integrated to a multilevel view of the level-set is another open issue. Up to now (2004), conventional domain decomposition has been implemented to parallelize level-set (Croce et al. (2004)). Treurniet (2002) has split the computational domain in two: one to study the interaction of the flame front with homogeneous turbulence and a second to compute the flow and the development of the flame front around a square cylinder.

The use of the multiresolution approach can be another way to justify that a procedure, similar to that of section 5.3.1, is applicable for the filtered $G$ equation. The filtered $G$ equation, valid in both the corrugated flamelets and the thin reaction zone, has already been given by (Peters (2000) p. 154) and it, not surprisingly, resembles (5.20). However, an interconnection between subgrid viscosity from (V)LES and the RANS eddy viscosity should be included already here, as pointed out by Ewald (2003 a). Thus, the equations for $\tilde{G}$ and $\tilde{G}''$ are:

\[
\hat{\rho} \frac{\partial \tilde{G}}{\partial t} + \hat{\rho} \vec{v} \cdot \nabla \tilde{G} = (\hat{\rho} s_l^0 |\nabla \tilde{G}| - \hat{\rho} \hat{D}_l \hat{\kappa} |\nabla \tilde{G}|) \tag{5.22}
\]

\[
\hat{\rho} \frac{\partial \tilde{G}''}{\partial t} + \hat{\rho} \vec{v} \cdot \nabla \tilde{G}'' = 2\hat{\rho} \hat{D}_l (\nabla \tilde{G}'' \cdot \nabla \tilde{G}'') - c_s \hat{\rho} \frac{\hat{\kappa}}{\hat{\epsilon}} \hat{\tilde{G}}'' + \nabla \cdot (\hat{\rho} \hat{D}_l \nabla \tilde{G}'' \cdot \vec{v}) \tag{5.23}
\]

where the hat $\hat{\cdot}$ denotes a spatial filtering while the wide hat with the wide tilde $\tilde{\cdot}$ a spatial Favre filtering. The equation (5.23) is obtained following a similar procedure applied to get (5.21). Both (5.22) and (5.23) share the physical-mathematical properties with (5.20) and (5.21), with the corresponding difference in terms of average and filtering. Those differences are
5.3. PREMIXED TURBULENT COMBUSTION MODELING WITH LEVEL SET

tackled in this work with the Willems(1996) model, i.e.:

\[
\tilde{\varepsilon} = \tilde{\varepsilon} (5.24)
\]

\[
\tilde{k} = \left( \frac{\Delta f_j}{\ell} \right)^{2/3} \cdot \tilde{k} (5.25)
\]

\[
\tilde{D}_t = \left( \frac{\Delta f_j}{\ell} \right)^{4/3} \cdot D_t (5.26)
\]

\[
\tilde{G}_{\text{avg}} = \{ \text{from the time evolution of the } \ell_{F,t} \}
\]

\[
\text{Peters (2000) p. 120, 122, 123 and Ewald (2003 a)} =
\]

\[
= \frac{2 \tilde{D}_t}{c_s} \tilde{k} = \{ \text{with (5.26) and (5.25)} \} = \left( \frac{\Delta f_j}{\ell} \right)^2 \tilde{G}_{\text{avg}}
\]

(5.27)

where, in the general perspective, \( \Delta f_j \) can be seen as the filter width at \( j \)-level (Figure 4.4). Because of these interconnections (5.24)-(5.27), the coding of (5.22) and (5.23) is very simple, once (5.20) and (5.21) are already in GMTEC.

5.3.3 A Model Equation for the Flame Surface Area Ratio and its Closures

It has been said that a well-defined turbulent burning velocity \( s_{0T} \) is a must in the formulation of the equations. Two effects to consider in the modelling of the turbulent burning velocity:

- the effect of curvature, which is important in the small scale turbulent regime.
- the effect of laminar flame propagation, which is important in the large scale turbulent regime.

Since the \( s_{0T} \) is related to the mean gradient \( \tilde{\sigma} \) by \( (\tilde{\rho} s_{0T}) |\nabla \tilde{G}| = (\tilde{\rho} s_{0L}) \tilde{\sigma} \) (Peters (2000) p. 118), a modeled equation for the flame surface area ratio \( \frac{A_T}{A} = \tilde{\sigma} \) is enough (Peters (2000) p. 129). The \( \tilde{\sigma} \) represents the mean gradient \( \tilde{\sigma} = |\nabla \tilde{G}| + \tilde{\sigma}_t \). Therefore, the model equation for the unconditional \( \tilde{\sigma}_t \) is needed,
which is (Peters (2000) p. 130):

\[ \rho \frac{\partial \bar{\sigma}_t}{\partial t} + \bar{\rho} \mathbf{v} \cdot \nabla \bar{\sigma}_t = \nabla \parallel (\bar{\rho} D \nabla ||\sigma_t) + c_0 \bar{\rho} \left( -\nabla \parallel \mathbf{v}_\alpha \mathbf{v}_\beta \right) \frac{\partial \bar{\mathbf{v}}_\alpha}{\partial x_\beta} \bar{\sigma}_t \]

local rate of change

\[ + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \bar{\sigma}_t \]

convection

\[ = \nabla \nabla (\bar{\rho} D \nabla \bar{\sigma}_t) + \frac{c_1 \bar{\rho}}{k} \frac{\partial \tilde{\mathbf{v}}_\alpha}{\partial x_\beta} \bar{\sigma}_t \]

