Direct Numerical Simulation of Premixed Turbulent Combustion

Theo Treurniet

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Theodoor Cornelis TREURNIET
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Dit proefschrift is goedgekeurd door de promotor:

Prof.dr.ir. F.T.M. Nieuwstadt

Samenstelling promotiecommissie:

Rector Magnificus, voorzitter

Prof.dr.ir. F.T.M. Nieuwstadt, Technische Universiteit Delft, promotor

Prof.dr.ir. P. Wesseling, Technische Universiteit Delft

Prof.dr.ir. D.J.E.M. Roekaerts, Technische Universiteit Delft

Prof.dr.ir. Th.H. van der Meer, Universiteit Twente

Prof.dr. L.P.H. de Goeij, Technische Universiteit Eindhoven

Prof.dr. H.B. Levinsky, Rijksuniversiteit Groningen

Dr.ir. B.J. Boersma, Technische Universiteit Delft

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Stellingen behorend bij het proefschrift van Theo Treurniet

1. De hydrodynamische instabiliteit leidt bij lage turbulentie intensiteit tot een sterke productie van turbulentie die dus niet, zoals vaak gedacht, toegeschreven kan worden aan barocline processen.
2. Door toepassen van Favre middeling worden essentiële processen in de dynamica van een vlam, zoals hydrodynamische instabiliteit, geconcentreerd in termen waarvoor geen correcte sluitingshypothese bekend is.
3. In de interactie tussen een vlamfront en een obstakel in de stroming spelen zowel de vervorming van het vlamfront door de turbulentie in het zog als de vervorming door het gemiddelde stromingsveld een belangrijke rol.
4. Zonder numerieke simulaties is het onmogelijk om inzicht te krijgen in complexe fysische processen zoals de dynamica van een vlamfront.
5. Menselijk verantwoordelijkheidsgevoel is het belangrijkste op het gebied van veiligheid. Als technische hulpmiddelen of regelgeving dit verantwoordelijkheidsgevoel belemmeren, vergroten ze de onveiligheid.
6. Onderzoek, zoals dat aan de universiteit wordt uitgevoerd, kenmerkt zich door het idealiseren en vereenvoudigen van het bestudeerde probleem, terwijl onderzoek, zoals dat wordt uitgevoerd in een industrieel laboratorium richt zich op het oplossen van problemen die extra gecompliceerd worden door commerciële en technische beperkingen. Het gebrek aan aandacht voor deze extra complicaties in de opleiding aan een technische universiteit levert uitstekende wetenschappers, maar slechte ingenieurs op.
7. De aandacht die in standaardwerken op het gebied van warmtetransport wordt gegeven aan transport door middel van straling, staat niet in verhouding tot de complexiteit en het belang van stralingstransport in veel toepassingen.
8. De gedachte dat de klant koning is, leidt tot een republikeinse houding van veel bedrijven.
9. Het is goed voor een huwelijk, als de echtgenoten elkaar vak inhoudelijk slecht begrijpen.
10. De beste oplossing is de eenvoudigste.

Wie mat de wateren met zijn holle hand, bepaalde de omvang der hemelen met een span, vatte met een maat het stof der aarde, woog de bergen met een waag en de heuvelen met een schaal? Wie bestuurde de Geest des HEREN en onderrichte Hem als zijn raadsman? Wie raadpleegde Hij, dat deze Hem inzicht zou geven, het rechte pad zou leren. kennis bijbrengen en de weg des verstands doen kennen?

Jesaja 40:12-14

Voor Jolien

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Summary

We consider the Direct Numerical Simulation (DNS) of a premixed flame in a homogeneously turbulent flow. The combustion takes place in the flamelet regime which means that combustion occurs in a very thin layer, called the flame front. The position of the flame front is modelled by means of the G -equation, in which the flame front is represented by an isosurface G_0 of a scalar field $G(\mathbf{x}, t)$. The flow is described by the Navier-Stokes equations in the low-Mach number limit, which allows for the inclusion of gas expansion due to the temperature increase by the combustion. The advantage of the low-Mach number approximation is that efficient numerical methods, used for incompressible flows, can be applied to solve the discretised equations.

The numerical method uses a Finite Volume Method (FVM) for the spatial discretisation and an explicit Predictor-Corrector method for the temporal discretisation. This method is implemented on a parallel computer with a domain decomposition approach, which results in an efficient method, which scales very good on a parallel computer.

The calculations are carried out in two different geometries. The first geometry is a box with homogeneous isotropic turbulence. The second geometry is the flow around a square cylinder.

In the first geometry, a homogenous isotropic turbulent flow is introduced. In addition, a uniform mean velocity is imposed with a inflow boundary condition at $x = 0$. The inflow velocity is adjusted such that the mean position of the flame is stabilised at a fixed position. This allows us to use time averaging to obtain accurate statistics, which are very difficult to obtain when the flame is allowed to propagate. In the y - and z -direction, periodic boundary conditions are applied.

The numerical code has been checked with a well-known theoretical result, the so-called Darrius-Landau instability of a thin flame front. The results show

a good agreement between the computed growth rate and the theoretical value when the thickness of the flame front is much smaller than the wave length of the disturbance. When this condition is not met, the growth rate becomes lower than the theory in agreement with the restriction under which the theory is valid.

For the computations in homogeneous turbulence, the results show an increase in the turbulent flame speed with increasing turbulent intensity at the position of the flame front. This is in good agreement with experimental data and theory. The turbulent flame speed shows also an increase as function of the heat release parameter. This is due to the fact that disturbances on the flame front, induced by the turbulence, are enhanced by the Darrieus-Landau instability.

The budgets of the turbulent kinetic energy and the enstrophy show that the expansion of the gas across the flame front suppresses the turbulence. At higher expansion rates, turbulence in the direction of the mean velocity increases and as a result turbulence becomes strongly anisotropic. The increase is due to two processes. The first is the influence of the Darrieus-Landau instability already mentioned above. The second is the baroclinic production of vorticity due to the fact that at the flame front density and pressure gradients are not aligned.

In the second geometry, the development of a flame front around a square cylinder and in the turbulent wake behind the cylinder are studied. We have first performed a simulation without combustion in order to check our computational techniques. The results show a good agreement with experiments and other simulations. Next, the simulations with combustion have been carried out, which show an increase in flame speed in the wake of the square cylinder. This is caused by two phenomena. The first is the presence of regions with high shear in the mean velocity field behind the square cylinder. In these regions, the flame is stretched and the area of the flame front is increased. The second is due to the turbulence in the wake which increases the flame speed even further. After the flame front the turbulence is suppressed strongly as a result of the expansion of the gas in the combustion zone.

Samenvatting

We beschouwen de Directe Numerieke Simulatie (DNS) van een voorgemengde vlam in een turbulente stroming. De verbranding vindt plaats in het flamelet regime, wat betekent dat de verbranding plaats vindt in een dunne laag, genaamd het vlamfront. De positie van het vlamfront wordt gemodelleerd door middel van de G -vergelijking, waarin het vlamfront wordt voorgesteld door een isooppervlak G_0 van een scalair veld $G(\mathbf{x}, t)$. De stroming wordt beschreven door de Navier-Stokes vergelijkingen in de laag-Machgetal limiet, waardoor het effect van uitzetting van het gas als gevolg van de toename in temperatuur door de verbranding meegenomen kan worden. Het voordeel van de laag-Machgetal benadering is dat efficiënte numerieke methodes die gebruikt worden in incompressiebele stromingen, kunnen worden toegepast voor het oplossen van de gediscretiseerde vergelijkingen.

De numerieke methode gebruikt een Eindige Volume Methode (FVM) voor de ruimtelijke discretisatie en een expliciet Predictor Corrector methode voor de tijds discretisatie. Deze methode is geïmplementeerd op een parallelle computer door middel van een domein decompositie benadering. Het resultaat is een efficiënte methode die erg goed schaal op een parallelle computer.

De berekeningen zijn uitgevoerd in twee verschillende geometriën. De eerste geometrie is een doos met homogene isotrope turbulentie. De tweede geometrie is de stroming rond een vierkante cilinder.

In de eerste geometrie wordt een homogeen isotroop turbulent veld ingevoerd. Daarbij wordt een uniform instroom snelheid opgelegd met een instroom randvoorwaarde bij $x = 0$. De instroom snelheid wordt aangepast, zodat de gemiddelde positie van de vlam stabiel wordt gehouden op een vaste positie. Als gevolg hiervan kunnen we middeling in de tijd toepassen om nauwkeurige statistieken te bepalen, die moeilijk te verkrijgen zijn als we toelaten dat de vlam zich verplaatst. In de y - en z -richting zijn periodieke randvoorwaarden

toegepast.

De numerieke code is geverifieerd met een bekend theoretisch resultaat, de zogenaamde Darrieus-Landau instabiliteit van een dun vlamfront. De resultaten laten een goede overeenkomst zien tussen de berekende groeisnelheid en de theoretisch waarde, als de dikte van het vlamfront veel kleiner is dan de golflengte van de verstoring. Als aan deze voorwaarde niet is voldaan, wordt de groeisnelheid lager dan de theorie, wat in overeenstemming is met de beperking waaronder de theorie geldig is.

De resultaten voor de berekeningen in homogene turbulentie laten een toename van de turbulente vlamsnelheid zien, bij een toename van de turbulentie intensiteit op de positie van het vlamfront. Dit komt goed overeen met experimentele gegevens en de theorie. De turbulente vlamsnelheid laat ook een toename zien, als functie van de warmte afgifte. Dit is een gevolg van het feit dat verstoringen op het vlamfront die veroorzaakt zijn door de turbulentie, worden versterkt door de Darrieus-Landau instabiliteit.

De budgetten van de turbulente kinetische energie en de enstrofie laten zien dat de uitzetting van het gas over het vlamfront de turbulentie onderdrukt. Bij hogere uitzetting neemt de turbulentie in de hoofd stroomrichting versterkt, waardoor de turbulentie sterk anisotroop wordt. Deze toename is het gevolg van een tweetal processen. Het eerste is de invloed van de Darrieus-Landau instabiliteit. Het tweede proces is de barocline vortciteitsproductie als gevolg van het feit dat op de plaats van het vlamfront de dichtheids- en drukgradiënten niet in dezelfde richting staan.

In de tweede geometrie wordt de ontwikkeling van een vlamfront rond een vierkante cilinder en in het zog achter de cilinder bestudeerd. Allereerst hebben we een simulatie zonder verbranding uitgevoerd om de numerieke technieken te controleren. De resultaten laten een goede overeenkomst zien met experimenten en andere simulaties. Vervolgens zijn er simulaties uitgevoerd met verbranding, die een toename in de vlamsnelheid in het zog van de vierkante cilinder laten zien. Dit wordt veroorzaakt door twee verschijnselen. Het eerste is de aanwezigheid van gebieden met een grote afschuiving in het gemiddelde snelheidsveld. In deze gebieden wordt de vlam uitgerekt en het oppervlak van het vlamfront vergroot. Het tweede verschijnsel is het gevolg van de turbulentie in het zog, wat ervoor zorgt dat de vlamsnelheid nog verder toeneemt. Na het front wordt de turbulentie sterk onderdrukt als gevolg van de uitzetting van het gas in de verbrandingszone.

Chapter 1

Introduction

1.1 Background and motivation of this study

Combustion processes are applied in many different areas, ranging from domestic applications like heating and cooking to applications in chemical industry, power plants and engines in all kinds of automotive applications. Because of the importance of combustion processes in our society, knowledge of all aspects of these processes is needed to utilise them in an efficient, safe and environmental friendly way. Besides the applications of combustion processes, understanding of the processes is needed to estimate and minimise the risks, which occur at the production, transport and refining of fossil fuels like crude oil and natural gas.

Much effort has been put already in understanding the process of combustion. However the study presented in this thesis is motivated by the fact that certain aspects of combustion are still not fully understood. This thesis focuses on the interaction between turbulence in the flow and the combustion process in premixed combustion. It is known that the combustion process is strongly enhanced by turbulence in the gas flow, which means that it plays an important role in the development of gas explosions and other events in which premixed combustion plays an important role. Knowledge on the interaction between turbulence and premixed combustion is for instance needed in the design of chemical plants and other constructions with an increased risk of gas explosions. In that case care should be taken to avoid the generation of turbulence by optimising the layout of the plant and removing obstacles from the flow gen-

erated by a possible explosion. To carry out such studies we need tools to study the propagation of gas explosions in complex flow conditions such as urban areas, chemical plants and other large scale constructions. These tools need a parameterisation for the influence of turbulence on the combustion. However it is felt that, because of the importance of the influence of turbulence, the existing parameterisations (van den Berg and Lannoy, 1993; Hjertager and Solberg, 1999), need to be improved. This thesis is motivated by this need and tries to provide more insight in the complex process of premixed turbulent combustion. To this end, we focus on the interaction of three phenomena which occur in premixed combustion, namely the deformation of the flame front, hydrodynamic instability of the flame front and baroclinic vorticity production at the position of the flame front. In the following, we will introduce each of these effects.

Premixed combustion assumes that the gaseous fuel and oxidiser are already fully mixed before combustion takes place. After ignition and when the chemical process is sufficiently fast the combustion then proceeds in the form of a thin flame sheet which propagates through the mixture. The process of propagation depends in first approximation on the diffusion of heat in front of the flame, by which the unburnt gas is heated up until the ignition temperature is reached. As this process is dominated by diffusion, the speed of the flame front is low. It is known that the combustion rate and the flame speed is strongly influenced by turbulence in the flow in which the explosion occurs. The turbulence in the gas flow will deform the flame front, which causes the total area of the flame front to increase. As a result the total rate of combustion, which is more or less proportional with the total area of the flame front, increases. This is the first important phenomenon in the interaction between turbulence and premixed combustion. The flow of the gas mixture, in which the explosion or combustion process occurs, might be generated by the gas expansion accompanying the combustion process itself. Turbulence is then generated near walls or in the wake behind obstacles. Turbulence increases the combustion rate, which generates an even stronger flow with more turbulence. In other words, turbulence acts as a positive feedback on the whole combustion process. This effect plays a very important role in the development of gas explosions in confined areas like chemical plants and offshore installations.

A second phenomenon, which occurs in premixed combustion is the fact that a flame front is unconditionally unstable. This means that small disturbances on an otherwise flat flame front will grow as a result of the expansion of the gas at the position of the flame front. This effect is called hydrodynamic instability of the flame front. These small disturbances might be caused by turbulence in the gas flow. In practise, some turbulence and therefore some small disturbances

are nearly always present. This means that a flat flame front will nearly always develop into a wrinkled flame front. This increases the total area of the flame front and thus the total combustion rate.

A third aspect which will be of importance in the modelling of premixed combustion, is the fact that vorticity can be generated at the flame front. Since heat is released by the combustion process, the gas will expand at the position of the flame front. This results in a large gradient in the density over the flame front. When the density and the pressure gradient are not aligned, vorticity will be generated at the position of the flame front. This is called baroclinic vorticity production and means that the flow field is effected by the combustion process.

Although these different phenomena, which occur in premixed turbulent combustion, are more or less known, it is the interaction between the different effects which makes the whole process difficult to understand and to model. To perform experiments is not the solution to obtain more information, since the high temperatures and pressures which occur in combustion make it difficult to perform detailed measurements on the turbulence in the gas flow.

1.2 Simulation premixed turbulent combustion

Due to continuing increase in computing power, it has become possible to perform detailed computer simulations of premixed turbulent combustion. The set of equations which describe the evolution of flow field and the combustion process in time are known and can be solved numerically for simple geometries these days. This approach is also used in this study. A so called Direct Numerical Simulation (DNS) of the flow field is performed, together with a model to compute the evolution of the flame front in the turbulent flow field. This model gives the opportunity to perform simulation of the complex interaction between premixed combustion and turbulence and will provide detailed information on the process, which will lead to a better insight in the process and eventually to better modelling.