turbulent transport

\[ + c_0 \bar{\rho} \left( -\nabla \parallel \mathbf{v}_\alpha \mathbf{v}_\beta \right) \frac{\partial \bar{\mathbf{v}}_\alpha}{\partial x_\beta} \bar{\sigma}_t \]

production of \( \frac{\partial \bar{\sigma}_t}{\partial x_\beta} \) by mean velocity gradients

\[ + c_1 \bar{\rho} \left( \frac{\nabla \parallel \tilde{G}}{G^\nu} \right)^2 \bar{\sigma}_t \]

turbulent production of \( \frac{\partial \bar{\sigma}_t}{\partial x_\beta} \)

\[ - c_2 \bar{\rho} \frac{s_L^0 \sigma_t^2}{(|\nabla \tilde{G}|)^{1/2}} \]

kinematic restoration of \( \frac{\partial \bar{\sigma}_t}{\partial x_\beta} \)

\[ - c_3 \bar{\rho} \frac{D \sigma_t^3}{G^\nu} \]

dissipation of \( \frac{\partial \bar{\sigma}_t}{\partial x_\beta} \)  

(5.28)

where the constant \( c_0 = c_{x,1} - 1 = \{\text{from (4.17)}\} = 0.44 \), \( c_1 = 4.63 \) (Wenzel (2000)), while \( c_2 = 1.01 \) and \( c_3 = 4.63 \) when steady planar flame is assumed (Peters (2000) p. 132). It is worth notice that an unsteady approach would require an initial value of \( \bar{\sigma}_t \). Because of steadiness, the \( \frac{\partial \bar{\sigma}_t}{\partial x_\beta} \) term in (5.28) disappears. The planar case implies that the convective and the turbulent transport term vanish. Also, the second term on the r.h.s. is neglected because of production term \( \ll \) turbulence production. Thus, the result is a balance equation which assumes production = kinematic restoration + dissipation. Then,

\[ 0 = c_1 \frac{D_L}{\ell_2^2} - c_2 \frac{s_L^0}{\ell_1} \bar{\sigma}_t - c_3 \frac{D}{\ell_1^2} \bar{\sigma}_t^2 \]

(5.29)

Using the quadratic equation in (5.29) and taking only the positive root, the algebraic \( \sigma_t \)-equation is

\[ \bar{\sigma}_t = -\frac{c_2 s_L^0}{2c_3 D} \ell_1 + \sqrt{\left( \frac{c_2 s_L^0}{2c_3 D} \right)^2 \ell_1^2 + \frac{c_1 D_L}{c_3 D} \left( \frac{\ell_1}{\ell_2} \right)^2} \]

(5.30)

where length scales \( \ell_1 \) and \( \ell_2 \) are needed to close the source and destruction terms in (5.30). Two main possibilities show up (1 and 2), whose combinations give a total of four:

1. \( \ell_1 = \ell_2 = \ell_{F,t} = (G^\nu)^{1/2} / ||\nabla \tilde{G}|| \) for steady planar flame (Peters (2000) p. 131).

2. \( \ell_1 = \ell_2 = b_2 \ell \) for the limit of a steady state planar flame where the flame brush thickness \( \ell_{F,t} \) is proportional to the integral length scale \( \ell \). The constant \( b_2 = 1.78 \) (Peters (2000) p. 132).
3. $\ell_1 = \ell_{F,t}$ and $\ell_2 = b_2 \ell$. Tested by Ewald, J. (2003 b) and confirmed in this thesis.

4. $\ell_1 = b_2 \ell$ and $\ell_2 = \ell_{F,t}$.

The $\ell_{F,t} = 0$ is assumed immediately after spark ignition, but $\ell_{F,t}$ evolves subsequently. A 10 ms ignition delay case is studied in this thesis (section 6.3). The results from RANS confirm previous work by Ewald, J. (2003 b), i.e. version 3 for the algebraic flame surface area equation yields best results for the initial turbulent flame evolution. In addition, a VLES is carried out for the first time ever. In this second study, version 2 provides consistent results.

5.3.4 Wall Modell

Some wall modeling is necessary for the flame brush thickness $\ell_{F,t}$. Close to the wall, the turbulent length scale is approximated to large Reynolds numbers by $L = C_L y$ where $C_L \approx 2.5$ and $y$ is the normal wall distance (Pope (2000), Ewald (2003 c)). Because of the non-normalized flame brush thickness is $\ell_{F,t} = \widetilde{G''}$, then

$$\widetilde{G''}_\text{wall} = \min \left( \widetilde{G''}_\text{transport} - C_{G \var} y^2 \right) \quad (5.31)$$

where $C_{G \var} = \sqrt{C_L C_D b_2} = \sqrt{2.5 \cdot 2.01 \cdot 1.78} = 0.95$.