To reach our goal, the DNS should be able to reproduce the three aforementioned effects, i.e. distortion of the flame front, flame front instability and baroclinic vorticity production. The simulation of the first effect, distortion of the flame front is straightforward, since in a DNS all turbulent length scales are resolved so that the deformation of the flame front can be computed directly. Instability of the flame front and baroclinic vorticity production are a result of gas expansion at the position of the flame front so that compressibility effects

should be taken into account in our simulation. To accomplish this we consider the compressible Navier-Stokes equations in the low Mach-number limit (Najm et al., 1998). The advantage of this limit is that it allows us the use of the efficient numerical methods, developed for incompressible flows. In previous studies, gas expansion has not been included or it has been included in such a way that does not allow for baroclinic vorticity production. To our knowledge the study presented here is the first DNS of premixed combustion in the flamelet regime, which includes all the aforementioned effects. A comparison of the results obtained from our simulation with the results of other computations will thus allow for an investigation of the additional effects due to compressibility of the gas.

Since we consider premixed combustion in the flamelet regime, the actual combustion takes place in a very thin layer, the so-called flame front. A resolution of this flame front on the numerical grid, on which the flow is to be computed, would lead to inaccessible requirements in terms of computational power. Therefore we have chosen to model the flame front by means of a so-called level set approach (Sethian, 1999). In this approach, the position of the flame front is represented by an isosurface G_0 of a scalar field $G(\mathbf{x}, t)$. The scalar field propagates with respect to the flow field with a flame velocity s_f . With the value of this flame velocity, all the internal structures of the flame region, which we cannot resolve on our numerical grid, is taken into account. The result is an equation which describes the evolution of the scalar field G in time, the so-called G -equation, (Williams, 1985a). The expansion of the gas is included by imposing a certain temperature and density profile at the position of the propagating flame. The size of the temperature jump over the flame front is determined by the properties of the chemical reaction and has to be known in advance. The same is true for the flame speed s_f , which is also assumed to be a known parameter.

1.3 Outline of this thesis

Chapter 2 of this thesis will provide the theoretical background for this thesis. In this chapter a brief introduction in the field of turbulent combustion is given and the actual model which is used for the DNS is derived. In chapter 3 the numerical method of the DNS is described, together with the implementation of this method on a parallel computer. Some results, concerning the parallel performance of this method are also presented in this chapter. Chapter 4 discusses the simulation results of the interaction of a flame front with decaying

homogeneous isotropic turbulence. In this simple geometry, the flame can be stabilised and proper statistics for the turbulent flow and the behaviour of the flame front are obtained. Chapter 5 describes the propagation of the flame front around a square cylinder. This geometry is more complicated than the geometry used in chapter 4 and show the interaction between a flame front and an obstacle. Due to the complexity of the geometry, it is difficult to obtain proper statistics. However the results show a strong influence of the obstacle, due to the turbulence in the wake and in the shear, which is present in the mean flow behind the cylinder.

Chapter 2

Theory on Premixed Turbulent Combustion

This chapter will provide the theoretical background for the remainder of this thesis. A short overview of the theory of combustion will be given. We start with a section which distinguishes between different kinds of combustion, namely premixed and non-premixed combustion and deflagration and detonation. After this, we focus on the kind of combustion which will be treated in the remainder of this thesis: deflagrating premixed turbulent combustion. Some effects, which will occur in deflagrating premixed turbulent combustion, are the deformation of the flame front by the turbulence, the hydro-dynamic instability of the flame front and baroclinic vorticity production. These effects will be discussed, after which we will derive a set of equations which describes the flow field and the chemistry for our application. Next the equations for the turbulent kinetic energy, the vorticity and the enstrophy of the flow will be derived. These quantities will become important in the discussion about the interaction between combustion and turbulence. The remainder of this chapter discusses the previous work done on the modelling and DNS of premixed turbulent combustion

2.1 General Combustion Theory

Combustion is defined as a chemical reaction between a fuel and oxygen at which heat is released. In order for combustion to take place, certain conditions have to be met. First, an amount of fuel and oxygen has to be mixed and

second, enough heat must be present in order to ignite this mixture. When these conditions are met and the reaction proceeds sufficiently fast, a flame will start to propagate through the medium. A flame is defined as the self-sustaining propagation of a chemical reaction zone in space. This means that the energy, released in the chemical reaction, ignites the surrounding gas mixture, causing the flame to propagate. We can make several classifications in combustion. The first is based on the fact how the reactants, fuel and oxygen, are to be mixed and this will be discussed in the next section. The second classification distinguishes between the mechanisms for flame front propagation: detonation and deflagration.

2.1.1 Non-premixed and premixed combustion

The first classification is based on the fact that the reactants have to be mixed, in order to react. When the reactants initially are *not* mixed, the process is called non-premixed combustion and the mixing process will strongly influence the development of the flame. In case of a chemical reaction with a high reaction rate, the combustion process can be completely determined by the mixing process. Since turbulence is known to play an important role in the mixing of different species, it will also play an important role in non-premixed combustion. In this thesis, this type of combustion is not considered and for an extensive discussion on non-premixed turbulent combustion we refer to (Peters, 2000, chapter 2).

The case where the reactants are already well mixed when the gas is ignited is called premixed combustion. After ignition, a flame will start to propagate through the gas mixture. In premixed combustion, the reaction will not be influenced by the mixing process, but the reaction rate is only determined by the properties of the gas mixture itself. We can distinguish two different classes of a premixed flame propagation through the gas mixture: deflagration and detonation.

2.1.2 Deflagration and detonation

When a premixed flame runs through the medium, heat will be released, the gas will expand and the pressure will rise. This pressure disturbance will run through the gas with the speed of sound and due to compression it will heat up the gas mixture. In case of strong compression, the gas might be heated up above the ignition temperature and will ignite, resulting in a flame which runs with the speed of sound. This phenomenon is called detonation and occurs in

gas mixture only in case where a large amount of heat is released in a long, closed area like a pipe or a tunnel.

It is more common that the flame propagates through the medium by deflagration. In that case, the reaction heat is transported from the reaction area to the burnable mixture in front of the flame by the diffusion of heat. The gas will heat up and ignite, when it reaches the ignition temperature. This method of flame propagation is called deflagration and results in flame speeds, determined by the diffusion of heat, in the order of several meters per second. In contrast, the detonation flame reaches a speed in the order of several hundreds of meters per second. In the remainder of this thesis, we will focus on deflagration flames.

2.1.3 Reaction equations

Chemical reactions can be very complex and a lot of different species can be involved in the reaction. The mass fraction of a species i is defined as the ration between the density of that species and the total density as

$$Y_i = \frac{\rho_i}{\rho}. \quad (2.1)$$

When we consider the mass fraction Y_i for the species $i = 1, 2, \dots, n$, where n is the number of species, we can write the following set of balance equations for the mass fraction (Williams, 1985b):

$$\rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{u} \cdot \nabla Y_i = -\nabla \cdot \mathbf{j}_i + w_i, \quad (2.2)$$

where ρ is the density of the total gas mixture and $\mathbf{u}$ its velocity. The $\mathbf{j}_i$ is the diffusive flux and w_i the chemical source term. This balance indicates that the rate of change of the mass fraction Y_i at a given position is determined by convective and diffusive fluxes and by the chemical source term w_i . Real life reaction are very complicated. For instance the complete reaction mechanism of methane and oxygen consist of 125 reactions with 30 different species, (Li and Williams, 1999). The reaction between oxygen and hydrogen is relatively simple and can be described with only 15 reactions between 8 species. Therefore, this reaction has been used in the only DNS with complex chemistry so far, (Baum et al., 1994). This complexity makes it difficult to find an exact expression for w_i , since the species i can occur in several reactions which all contribute to w_i . Further, w_i strongly depends on the temperature.

In order to overcome the problems of very complex reaction mechanisms, reduced reaction mechanisms are introduced. Peters and Williams (1997) have

reduced the complex methane-air reaction mechanism to a mechanism with four steps. These reduced mechanisms are derived by introducing steady state and partial equilibrium assumptions from the complete reaction mechanism. The advantage is, that these reduced mechanisms still describe the most important chemical properties of the complete mechanisms and parameters like the reaction rate can be derived from the complete mechanism. A disadvantage is that they are usually still too complex to solve in a turbulent flow simulation.

An even more simple model for combustion is a one-step global reaction between fuel F and oxygen O_2 , resulting in a product P :

where ν are the stoichiometric coefficients of F , O_2 and P . The reaction rate is written as:

$$w = A \left(\frac{\rho Y_F}{W_F} \right)^{n_F} \left(\frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{O_2}} e^{-\frac{E}{RT}}, \quad (2.4)$$

where A is the pre-exponential factor, n is reaction order of F and O_2 , W the molecular weight and E the activation energy. R is the universal gas constant. All these constants have to be obtained empirically, since they can not be derived from the complete reaction mechanism. This approach is called the simple chemistry approach. Although this model might be too simple to study the chemical details of combustion, it is often used to study the fluid dynamical aspects of systems with combustion.

2.2 Regimes in Premixed Turbulent Combustion

When a mixture of fuel and oxidiser is ignited, a flame will propagate through the medium in the shape of a thin sheet-like region. This is called the flame zone or flame front. It propagates with a speed determined by two processes: the diffusion of heat and the chemical reaction rate w . w is the amount of fuel mass which burns per unit volume per unit time. The unburnt gas in front of the flame will be heated as a result of heat transfer due to diffusion and ignites when it reaches the ignition temperature. This diffusion depends on the thermal diffusivity $\lambda/\rho_u c_p$ in which λ is the thermal conductivity, ρ_u the density of the unburnt gas and c_p the specific heat at constant pressure of the unburnt gas. In case of a flat flame front in a laminar flow the so-called laminar flame speed s_l

Figure 2.1: The structure of a premixed flame. ℓ_f is the total flame thickness, ℓ_δ is the thickness of the reaction zone, where the actual reaction takes place and ℓ_o is the oxidation layer where the final reaction products are formed.

becomes proportional to (Williams, 1985b):

$$s_{fl} \approx \frac{1}{\rho_u} \sqrt{\frac{\lambda w}{c_p}}. \quad (2.5)$$

In Zeldovich et al. (1985) it is shown that this flame speed strongly depends on the composition of the fuel mixture and on the temperature. This can be explained by the dependence of the reaction rate on the temperature and on the concentration of the reactants. To determine this flame speed one often uses 1-dimensional complex chemistry simulations.

As we have argued above the actual chemical reaction takes place in a very thin layer, the flame zone. Let us look at this flame zone in a some more detail. A sketch of the flame zone is plotted in figure 2.1. It consists of three regions: a preheat zone, in which the gas is heated by diffusion; a region called the inner zone in which the fuel is oxidised to intermediate components such as CO and H₂ and a post-flame oxidation layer where the final combustion products are formed and most of the heat is released. These two latter regions form the

so-called reaction zone. The preheat zone determines for a large part the flame thickness ℓ_f . The inner zone, in which the fuel is oxidised, controls the structure of the flame. The thickness of this layer which is denoted by ℓ_δ , is usually in the order of $0.1\ell_f$. The thickness of the post-flame oxidation layer, ℓ_o is of the same order as the inner zone.

Based on the relevant time and length scales for the combustion and turbulence, we can distinguish several regimes in premixed turbulent combustion, see figure 2.2 (Peters, 2000). We first introduce the Karlovitz number, which is defined as the ratio between the chemical time scale $\tau_f = \ell_f/s_{fl}$ and the Kolmogorov time scale τ_η :

$$Ka = \frac{\tau_f}{\tau_\eta} = \frac{\ell_f^2}{\eta^2} \quad (2.6)$$

where η is the Kolmogorov length scale. When this ratio is smaller the unity, the smallest turbulent scales will be too slow to change the structure of the flame. In this regime, called the flamelet regime, the flame front will be deformed by the turbulent eddies, but the inner structure of the flame will not be changed.

We can define another Karlovitz number Ka_δ base on the reaction zone thickness as

$$Ka_\delta = \frac{\tau_\delta}{\tau_\eta} = \frac{\ell_\delta^2}{\eta^2} = \delta^2 Ka. \quad (2.7)$$

In the situation, when the Kolmogorov scale become smaller and faster, the Karlovitz number Ka increases. When $Ka > 1$, while $Ka_\delta < 1$, the Kolmogorov eddies become small enough to enter the preheat zone. In this regime, called the thin reaction zones regime, the diffusion of heat in the preheat zone will be also influenced by the turbulence and turbulent diffusion has to be taken into account to determine the flame speed s_f . However, since $Ka_\delta < 1$ the inner reaction zone is not affected by the turbulence and the actual reaction zone remains thin, hence the name 'thin reaction zones regime'.

In case of $Ka_\delta > 1$, the inner reaction zone is disturbed by the smallest turbulent eddies. In that case the regime is called distributed reaction zones. This only occurs at slow reaction rates or in well-mixed reactors. We refer to Peters (2000) for a more extensive discussion on this topic.

Let us now go back to the flamelet regime where $Ka < 1$. We can define a length scale ℓ_G , also called the Gibson scale, as the size of an eddy with a turnover velocity equal to the laminar flame speed s_{fl}

$$\ell_G = \frac{s_{fl}^3}{\epsilon}, \quad \text{or} \quad \frac{\ell_G}{\ell} = \left(\frac{s_{fl}}{u'} \right)^3, \quad (2.8)$$

Figure 2.2: Different regimes in premixed turbulent combustion. ℓ denotes turbulent macro scale, ℓ_f the flame thickness and η the Kolmogorov scale. s_L is the laminar flame speed and u' is the root-mean-square velocity fluctuation of the turbulent field. The Karlovitz number Ka is defined as the ratio between the chemical and the Kolmogorov time scale. $Ka = \frac{\tau_l}{\tau_\eta}$ and $Ka_\delta = \frac{\tau_\delta}{\tau_\eta}$

where ℓ is the integral turbulent length scale, u' a scale for the turbulent velocity fluctuations and ϵ the dissipation rate. The situation that $\ell_G < \ell$, or $s_{fl} < u'$, corresponds to the corrugated flamelet regime. In that regime, the turbulence corrugates, i.e. makes large scale disturbances in, the flame front, while in case $\ell_G > \ell$ and $s_{fl} > u'$, the turbulence is not able to deform the flame front substantially. This regime is called the wrinkled flamelet regime, see figure 2.2.

2.2.1 Turbulent distortion of the flame front

Although for $Ka < 1$ the turbulence is not able to influence the inner structure of the flame, larger turbulent eddies are able to deform the flame as a whole, especially in the corrugated flamelet regime. Therefore, the flame front is no longer flat, but becomes distorted, which we may denote as a kinematic interaction. The effect of this distortion is an increase in the total the flame front area and therefore in the total combustion rate. Let us define a mean turbulent flame speed s_{fl} by

$$s_{fl} = s_{fl} \frac{A_t}{A_l}, \quad (2.9)$$

where A_t is the total area of the turbulent flame front and A_l the projected area of the flame front on a flat plane, which would be the geometry of the flame in laminar flow conditions. Damköhler (1940) related the increase in flame area to some measure of the turbulent velocity fluctuations u' as follows:

$$\frac{A_t}{A_l} = \frac{s_{fl} + Cu'}{s_{fl}}, \quad (2.10)$$

where C is a coefficient with a value of the order of unity. Combined with (2.9), this gives:

$$s_{fl} = s_{fl} + Cu', \quad (2.11)$$

which suggests that the turbulent flame speed in the flamelet regime is linearly proportional to the turbulent velocity fluctuations.