5.4 On the Regime Diagram for LES of Premixed Turbulence Combustion

In Peters regime diagram (Figure 3.3), $\nu'/s_L$ is a function of $\ell/\ell_F$ where $\nu'$ is the turbulent velocity fluctuation at the integral length $\ell$, $\ell_F$ is the flame thickness and $s_L$ is the laminar burning velocity. Since filter width $\Delta_f$ replaces $\ell$ as known from turbulent flows, the location in the regime depends on the LES filter width $\Delta_f$. 
Pitsch and de Lageneste (2002) have created a new regime diagram for LES to distinguish between changes of the turbulent/chemistry interaction and the numerical treatment in an LES by replacing $\ell$ with $\Delta f_i$ (Figure 5.5). This replacement affect the Reynolds number $Re_{\Delta f_i} = \frac{u'_{\Delta f_i} \Delta f_i}{\nu}$ and Damköhler number $Da_{\Delta f_i} = \frac{s_L \Delta f_i}{u'_{\Delta f_i} \ell_F}$, where $u'_n$ is the subgrid velocity fluctuation. On the other hand, the Karlovitz number $Ka = \frac{t_F}{t_q} = \frac{t_F^2}{\nu}$ remains the same. It only depends on the laminar flame scales and the turbulent kinetic energy transfer rate $\varepsilon$ due to $Ka^2 = \frac{t_F}{t_q} = \frac{t_F^2}{\nu} = \left( \frac{u'_{\Delta f_i}}{s_L} \right)^3 \frac{t_F}{\ell_F}$. Thus, $Ka$ is used as the independent variable and $\frac{u'_{\Delta f_i}}{s_L}$ or $\frac{\Delta f_i}{\ell_F}$ as the dependent variable in the new regime diagram. Since the influence of the in the regime is desired to analyze, $\frac{\Delta f_i}{\ell_F}$ is the chosen dependent variable. Finally, the LES regime diagram is constructed using $\frac{\Delta f_i}{\ell_F}$ to write $Re_{\Delta f_i}$ and $Da_{\Delta f_i}$ in term
5.4. ON THE REGIME DIAGRAM FOR LES OF PREMIXED TURBULENCE COMBUSTION

5.4.1. The Regime Diagram for LES of Premixed Turbulence Combustion

of $Ka$:

$$Re_{\Delta_f_i} = Ka^{2/3} \left( \frac{\Delta_f_{i}}{\ell_F} \right)^{4/3} = Ka^{-2} \left( \frac{v'_{\Delta_f_i}}{s_L} \right)^4 \quad (5.32)$$

$$Da_{\Delta_f_i} = Ka^{-2/3} \left( \frac{\Delta_f_{i}}{\ell_F} \right)^{2/3} = Ka^{-2} \left( \frac{v'_{\Delta_f_i}}{s_L} \right)^2 \quad (5.33)$$

Only the eddies with Gibson length scale $\ell_G$ interact with the flame front. They have a turnover velocity fluctuation $v' = s_L$. On the other hand, the eddies with $\ell < \ell_G$ have $v' < s_L$ and do not even wrinkle the flame front (Peters 2000 p. 81). The MRA can be inserted here as well. When moving upward $j \rightarrow -\infty$ (Figure 4.5), the filter width $\Delta_{f_i}$ decreases as the grid get finer (Figure 4.4). Therefore, once $\Delta_{f_j} < \ell_G$ the $v'_{\Delta_f_i} < s_L$ and the modeled part from the corrugated flamelets regime changes to the wrinkled flamelets. Then, the corrugation of flamelets may show up at the resolved scales and not in the subgrid modeled part. The filter width can be decreased further such that $\Delta_{f_j} < \eta$ but still $\Delta_{f_i} > \delta$, where $\eta$ is the Kolmogorov length scale and $\delta$ is the reaction zone thickness. In this case, the subgrid modeled part of the flow becomes laminar and it is known as the $G$-equation DNS regime due to all relevant length scales are resolved. In this thesis, the VLES imply that the $\Delta_{f_i} = (\text{minimum cell volume})^{1/3}$ is large enough. The grid in VLES is as coarse as the used in RANS.
5.5 Fast Marching Method for the $G$-equation

Given a level set function $G$, Adalsteinsson and Sethian (1999) show how to simultaneously construct a signed distance function and an extension velocity $F_{\text{ext}}$ very rapidly using the Fast Marching Method. $F_{\text{ext}}$ is then used to update the level set function $G$. The analysis starts with the construction of the initial value PDE in (5.34) - (5.35)

$$\frac{\partial G}{\partial t} + F|\nabla G| = 0 \quad \text{at} \quad G = G_0 \tag{5.34}$$

$$|\nabla G| = 1 \quad \text{at} \quad G \neq G_0 \quad \text{(reinitialization constraint)} \tag{5.35}$$

leading to

$$\frac{\partial G}{\partial t} + F_{\text{ext}}|\nabla G| = 0 \tag{5.36}$$

This implies that $F_{\text{ext}}$ in (5.36) is now defined on the whole computational domain for all the level set and not just at the zero level set on the interface itself. On the other hand, the velocity at the interface only has meaning at the front itself in combustion. Therefore, the extension velocity in (5.36) must be specifically constructed with the following two properties:

1) $F_{\text{ext}} = F$ at the interface $G_0$, which is placed straight ahead from the flame front.