2.2.2 Restoration of the flame front

Due to the fact that the flame front propagates in the direction, normal to its surface, it has a tendency to restore disturbances which are present on the flame front. This is called the Huygens effect in flame propagation, analog to a similar effect which occurs in non-linear optics. A schematic illustration of this process, is given in figure 2.3, which shows the propagation of a flame from the right to

Figure 2.3: Schematic illustration of the process of flame front restoration. The flame propagates from the right to the left, while the unburnt gas is at rest.

the left, while the unburnt gas is at rest. This figure shows that the amplitude of the disturbance on the flame front decreases while the flame propagates through the medium. This is a result of the fact that the flame propagates in the normal direction to the flame front, indicates with the vectors in the figure, which is a purely kinematic effect.

2.3 Flame front instabilities

There are several different kinds of instabilities which may occur in combustion. The first instability considered here is the hydrodynamic instability. Landau (1944) considered the flame front as a plane discontinuity. The flame has a small displacement in the x -direction, $\zeta(y, t)$, see also figure 2.4

$$\zeta = D e^{iky - i\omega t}. \quad (2.12)$$

If $u_u < u_b$ or $\rho_b < \rho_u$, the growth rate $\Omega = -i\omega$ has a real and positive root, given by

$$\Omega = k u_u \frac{\tau + 1}{\tau + 2} \left(\sqrt{2 + \tau - \frac{1}{\tau + 1}} - 1 \right), \quad (2.13)$$

Figure 2.4: Schematic illustration of the mechanism of hydrodynamic instabilities

where k is the wave number, u_u the velocity of the unburnt gas and τ the heat release parameter $(\rho_u - \rho_b)/\rho_b$. This means that a plane discontinuity in the density, as it occurs in premixed combustion, is unconditionally unstable. This can also be explained by looking at the schematic illustration in figure 2.4. The velocity can be decomposed in a component perpendicular and a component tangential to the flame front. The tangential component is continuous, while the perpendicular component will increase from the unburnt to the burnt gas. This results in a change in the flow direction, which causes an increase in the flow rate where ζ is positive and a decrease where ζ is negative. Therefore a disturbance will be amplified and the flame front will be unconditionally unstable.

Let us now consider the effect of the flame-front deformation on the density and velocity fluctuations. To this end we consider the points denoted with a and b in figure 2.4. In case of an undisturbed flame, the density and velocity in point a would be ρ_b and u_b , respectively. As a result of the deformation of the flame front, the density is equal to ρ_u and velocity will be of the order of u_u . As a result $\rho' = \rho_u - \rho_b > 0$ and $u' \approx u_u - u_b < 0$ so that the product $\rho'u' < 0$. For point b the undisturbed values are ρ_u and u_u . The fluctuations related to the flame-front deformation then become $\rho' = \rho_b - \rho_u < 0$ and $u' \approx u_b - u_u > 0$ and again the product $\rho'u' < 0$. We can conclude that the gas expansion across the flame front together with a deformation with respect to its average

position, always leads to a negative value for the product $\rho'u'$, independent of the deformation mechanism. This means that this effect occurs as a result of flame-front deformation due to the hydrodynamic instability mechanism, discussed in this section, but it will also occur as a result of deformation due to turbulence.

2.4 Baroclinic vorticity production

A third effect, which may occur in premixed turbulent combustion, is the production of vorticity at the position of the flame front, due to the interaction between the pressure and the density gradient. In figure 2.5 a sketch of this process is given. This mechanism of vorticity production is called baroclinic vorticity production, because it occurs when the density gradient and the pressure gradient are not aligned. This is the case when the flame front is disturbed by either turbulence in the flow field or by instability processes. In that case the density gradient is perpendicular to the flame front, while the pressure gradient is not influenced. The vorticity generated alters the turbulent flow field behind the flame front, which may have an effect on the propagation of the flame front itself. This effect has been studied by Rutland and Ferziger (1991), who carried out a 2 dimensional simulation. More recently, Mueller et al. (1998) performed PIV measurements of the interaction between a vortex pair and a premixed flame, which provide the first quantitative experimental results of the generation of vorticity in premixed combustion. Louch and Bray (1998) have performed 2D simulations of Mueller's experiments.

2.5 Modelling Premixed Turbulent Combustion

The description of the actual chemical process of combustion is mostly very complex. Depending on the chemical species involved, the complete reaction mechanism may consist of more than 100 reactions. Because of the high reaction rate of some of these reactions, the resulting system of differential equations can become very stiff. Furthermore, the resulting chemical length scales are too small to be resolved on a three dimensional mesh. Although the use of reduced reaction mechanisms can solve these problems partially, it is still not feasible to perform a three dimensional time dependent full simulation of a combustion process.

In the flamelet regime, which is the regime of interest here, the chemical length scales are by definition smaller than the Kolmogorov scale. The combus-

Figure 2.5: Sketch of the baroclinic vorticity production mechanism

tion can then be described only in terms of the flame speed s_f and the amount of energy released per unit mass. Also when the chemical time scales are shorter than the time scales of the flow, the inner structure of the flame will not be affected by larger and slower flow structures. So when we stay in the flamelet or in the thin reaction zones regime, we do not have to resolve the structure of the flame with a complex chemistry model in order to study the interaction between the flame front and turbulence in the flow. As long as it provides us with the propagation of the flame front and the amount of energy released by the combustion process, the chemical model is sufficient.

An approach which obeys these criteria is the level-set approach (Sethian, 1999), which has been introduced by Williams (1985a). In this approach, the position of the flame front is represented by the isosurface G_0 of a scalar field G .

$$G(\mathbf{x}, t) = G_0 \quad (2.14)$$

The flame front is advected with the flow field and propagates with respect to the flow with the flame speed s_f in the direction to its normal $\mathbf{n}$

$$\frac{d\mathbf{x}_f}{dt} = \mathbf{u} + \mathbf{n}s_f. \quad (2.15)$$

Differentiating (2.14) with respect to t gives

$$\frac{\partial G}{\partial t} + \nabla G \cdot \frac{d\mathbf{x}_f}{dt} = 0. \quad (2.16)$$

With

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|} \quad (2.17)$$

one can derive then the following equation for G :

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = s_f |\nabla G| \quad (2.18)$$

which is known as the G -equation. All the chemistry is now included in the velocity of the flame front s_f .

2.5.1 Effects of curvature and strain on s_f

In case of the flamelet regime, s_f can be taken equal to the laminar flame speed s_{fl} , corrected for effect flame stretch. This correction is done with the Markstein length $\mathcal{L}$, which relates the total stretch rate α to the velocity:

$$s_f - s_{fl} = \mathcal{L}\alpha \quad (2.19)$$

The total stretch has a contribution of the curvature and the strain which gives

$$s_f = s_{fl} - s_{fl}\mathcal{L}\kappa - \mathcal{L}S, \quad (2.20)$$

The curvature κ is defined by

$$\kappa = \nabla \cdot \mathbf{n} \quad (2.21)$$

where the unit normal vector $\mathbf{n}$ can be written in terms of the G -field as

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}. \quad (2.22)$$

The S is the strain rate, imposed on the flame, is given by

$$S = -\mathbf{n} \cdot \nabla \mathbf{u} \cdot \mathbf{n}. \quad (2.23)$$

According to Peters (2000), the Markstein length $\mathcal{L}$ is positive for most practical applications of premixed hydrocarbon combustion and is in the order of the laminar flame thickness ℓ_f . For positive values of $\mathcal{L}$, the contribution of the

Figure 2.6: A sketch of a one dimensional flame

curvature will suppress instabilities in the flame front. For negative values of $\mathcal{L}$, which occur in hydrogen-air mixtures, thermo-diffusive instabilities, as mentioned in section 2.3, will occur, leading to an increase in flame area and strong flame accelerations. The occurrence of negative values of $\mathcal{L}$ will also lead to numerical problems, since they are equivalent with negative diffusion in the G -equation.