2) $F_{\text{ext}}$ moves the neighboring level sets in such way that the signed distance function is preserved. This is achieved with

$$\nabla F_{\text{ext}} \cdot \nabla G = 0 \tag{5.37}$$

assuming that both $F$ and $G$ are smooth for $|\nabla G| = 1$ and is shown below:

$$\frac{\partial |\nabla G|^2}{\partial t} = \frac{\partial}{\partial t}(\nabla G \cdot \nabla G) = 2\nabla G \cdot \frac{\partial}{\partial t}\nabla G$$

$$= \{ \text{inserting (5.36)} \}$$

$$= -2 \nabla G \cdot \nabla F_{\text{ext}} |\nabla G| - 2\nabla G \cdot \nabla |\nabla G| F_{\text{ext}}$$

$$= 0 \quad \text{due to (5.37)} \quad \text{and} \quad |\nabla G| = 1$$

The algorithm (Adalsteinsson and Sethian (1999)) is represented in Figure 5.6.
5.5. FAST MARCHING METHOD FOR THE G-EQUATION

Figure 5.6. The algorithm i) starts with the level set function $G^n$ at time step $n\Delta t = 0$. ii) Construct a signed distance function $G^{n,\text{temp}}$ around the zero level set using Fast Marching Method and simultaneously construct the extension velocity $F_{\text{ext}}$ satisfying $\nabla G^{n,\text{temp}} \cdot \nabla F_{\text{ext}} = 0$ with $G^{n,\text{temp}} = G^n$ at $G^0$ and $F_{\text{ext}} = F$ at $G^0$. iii) use the computed $F_{\text{ext}}$ to advance $G^n$ to a new $G^{n+1}$ by solving (5.36).

The algorithm in Figure 5.6 can be extended. Ewald (2000) has proposed the use of two temporal functions to advance the front: one function $G^{n,\text{temp}}$ that takes $G^n$ close to the interface and $G^{n,\text{temp}1}$ farer away from it.

5.5.1 Fast Marching Method

The signed distance $G^{n,\text{temp}}$ to the front is computed using the Fast Marching Method, which is overviewed here. The reader is referred to Sethian (1999) for more details. The analysis starts with some definitions:

- The interceptions between the interface and the grid are considered accepted points $P_a$.

- Neighbors of accepted points are considered close points $P_c \in S_c$ while the rest are far points $P_f \notin S_c$. $S_c$ is the set of all close points.

The interface front advances as follows:

1. The interface $G = G_0$, which separates $G < G_0$ from $G > G_0$ (Figure 5.1), moves towards the low values of $G$. A point $P_l \in S_c$ with the lowest value of $G$ is the closest point to the interface $G = G_0$. Transfer $P_l$ from $S_c$ to $S_a$.

2. Move the interface $G = G_0$ outward into the accepted points.

3. The above steps may change the values of the points in $S_c$ and some far points may move to $S_c$. Thus, redistribute and redefine the points in $S_f$, $S_c$ and $S_a$ again and go to step 1.
Although the Fast Marching Method is very fast \( O(N\log N) \), \( N \) = number of points) compared to the level-set, still it is a costly procedure. Nevertheless, there exist some possible ways to decrease the computational costs. For instance, one of the main issues in Fast Marching Method is to efficiently locate the smallest value of \( G \) in \( S_c \). This is achieved by an adapted heap method, which organizes the database of all closure points. Mu (2002) has presented a parallel multiple-heaps algorithm which may find application here. The view of level-sets as multiresolution grids could be linked to (algebraic) multigrid methods. These last methods have well-documented parallel algorithms. Further work is needed to determine the appropriate method.
Chapter 6

Computational Fluid Dynamics (CFD)

Any result from Computational Fluid Dynamics (CFD) is qualitative and partial quantitative when measurements are available. It starts with the generation of a grid, followed by the insertion of initial estimations, and initial and boundary conditions when they are demanded. Once the numerical results are obtained, a comparison with eventual measurements is carried out. The procedure continues by improving the grid and running the problem again until satisfactory results are reached (Figure 6.1). Numerical turbulent combustion requires more time than any CFD work. Hence, it requires long-time projects to complete the circle. Because a master thesis is very time-limited project, any result should be considered qualitative.

\textbf{Figure 6.1} CFD circle

\textsc{GMTEC} is an unstructural grid CFD FORTRAN code, consisting of straight edged cells arbitrary shaped of (predominatly) hexaedral form. The
cells are joined face-to-face in arbitrary manner, filling any domain of any complexity. The N-S equations and continuity equation are solved using Finite Volume (Control-Volume) discretization. These equations are (linear) coupled through the pressure using a modified PISO (Pressure Implicit Split Operator). This modified algorithm reduces to a SIMPLE-like method in the case of a single outer loop (momentum predictor) and a single inner loop (pressure/velocity corrector) per time step (or per global iteration, in the case of a steady solution algorithm). The essential steps in the pressure/momentum/continuity coupling to advance the solution over one computational time step are (Ewald et al. (2003) p. 148):

1. **Momentum predictor**: compute a new velocity field using the current pressure field. This velocity field does not satisfy continuity.

2. **Pressure/velocity correctors**: compute corrections to the pressure and velocity fields to enforce continuity. The momentum predictor and pressure corrector each require the solution of a sparse implicit linear system that corresponds to a linearized discretized form of the governing PDE. The velocity corrector is explicit. Equations for additional quantities (e.g., internal energy/enthalpy, species) may be included in each pressure/velocity corrector step to maintain tight coupling among the equations. At the end of the pressure/velocity corrections, equations requiring a lesser degree of coupling are solved (e.g., turbulence model equations). The process then is repeated as necessary, starting from the momentum predictor, to obtain a converged solution for the current time step or global iteration.

Figure 6.2 represents three levels of iteration employed on each time step: an outer iteration and an inner iteration.
Figure 6.2. Flowchart to a compressible case (internal energy/enthalpy equation included in the inner iterations) using an energy/enthalpy predictor (versus explicit corrector) for each inner iteration. Small green loops correspond to iterations in the linear equation solvers. The actual number of iterations in each case depends on several user-specified convergence parameters. For each computational time step there are up to MOUTER outer iterations (momentum predictors), up to MAXCCP inner iterations (pressure/velocity correctors) per outer iteration, and up to MCON iterations in the sparse implicit linear equation solver per equation. In the group of active species can be found the fuel and the air, while the mean of $G$ and its variance are among the passive species. (Ewald et al. (2003) pp. 149, 153)

In general, the steps are:

1. **Start at $t_0 = 0$ seconds and/or continue from $t_n$.**
   - (a) Solve momentum (N-S) equation (a cycle is started at $t_{\text{fixed}}$)
     - Solve pressure/velocity corrector, active species and enthalpy until convergence using $\sum |\text{mass residuals}| \leq \text{convergence tolerance for inner loop (pressure/velocity corrections)}$, but not more than 20 pressure/velocity corrections per outer iteration.
   - (b) Solve turbulent passive species until absolute/relative convergence to, say $10^{-8}$, but not more than, say 500, iterations for iterative linear equation solvers for dependent variable.
   - (c) Solve turbulent quantities $k$ and $\varepsilon$ until convergence but not more than 1 cycle through the turbulence model equations per outer...
CHAPTER 6. COMPUTATIONAL FLUID DYNAMICS (CFD)

iteration

(d) Check convergence tolerance for outer loop, say $10^{-3}$, but no more than, say 3, outer iterations per time step. If it is not convergent, go to (a).

2. if $t_n \leq$ final time (in seconds) go to 1 by adding $\Delta t$ to the next time interval. Otherwise, stop the calculations

• NOTE: Although not used in the vessel case, another convergence criteria should be added when a moving oscillating surface (such as a piston) is present. In such cases, the endt is not the stopping calculating variable anymore, but the differences between the residual from two consecutive cycles. That difference is calculated until it reaches very small values (i.e. an added convergence criteria) after certain time $t_n$

In CFD computations based on Flamelet approach, species concentration $Y_i$ of all species are not required. The heat capacity $c_p$, the enthalpy $h = \Delta h_f^0 + c_p|^{T}_{T_0}(T - T_0)$ and other thermodynamics states are stored in flamelet libraries as coefficient of polynomial expressions. Therefore, no equations are given here for those quantities.

Figure 6.3 Level Set module and flamelet library interaction with CFD-code. The $\sim$ represents the Favre (Ewald (2003 c) p.11).
6.1 On the Numerics of the $G$-equation

The $G$-equation is itself calculated using finite difference method. The value of $G_p$ and $F_{\text{ext},p}$ at a point $p$ inside a cell are computed based on neighbors $i_k$ for $k = 1, 2, \cdots, 6$ (Figure 6.4). In the Fast Marching Method, the $i_k \in S_a$. For continuity sake, the analysis continues from the last part of the previous chapter. This follows the work of Ewald (2000), which is based on Sethian (1999).

Based on Figure 5.6, two equations are evaluated simultaneously in the grid (Figure 6.4) as follows:

- $|\nabla G| = 1$ is solved for $G_p$, which leads to a quadratic equation (Sethian (1999) p. 134-135). The purpose is to minimize $|G_p|$ for $|G_p| > |G_{i_k}|$.

- $\nabla G \cdot \nabla F_{\text{ext}} = 0$ gives an expression for $F_{\text{ext},p}$ which shares the same neighbors used for $|\nabla G| = 1$. The minimization of $|G_p|$ consists of evaluating it for all possible neighbors combinations. For simplicity, the 2D example is used (Ewald (2000) p. 6-7).
At the same time, the constraint $|\nabla G| = 1$ is resolved with $\Delta x_{ik} = x_p - x_{ik}$ to

- one neighbor: $G_p = S_e |\Delta x_{ik}| + G_{ik}$, $F_{\text{ext},p} = F_{\text{ext},ik}$.

- two neighbors: The stencil (Figure 6.4) is rotated into a 2D coordinate system ($\eta$, $\xi$) and the equations (6.1)-(6.2) are solved

$$
\Delta \eta_{i_1} G_\eta + \Delta \xi_{i_1} G_\xi = G_p - G_{i_1} \quad (6.1)
$$
$$
\Delta \eta_{i_2} G_\eta + \Delta \xi_{i_2} G_\xi = G_p - G_{i_2} \quad (6.2)
$$

to obtain $G_\eta$ and $G_\xi$. The $G_p$ is obtained from $G_{\eta}^2 + G_{\xi}^2 = 1$.

On the other hand, $F_{\text{ext},p}$ can be obtained from

$$
\Delta \eta_{i_1} F_\eta + \Delta \xi_{i_1} F_\xi = F_{\text{ext},p} - F_{\text{ext},i_1} \quad (6.3)
$$
$$
\Delta \eta_{i_2} F_\eta + \Delta \xi_{i_2} F_\xi = F_{\text{ext},p} - F_{\text{ext},i_2} \quad (6.4)
$$

whose solution is inserted into $G_\eta F_\eta + G_\xi F_\xi = 0$.

The $\nabla G$ has to fulfill the Courant-Friedrichs-Lewy (CFL) condition (Figure 6.4).

The implementation of the $G$-equation model contains the field variables: mean value $\bar{G}$, its fluctuations or variance $G''$, and the turbulent flame surface area ratio, together with its filtered counterparts. (Because filtered are linked to the mean values through the interconnections (5.24)-(5.27), only the mean values are explained from now on).