2.5.2 Effect of gas expansion on s_f

Since heat is released at the position of the flame front, the gas will expand and the density of the burnt gas ρ_b will be lower than the density of the unburnt gas ρ_u . When we look at a one dimensional, stationary flame, as sketched in figure 2.6, we see that the mass flux ρu must be constant over the flame in order to obey conservation of mass. Since the situation is stationary, G is constant in time. Therefore, there must be a balance between the advection of G and the propagation of G with the flame speed: $s_f = u$. When we define the laminar flame speed as the flame speed with respect to the unburnt gas, then the actual flame speed, has to be corrected for the expansion of the gas with

$$s_f = s_{fl} \frac{\rho_u}{\rho}. \quad (2.24)$$

When we combine (2.20) and (2.24), we end up with the following expression for s_f in the G -equation (2.18):

$$s_f = (s_{fl} - s_{fl}\mathcal{L}\kappa - \mathcal{L}S) \frac{\rho_u}{\rho}. \quad (2.25)$$

2.5.3 Reinitialisation of G

In principle the value of G outside G_0 , i.e. the position of the flame front, can be chosen freely. It has been found useful, however, to define G as a distance function, i.e. the value of G at some position gives the distance to the flame front. This implies that $|\nabla G| = 1$ everywhere. This allows for a direct coupling between the G -field and the temperature of the gas, without having to estimate the position of the flame front, section 2.6.2. To keep G a distance function a reinitialisation of G must be carried out after every time step in the solution procedure. The reason for this is the fact that the G -equation can be characterised as an advection equation. Using upwind methods to solve such equation may lead to inaccuracies in the computed G -fields, which results in considerable errors in the position of the flame front, especially in regions where large gradients in the G -field occur. The reinitialisation procedure addresses this problem by adjusting G in a way that it remains a distance function. In this way large gradients in G , which are difficult to resolve numerically, are avoided while the level G_0 is not affected.

Sussman et al. (1994) achieved this by solving

$$\frac{\partial G}{\partial t} = S(G^0 - G_0) (1 - |\nabla G|) \quad (2.26)$$

until a steady state is reached, starting with the initial condition $G(t = 0) = G^0$. $S(\dots)$ is the sign function. Equation (2.26) has the property that G remains unchanged at the interface G_0 and that away from the interface G will converge to $|\nabla G| = 1$, which is equivalent to G being a distance function. The advantage of G being a distance function is that it is now not necessary to track the position of flame front in order to determine the distance from the flame front at a certain point $\mathbf{x}$ since this distance is now given by $G(\mathbf{x}) - G_0$.

2.6 Flow equations

The flow can be described by the Navier Stokes equations in compressible form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{m} = 0 \quad (2.27)$$

and

$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{m}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (2.28)$$

Where $\mathbf{u}$ is the velocity, ρ is the density, p is the pressure and $\boldsymbol{\tau}$ the deviatoric stress tensor. The equations (2.27) and (2.28) are written in dimensionless form where we used the laminar flame speed s_{fl} as velocity scale and of the density of the unburnt gas ρ_u as density scale. The length scale, which we denote by L , depends on the simulation geometry and can not be determined at this stage, but will be defined at the description of the numerical geometry. The tensor $\boldsymbol{\tau}$ can be written in dimensionless form as

$$\boldsymbol{\tau} = \frac{\mu}{Re} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} \Delta I \right), \quad (2.29)$$

where Re is the Reynolds number, defined by

$$Re = \frac{\rho_u s_{fl} L}{\mu_u}. \quad (2.30)$$

Δ is the relative change in volume:

$$\Delta \equiv tr(\nabla \mathbf{u}) \equiv \nabla \cdot \mathbf{u} = -\frac{1}{\rho} \frac{D\rho}{Dt}. \quad (2.31)$$

The dynamic viscosity μ is scaled with the viscosity of the unburnt gas μ_u . In principle the viscosity may depend on the temperature so that the viscosity may vary. However here we assume a constant viscosity. With these relations, the gradient of the stress tensor in (2.29) can be written as:

$$\nabla \cdot \boldsymbol{\tau} = \frac{1}{Re} \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{u}) \right), \quad (2.32)$$

resulting in the following expression for the momentum equation:

$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{m}\mathbf{u}) = -\nabla p + \frac{1}{Re} \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{u}) \right). \quad (2.33)$$

2.6.1 Coupling between flow and chemistry

The system of equations is closed with an equation of state, which relates the density to the pressure and the temperature $\rho = \rho(T, p)$. In case of combustion,

density will be determined mainly by temperature effects. Therefore we simplify the equation of state as $\rho = \rho(T)$:

$$\rho = \frac{1}{T}. \quad (2.34)$$

This simplification only holds in cases where the density fluctuation are small. This is the case in open geometries where the gas can flow out easily.

A consequence of equation (2.34) is that

$$\left(\frac{\partial \rho}{\partial p} \right)_s = \frac{1}{c_s^2} = 0, \quad (2.35)$$

where c_s is the speed of sound. Therefore (2.34) is called the equation of state in the zero Mach-number limit and can only be applied if the gas velocities are low, compared to c_s . An advantage of this formulation is that all the acoustic modes are eliminated from our problem and that efficient methods, used to solve incompressible flows, can be applied to our problem also.

2.6.2 Energy

To obtain the temperature one needs in principle to solve the energy equation. For instance, to obtain the exact temperature profile in the flame zone, one has to solve the entire system of chemical reactions combined with the energy equation. This is exactly what we wanted to avoid by using the G -equation approach and, besides that, we lack the resolution to solve all the chemical length scales. However, the use of the G -equation implies that the flame speed s_f is given or alternatively when applying the G -equation we have made already use of the energy equation. Therefore, we do not need to solve the energy equation so to speak for a second time. The consequence is the following. Let us assume that there are no energy losses due to radiation or diffusion across the boundaries of the domains. The total enthalpy, which is the sum of the thermal and chemical energy, can then be taken as constant before and after the flame has passed, i.e. in regions sufficiently far away from the flame where the temperature gradients are negligible. These regions are in our case given by the conditions $G > G_0$ and $G < G_0$. Given this constant enthalpy and the amount of heat released by the chemical reaction, we can determine the temperature of the burnt and the unburnt mixture, resp. T_b and T_u .

Since we can not solve the exact temperature profile in the flame zone, we have to assume one. For the numerical computation it has been found that

this profile has to span a few grid cells in order to avoid numerical instabilities but it has to be chosen as thin as possible in order to be consistent with our thin flame zone approximation. Since G can be interpreted as the distance to the flame front, we can couple the temperature directly to G and describe the temperature as:

$$T = T_u \left(1 + \frac{\tanh \left(\frac{G_0 - G}{\delta} \right) + 1}{2} \tau \right) \quad (2.36)$$

where δ determines the thickness of the temperature jump and therefore the numerical thickness of the flame. The fact that this artificial flame thickness will be much larger than the actual flame thickness ℓ_f , is not expected to have a big influence since it has no influence on the flame speed, which mainly determines the behaviour of the flame. The τ is the heat release parameter, which is defined as

$$\tau = \frac{T_b - T_u}{T_u} = \frac{\rho_u - \rho_b}{\rho_b}, \quad (2.37)$$

where the equation of state (2.34) is used to express τ in term is the density of the burnt and the unburnt gas. τ can be interpreted as the increase of volume, when a fluid element passes the flame front. The characteristic velocity scale of the chemical process is the laminar flame speed s_{fl} .

We can also define a characteristic velocity scale U of the flow field. Since the gas flow is driven by the expansion of the gas due to the combustion, we can express U in terms of the chemical process as

$$U = \tau s_{fl} \quad (2.38)$$

U can be interpreted as the outflow velocity resulting from an undisturbed flat flame running through a gas at rest.