The mean of $G$ and its variance equations are treated in a separate solver, called $G$-equation solver or simply $G$-solver. This, due to those equations have different properties compared to the regular transport equations (e.g. momentum eq., energy eq., etc). The $G$-equation solver is coupled to the PISO:
6.1. ON THE NUMERICS OF THE $G$-EQUATION

Figure 6.5. $G$-equation solver and PISO

where

- the level set variable, i.e. the geometrical distance $\tilde{G}$ is solved in the $G$-solver internally.

- the $G''$, defined on the iso-surface $\tilde{G} = G_0$, is solved in the $G$-solver internally.

- Also, the algebraic equation (5.30), i.e. the turbulent flame surface area ratio. Equation (5.30) is needed to calculate the turbulent mass burning rate and thereby the interface speed.

The equations to deal with in the $G$-solver are:

$$\frac{\partial \tilde{G}}{\partial t} = -F_{\text{ext}} |\nabla \tilde{G}|$$  \hspace{1cm} (6.5)

$$\frac{\partial \tilde{G}''}{\partial t} = P - \varepsilon \tilde{G}''$$  \hspace{1cm} (6.6)

where $F = F_{\text{ext}}$ is the already well-known boundary condition at the interface $G = G_0$. It determines the interface velocity by

$$F = F_{\text{ext}} = \frac{1}{\bar{\rho}} \left( -\bar{\rho} \bar{\nabla} \cdot \mathbf{n} - (\bar{\rho} \bar{s}_T) - \bar{\rho} D_r \right)$$  \hspace{1cm} (6.7)
Also, the term $P$ (= turbulent production + tangential diffusion + tangential convective) and the dissipation term $\varepsilon$ in (6.6) are evaluated at the interface

\[
P = -\left(\mathbf{n} \times (\mathbf{\tilde{v}} \times \mathbf{n})\right) \cdot \nabla \mathcal{G}^2 + \frac{1}{\bar{\rho}} \nabla \| \cdot \left(\bar{\rho} D_{\|} \nabla \mathcal{G}^2\right) + 2D_t(\nabla \mathcal{G})^2 \tag{6.8}
\]

\[
\varepsilon = c_s \frac{\mathcal{G}}{\kappa} \tag{6.9}
\]

Each term $F_{\text{ext}}, P$ and $\varepsilon$ are extended into the whole computational domain, following the algorithm given in Figure 5.6, as

\[
\nabla \phi \cdot \nabla \mathcal{G} = 0, \quad \phi \in \{F_{\text{ext}}, P, \varepsilon\} \tag{6.10}
\]

using the Fast Marching scheme. Before any other scalar is solved for the time level $n+1$, the fields $\mathcal{G}$ and $\mathcal{G}^2$ are predicted by

\[
\mathcal{G}^{n+1} = \mathcal{G}^n - \Delta t F_{\text{ext}}^n \tag{6.11}
\]

\[
\mathcal{G}^{n+1}_{\text{int}} = \mathcal{G}^{n}_{\text{int}} + \Delta t \left(P^n - \varepsilon^n \mathcal{G}^{n}_{\text{int}}\right) \tag{6.12}
\]

When all other scalars within the PISO algorithm are solved (Figure 6.2), the scalars $\mathcal{G}^{n+1}$ and $\mathcal{G}^{n+1}_{\text{int}}$ are corrected by

\[
\mathcal{G}^{n+1} = \mathcal{G}^n - \Delta t \left(F_{\text{ext}}^n + F_{\text{ext}}^{n+1}\right) \tag{6.13}
\]

\[
\mathcal{G}^{n+1}_{\text{int}} = \mathcal{G}^{n}_{\text{int}} + \frac{\Delta t}{2} \left(P^n - \varepsilon^n \mathcal{G}^{n}_{\text{int}} + P^{n+1} - \varepsilon^{n+1} \mathcal{G}^{n+1}_{\text{int}}\right) \tag{6.14}
\]

Because of GMTEC is a Licensee Derivative Product in the context of the Software License agreement between General Motors (GM) and Advanced Combustion GmbH (AC), the author has been subjected to a Condisclosure Agreement. Therefore, no implementation details existing in the General Motor CFD code are given. However, no novel discretisation schemes have been implemented beside those available in the literature. The reader can find many references about these schemes implemented on the level-set formulation of the $G$-equation (c.f. Sethian (1999), Schneider (1999), Herman (2000), Wenzel (2000), Repp (2001), Treurniet (2002), Lin (2003), Osher and Fedkiw (2003), Schuller (2003), Samuel et al. (2004)) As further work, the extended algorithm from Schmidt and Klein (2003) can be an interesting addition into GMTEC.
6.2 Initial Estimations

In the present work, the initial values are calculated based on the experiments done by Hamamoto et al. (1988).

- The turbulent length scale $\ell$ is 10% of the vessel diameter. Thus, $\ell = \frac{\text{vessel diameter}}{10} \approx 0.0125m$.
- The tangential velocity immediately before the spark is $U = 5m/s$. The turbulence intensity $T_I = 0.2/5 = 0.04$ is already given by Hamamoto et al. (1988). It has been normalized with the tangential velocity.
- The turbulent kinetic energy is $k = \frac{3}{2} (T_I U)^2 = \frac{3}{2} (0.2)^2 = 0.06$.
- The turbulent dissipation is $\varepsilon = C_\mu \frac{k^{3/2}}{\ell} = \{ \text{with } C_\mu = 0.09 \} = 0.1058$
- The eddy viscosity $\nu_t = C_\mu \frac{k}{\varepsilon} = \{ \text{with } C_\mu = 0.09 \} = 0.0031$
- A stoichiometric mixture of propate and air is assumed. (c.f Turn (2000)).