2.7 Turbulent Statistics

2.7.1 Turbulent Kinetic Energy

In order to derive some expressions for the turbulent kinetic energy it is convenient to write conservation of mass (2.27) and the momentum equation (2.28) in Cartesian tensor notation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial m_i}{\partial x_i} = 0 \quad (2.39)$$

and

$$\frac{\partial m_i}{\partial t} + \frac{\partial m_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}. \quad (2.40)$$

The kinetic energy per unit volume is defined as $k = \frac{1}{2} \rho u_i^2$. An equation for k can be obtained by multiplying the momentum equation (2.40) with u_i

$$\frac{\partial k}{\partial t} + \frac{\partial u_j k}{\partial x_j} = -u_i \frac{\partial p}{\partial x_i} + u_i \frac{\partial \tau_{ij}}{\partial x_j}. \quad (2.41)$$

In our case of a turbulent flow we will compute various flow statistics with the help of a Reynolds decomposition where each variable is written as the sum of a mean value and a fluctuation, i.e. $u = \bar{u} + u'$. Here the overbar indicates an ensemble average and the prime the fluctuation around this average. When we apply this procedure to the definition of the kinetic energy, we obtain the following expression for the mean kinetic energy $\bar{k}$,

$$\bar{k} = \frac{1}{2} \bar{\rho} \bar{u}_i^2 + \overline{\rho' u_i' \bar{u}_i} + \frac{1}{2} \bar{\rho} \overline{u_i'^2} + \frac{1}{2} \overline{\rho' u_i'^2} \quad (2.42)$$

and the kinetic energy fluctuations k' ,

$$k' = \frac{1}{2} \rho' \bar{u}_i^2 + \bar{\rho} \bar{u}_i u_i' + \rho' u_i' \bar{u}_i - \overline{\rho' u_i' \bar{u}_i} + \frac{1}{2} \bar{\rho} u_i'^2 - \frac{1}{2} \bar{\rho} \overline{u_i'^2} + \frac{1}{2} \rho' u_i'^2 - \frac{1}{2} \overline{\rho' u_i'^2}. \quad (2.43)$$

Due to the fact that we have taken into account density fluctuations, these expressions become more complicated than the expression for $\bar{k}$ and k' in incompressible flows. We must now make a distinction between the contribution to the kinetic energy by the mean flow and by the turbulence. We define the Galilei invariant part of (2.42) as the turbulent kinetic energy k_t and the non-Galilean part of (2.42) as the mean flow kinetic energy k_m , so that $k = k_m + k_t$. Both k_m and k_t can be divided in a mean and a fluctuating part which are given by:

$$\bar{k}_m = \frac{1}{2} \bar{\rho} \bar{u}_i^2 + \overline{\rho' u_i' \bar{u}_i} \quad (2.44)$$

$$k'_m = \frac{1}{2} \rho' \bar{u}_i^2 + \bar{\rho} \bar{u}_i u_i' + \rho' u_i' \bar{u}_i - \overline{\rho' u_i' \bar{u}_i} \quad (2.45)$$

and

$$\bar{k}_t = \frac{1}{2} \bar{\rho} \overline{u_i'^2} + \frac{1}{2} \overline{\rho' u_i'^2} \quad (2.46)$$

$$k'_t = \frac{1}{2} \bar{\rho} u_i'^2 - \frac{1}{2} \bar{\rho} \overline{u_i'^2} + \frac{1}{2} \rho' u_i'^2 - \frac{1}{2} \overline{\rho' u_i'^2} \quad (2.47)$$

An expression for $\bar{k}_m$ can be derived by applying a Reynolds decomposition to the momentum equation (2.40) and multiply the mean part,

$$\begin{aligned} & \overline{\rho \frac{\partial \bar{u}_i}{\partial t}} + \overline{\rho' \frac{\partial u'_i}{\partial t}} + \\ & \overline{\rho \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\bar{u}_j \rho' \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_j \frac{\partial \bar{u}_i}{\partial x_j}} = \\ & -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j}, \end{aligned} \quad (2.48)$$

with $\bar{u}_i$. This results in:

$$\begin{aligned} & \frac{\partial \bar{k}_m}{\partial t} + \frac{\partial \bar{u}_j \bar{k}_m}{\partial x_j} = -\frac{\partial \overline{u'_j k'_m}}{\partial x_j} - \bar{u}_i \frac{\partial \bar{p}}{\partial x_i} + \bar{u}_i \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \\ & \left(\overline{\rho' u'_i \frac{\partial \bar{u}_i}{\partial t}} + \overline{\rho u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}} \right). \end{aligned} \quad (2.49)$$

An expression for $\bar{k}_t$ can be found by taking the fluctuating part of the momentum equation,

$$\begin{aligned} & \rho' \frac{\partial \bar{u}_i}{\partial t} + \overline{\rho \frac{\partial u'_i}{\partial t}} + \rho' \frac{\partial u'_i}{\partial t} - \overline{\rho' \frac{\partial u'_i}{\partial t}} + \\ & \rho' \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \overline{\rho u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho \bar{u}_j \frac{\partial u'_i}{\partial x_j}} + \\ & \rho' u'_j \frac{\partial \bar{u}_i}{\partial x_j} + \rho' \bar{u}_j \frac{\partial u'_i}{\partial x_j} + \overline{\rho u'_j \frac{\partial u'_i}{\partial x_j}} - \\ & \overline{\rho' u'_j \frac{\partial \bar{u}_i}{\partial x_j}} - \overline{\bar{u}_j \rho' \frac{\partial u'_i}{\partial x_j}} - \overline{\rho u'_j \frac{\partial u'_i}{\partial x_j}} + \\ & \rho' u'_j \frac{\partial u'_i}{\partial x_j} - \overline{\rho' u'_j \frac{\partial u'_i}{\partial x_j}} = -\frac{\partial \bar{p}'}{\partial x_i} + \frac{\partial \bar{\tau}'_{ij}}{\partial x_j}, \end{aligned} \quad (2.50)$$

multiplying this with u'_i and averaging the result. This gives:

$$\begin{aligned} & \frac{\partial \bar{k}_t}{\partial t} + \frac{\partial \bar{u}_j \bar{k}_t}{\partial x_j} = -\frac{\partial \overline{u'_j k'_t}}{\partial x_j} - \overline{u'_i \frac{\partial \bar{p}'}{\partial x_i}} + \overline{u'_i \frac{\partial \bar{\tau}'_{ij}}{\partial x_j}} - \\ & \left(\overline{\rho' u'_i \frac{\partial \bar{u}_i}{\partial t}} + \overline{\rho u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}} + \overline{\rho' u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}} \right). \end{aligned} \quad (2.51)$$

Substitution of the expression for the deviatoric stress, equation (2.32), gives

$$\overline{u'_i \frac{\partial \tau'_{ij}}{\partial x_j}} = \frac{1}{Re} \left(\frac{\partial^2 \frac{1}{2} \overline{u_i'^2}}{\partial x_j^2} - \frac{1}{3} \overline{\left(\frac{\partial u'_i}{\partial x_j} \right)^2} + \frac{\partial \frac{1}{3} \overline{u'_i \Delta'}}{\partial x_i} - \overline{\Delta'^2} \right) \quad (2.52)$$

This, together with the assumption that the problem is stationary gives the following equation for the turbulent kinetic energy budget:

$$\frac{D\bar{k}_t}{Dt} = E_k + T_k + P_k + \Pi_k + D_k - \epsilon_k \quad (2.53)$$

with

$$\begin{aligned} E_k &= -\bar{k}_t \frac{\partial \bar{u}_i}{\partial x_i} \\ T_k &= -\frac{\partial \overline{u'_j k'_t}}{\partial x_j} \\ P_k &= -\left(\overline{\rho u'_i u'_j} \frac{\partial \bar{u}_i}{\partial x_j} + \overline{\rho' u'_i} \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \overline{\rho' u'_i u'_j} \frac{\partial \bar{u}_i}{\partial x_j} \right) \\ \Pi_k &= -\overline{u'_i \frac{\partial p'}{\partial x_i}} = -\frac{\partial \overline{p' u'_i}}{\partial x_i} + \overline{p' \frac{\partial u'_i}{\partial x_i}} \\ D_k &= \frac{1}{Re} \left(\frac{\partial^2 \frac{1}{2} \overline{u_i'^2}}{\partial x_j^2} + \frac{\partial \frac{1}{3} \overline{u'_i \Delta'}}{\partial x_i} \right) \\ \epsilon_k &= \frac{1}{Re} \left(\overline{\left(\frac{\partial u'_i}{\partial x_j} \right)^2} + \frac{1}{3} \overline{\Delta'^2} \right) \end{aligned}$$

E_k accounts for the effect of expansion on the kinetic energy. In our case, where the gas expands, $\frac{\partial \bar{u}_i}{\partial x_i} > 0$ and results in a decrease of the kinetic energy density. This can be explained by the fact that in case of gas expansion, the volume increases, resulting in a lower energy density. T_k is the turbulent transport of kinetic energy. P_k is the turbulent production of the mean flow and Π_k is the production of turbulent kinetic energy by the pressure. D_k accounts for the viscous transport and ϵ_k for viscous dissipation.