6.3 A 3-D Cylindrical Vessel Case with $GM$ code

The work starts from previous results, after more than two years of testing and calibrations, by Ewald (2003 b) (Figure 6.6).

![Figure 6.6](image-url)
The numerical study tries to mirror the experiments by Hamamoto et al. (1988) for 10 ms ignition delay case only. It consists of a cylindrical vessel of 125 mm diameter, 35 mm width and a total of 430 cm$^2$ comprising about 58400 computational cells. The stoichiometric propane air swirled mixture has $Sc_t = 0.7$ and is ignited at the center of the combustion chamber. Thus, the flame propagates almost axisymmetrical in the flow. The global pressure trace is the only experimental data available. Ewald (2003 b) adds a strong artificial swirl around the burnt cells (Figure 3.6) to overcome such unphysical ignition and to obtain a faster pressure increase. That trick does not consider the risk of 'laminarizing' the flow, and therefore is not implemented in this thesis. Good agreements with the pressure trace do not automatically imply that the other values are correct. Because of the nature of this work, no special emphasis is given on the turbulent combustion related results.

Figures 6.6 shows that version 3 (c.f. section 5.3.3) appears to be the appropriate closure for RANS in cylindrical vessels. It is confirmed in Figure 6.7. The VLES is tested in cylindrical configurations for the first time ever (Figure 6.7). It turns out that the pressure increases later in time. A 2.3 times widen filter width does not trigger the pressure increase enough sooner. However, it moves towards the RANS pressure trace as expected. It seems that VLES displaces the versions to the left. Thereby, Figure 6.6 reveals that version 2 should be next tested closure. It turns out that version 2 appears$^1$ to be the correct closure for VLES (Figure 6.7).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{pressure_trace.png}
\caption{Pressure trace for different closures in RANS and VLES}
\end{figure}

\footnote{Because of deadline issue, the case has been tested with a different $\Delta t$ and accuracy.}
6.3. **A 3-D CYLINDRICAL VESSEL CASE WITH GM CODE**

The evolution, from zero, of the flame brush thickness \( \ell_{F,t} = (G'')^{1/2} \), its algebraic version, the integral (turbulent) length scale \( \ell_{F,t,\text{alg}} = \sqrt{\frac{2c_p}{c_s c_s} \frac{E^{1.5}}{\pi}} \) = \( b_g \ell \) and their filtered counter parts are shown Figure 6.8. Because of the interconnections between averaged and filtered values, only the Favre \( \sim \) is written from now on.

![Figure 6.8. Length scales in RANS and VLES](image-url)
Chapter 7

Conclusions

The potential of analyzing turbulent combustion from the multiresolution perspective is aboard in this thesis. Its advantage is not repeated here and the reader is encouraged to read the work. From the numerical results, it can be said that:

- The existence of length scales $\ell_1$ and $\ell_2$ to close the source and destruction terms in (5.30) implies that no initial value for the turbulent contribution of the flame surface area ratio is needed.

- Length scales $\ell_1$ and $\ell_2$ model the temporal evolution of the flame front. $\ell_{F,t} = 0$ at the ignition and evolves during the front displacement.

- There exist two possibilities (Peters (2000) pp. 130-131)
  1. flame brush thickness $\ell_{F,t} = (\overline{G''})^{1/2}$.
  2. integral (turbulent) length scales $\ell_{F,t} = b_2 \ell$.

leading to a total of four combinations (c.f. section 5.3.3)

- The closures $\ell_1 = \ell_2 = \ell_{F,t} = (\overline{G''})^{1/2}$ and $\ell_1 = \ell_2 = b_2 \ell$ have been validated in Bunsen flame configurations for turbulent flame brush thickness by Herman (2000).

- The use of $\ell_1 = \ell_{F,t}$ and $\ell_2 = b_2 \ell$ in (5.30) for RANS has been validated in cylindrical vessels configurations by Ewald (2003 b) (Figure 6.6) given consistent result as confirmed in this thesis (Figure 6.7).

- The use of $\ell_1 = \ell_2 = b_2 \ell$ in (5.30) for VLES validated for cylindrical vessels configurations gives consistent result according to the results in this thesis (Figure 6.7). It should be confirmed with smaller $\Delta t$ and higher accuracy, as we have done in this thesis for the RANS.
CHAPTER 7. CONCLUSIONS

• Based on numerical experiments, the global pressure might increase little later when $\Delta t$ is decreased and accuracy is increased.

• Parameters from RANS seems to be overestimated, when they are compared to those from VLES.

• The $\ell_{F,t} > \ell_{F,t,\text{alg}}$.

• Minor disagreements with the measurements can be blamed, but not limited, to the use of:
  
  i) unphysical ignition.
  
  ii) no swirl model.
  
  iii) law-of-the-wall (Poinsot and Veynante (2001) pp. 345-354) for computational cost reasons. For confined places, the correct approach is Low Reynolds number turbulent models.

A considerable number of algorithms, propositions, ideas are given throughout this thesis. They can be implemented in G\textsuperscript{M}TEC, as well as in other CFD codes.
Appendix A

Appendix

Certainly for DNS and LES, the study of turbulence requires the injection, and sometimes the maintenance, of a fluctuating velocity field. The injection method is based on the turbulent kinetik energy spectra $E(\kappa)$, where $\kappa = \lambda/2\pi$ is the wavenumber and $\lambda$ is the wavelength, i.e. all various-sized eddies, which have a certain kinetic energy determined by vorticity or by intensity velocity fluctuation at a corresponding frequency, are arranged/organized in a plot $\log(E(\kappa))$ VS $\kappa$ to see how the eddies’ kinetic energy is distributed in frequency:

- the kinetic energy $k$ is the energy contained for the energy spectrum in the scales ensemble/sum, i.e.

$$k = \int E(\kappa) d\kappa$$ (A.1)

where $k = \frac{2}{3} u'^2$ for 3D

- the dissipation is

$$\varepsilon = 2\nu \int_{\kappa^2 E(\kappa)} D(\kappa) \frac{d\kappa}{\kappa^2 E(\kappa)}$$ (A.2)

where $D(\kappa)$ is the dissipation spectrum

- the integral length scale for 3D is

$$\ell = \frac{\pi}{2u^2} \int \frac{E(\kappa)}{\kappa} d\kappa$$ (A.3)

The goal is to obtain a field of fluctuating velocities $u'$ from the spectra of the turbulent kinetik energy $E(\kappa)$. 

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General steps to generate fluctuations and the entire log-log energy spectrum for a turbulent flow:

1. Choose a prescribed/theoretical model for $E_p(\kappa)$, for instance:
   - assuming that there is a self-similarity form of the power-law spectrum in dimensionless arguments, the generic form of $E_p(\kappa)$ is
     
     $$E_p(\kappa) = C_\eta \varepsilon^{2/3} \kappa^{-5/3} f(\kappa_r)$$  
     \hspace{1cm}\text{(A.4)}

     where $f(\kappa_r)$ is a damping function for large waves numbers.
   - For Pao spectrum is
     
     $$f(\kappa_r) = \exp\left(-\frac{3C_\eta^4}{2} \kappa_r^{4/3}\right)$$  
     \hspace{1cm}\text{(A.5)}

     where $C_\eta$ is the Kolmogorov constant $\sim 1.4$, $\varepsilon$ is the kinetic energy dissipation rate, $k$ is the kinetic energy, $\kappa$ (kappa) is the wavenumber is associated with the Kolmogorov scales and $\kappa_r$ is related to $\kappa$, $\nu$, $\varepsilon$ and the mesh (Pao (1965)).

2. Create a random velocity in space $u(\mathbf{x})$
   - $u(\mathbf{x}) = \text{random}$

3. Applied the Fast Fourier Transform algorithm to $u(\mathbf{x})$
   
   $$\text{FFT}(u(\mathbf{x})) = \tilde{u}(\kappa)$$  
   \hspace{1cm}\text{(A.6)}

4. Create the corresponding $E(\kappa)$ for $\tilde{u}(\kappa)$

5. Calculate the ratio($\kappa$)
   
   $$\text{ratio}(\kappa) = \frac{E(\kappa)}{E_p(\kappa)}$$  
   \hspace{1cm}\text{(A.7)}

6. Rescale $\tilde{u}(\kappa)$ by the ratio($\kappa$) in (A.7)

7. Rescale for total kinetic energy $k$
   
   $$k = (\text{constant}) \int E(\kappa)d\kappa$$  
   \hspace{1cm}\text{(A.8)}
8. Apply the Helmholtz decomposition of the velocity field

\[ \mathbf{u}(\mathbf{x}) = \mathbf{u}^I(\mathbf{x}) + \mathbf{u}^C(\mathbf{x}) \]  

(A.9)

where \( \mathbf{u}^I \) is the solenoidal and \( \mathbf{u}^C \) is the irrotational components of the velocity, i.e.:

\[ \nabla \cdot \mathbf{u}^I = 0 \]  

(A.10)

\[ \nabla \times \mathbf{u}^C = 0 \]  

(A.11)

- decompose only using (A.10) for incompressible flow, i.e. divergence free, hence \( \mathbf{u}(\mathbf{x}) = \mathbf{u}^I(\mathbf{x}) \)

9. Express the decomposition in Fourier space, i.e. \( \hat{\mathbf{u}}(\kappa) = \hat{\mathbf{u}}^I(\kappa) \) from (A.6)

\[ \hat{\mathbf{u}}^I = \hat{\mathbf{u}} - \kappa \cdot \frac{\kappa \cdot \kappa}{\kappa^2} \]  

(A.12)

10. Apply inverse fast fourier transform algorithm

\[ \text{IFFT}(\hat{\mathbf{u}}^I(\kappa)) = \mathbf{u}^I(\mathbf{x}) \]  

(A.13)

and the velocity field is finally obtained for every point in the mesh.

11. For the pressure

- Insert \( \mathbf{u}^I(\mathbf{x}) \) in the r.h.s. of the Poisson equation, i.e.

\[ \Delta P = \text{RHS}(\mathbf{u}^I(\mathbf{x})) \]  

(A.14)

12. Apply FFT to (A.14)

13. Apply Inverse FFT

Finally, both the \( \mathbf{u}^I(\mathbf{x}) \) and \( P \) for the entire field are obtained.
Bibliography


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BIBLIOGRAPHY