2.7.2 Vorticity

The vorticity $\boldsymbol{\omega}$ is defined as $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ and is a measure for the local rotational motion of the fluid. The momentum equation (2.40) can be written as:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \boldsymbol{\tau}. \quad (2.54)$$

When we introduce in this equation

$$\mathbf{u} \cdot \nabla \mathbf{u} = -\mathbf{u} \times \boldsymbol{\omega} - \frac{1}{2} \nabla (\mathbf{u} \cdot \mathbf{u}) \quad (2.55)$$

and take the curl of the result, we get the following expression for the vorticity:

$$\begin{aligned} \frac{\partial \boldsymbol{\omega}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\omega} &= \boldsymbol{\omega} \cdot \nabla \mathbf{u} - \boldsymbol{\omega} (\nabla \cdot \mathbf{u}) - \left(\nabla \frac{1}{\rho} \times \nabla p \right) + \\ &\quad \frac{1}{Re} \left(\frac{1}{\rho} \nabla^2 \boldsymbol{\omega} + \nabla \frac{1}{\rho} \times \left(\nabla^2 \mathbf{u} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{u}) \right) \right). \end{aligned} \quad (2.56)$$

To derive this equation, we made use of the following relations:

$$\nabla \cdot \boldsymbol{\omega} = 0 \quad (2.57)$$

$$\nabla \times (\nabla p) = 0 \quad (2.58)$$

$$\nabla \times \nabla (\mathbf{u} \cdot \mathbf{u}) = 0 \quad (2.59)$$

$$\nabla \times \nabla (\nabla \cdot \mathbf{u}) = 0 \quad (2.60)$$

The final two relations are valid since $\mathbf{u} \cdot \mathbf{u}$ and $\nabla \cdot \mathbf{u}$ are a scalar. Note that $\nabla \cdot \mathbf{u} \neq 0$ since the flow is compressible.

Let us first consider the terms in this equation which also appear in the vorticity equation for an incompressible flow (Batchelor, 1967, section 5.2). Apart from the terms on the left-hand side of the equation, this is the first term on the right-hand side $(\boldsymbol{\omega} \cdot \nabla) \mathbf{u}$, which describes the effect of deformation of the velocity field on the vorticity. One of the consequences of this term is that it causes a vortex to spin up, when it is stretched in the direction of its vorticity vector. The second term is $\nabla^2 \boldsymbol{\omega}$ and it accounts for the viscous destruction of vorticity.

Next we consider the terms which do not have an equivalent term in the incompressible vorticity equation. This is the term $-\boldsymbol{\omega} (\nabla \cdot \mathbf{u})$, which describes the effect of gas expansion. When the gas expands $\boldsymbol{\omega}$ will decrease since it is smeared out over a larger volume. The term $-\nabla(1/\rho) \times \nabla p$ is called the

baroclinic production term and it describes the production of vorticity when the pressure and density gradient are not aligned. For the same pressure gradient, the part of the flow with a low density will be accelerated faster than the part with the higher density, resulting in the production of vorticity. The last term, which is written as $\nabla(1/\rho) \times (\nabla \cdot \boldsymbol{\tau})$, is similar to the baroclinic term in a way that it accounts for the production of vorticity when the density gradient and the divergence of the stress are not aligned.

2.7.3 Enstrophy

In our analysis we will be primarily interested in the vorticity fluctuations. A measure of these fluctuations is the enstrophy Ω , which is defined as

$$\Omega = \overline{\frac{1}{2}|\boldsymbol{\omega}'|^2} \quad (2.61)$$

where $\boldsymbol{\omega}'$ is the vorticity fluctuation around the average vorticity $\bar{\boldsymbol{\omega}}$. An expression for Ω can be found by a similar procedure as used to obtain the equation for the turbulent kinetic energy. It is convenient to write the resulting equation with the help of the specific volume $v = 1/\rho$ and the quantity Ω' , defined as

$$\Omega' \equiv \frac{1}{2}|\boldsymbol{\omega}'|^2 = \frac{1}{2}\boldsymbol{\omega}' \cdot \boldsymbol{\omega}'. \quad (2.62)$$

The resulting equation for the enstrophy then becomes:

$$\frac{\partial \Omega}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \Omega = E_\omega + T_\omega + P_\omega + D_\omega + S_\omega - \epsilon_\omega \quad (2.63)$$

with

$$\begin{aligned} E_\omega &= -\Omega(\nabla \cdot \bar{\mathbf{u}}) \\ T_\omega &= -\nabla \cdot (\mathbf{u}'\Omega') \\ P_\omega &= -\overline{\boldsymbol{\omega}' \cdot (\nabla v' \times \nabla p')} + \overline{\boldsymbol{\omega}' \cdot (\nabla v' \times \nabla \cdot \boldsymbol{\tau}')} \\ D_\omega &= \frac{1}{Re} \bar{v} \nabla^2 \bar{\Omega}' + \frac{1}{Re} \overline{v' \nabla^2 \Omega'} \\ S_\omega &= \overline{\boldsymbol{\omega}' \cdot (\boldsymbol{\omega}' \cdot \nabla \bar{\mathbf{u}})} + \overline{\boldsymbol{\omega}' \cdot (\boldsymbol{\omega}' \cdot \nabla \mathbf{u}')} \\ \epsilon_\omega &= \frac{1}{Re} \bar{v} \overline{\|\nabla \boldsymbol{\omega}'\|^2} + \frac{1}{Re} \overline{v' \|\nabla \boldsymbol{\omega}'\|^2}, \end{aligned}$$

where E_ω is the effect of the expansion on the enstrophy. This term will lower the enstrophy density, due to the increase in volume in an expanding flow. T_ω

is the turbulent transport term. P_ω is the production of enstrophy, as a results of the normal and deviatoric stresses acting on a fluid with a density gradient. D_ω is the viscous transport term. S_ω is the production of enstrophy by the deformation of the velocity field and ϵ_ω is the viscous destruction of enstrophy.

2.7.4 Favre averaging

The complication that we have encountered in the sections 2.7.1 and 2.7.2 occur because of the fact that density fluctuations are present. This is usually avoided by introducing a so-called Favre averaging, which is defined as

$$\tilde{u}_i = \frac{\overline{\rho u_i}}{\bar{\rho}} \quad (2.64)$$

With this definition, the continuity equation results in

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0 \quad (2.65)$$

and the Favre mean momentum equation reads

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \bar{\rho} u_i'' u_j''}{\partial x_j} \quad (2.66)$$

where the velocity fluctuation u_i'' is defined by $u_i'' = u_i - \tilde{u}_i$.

The advantage of this description is that the equation (2.66) has the same form as the equation for the mean velocity in incompressible form. This is also the case for the Favre average kinetic energy, which is defined as

$$\tilde{k} = \tilde{k}_m + \tilde{k}_t = \frac{1}{2} \bar{\rho} \tilde{u}_i^2 + \frac{1}{2} \overline{\rho u_i''^2}. \quad (2.67)$$

The $\tilde{k}_t$ can be expressed in terms of the variables that we use here with as result

$$\tilde{k}_t = \frac{1}{2} \left(\overline{\rho u_i'^2} + \overline{\rho' u_i'^2} - \frac{\overline{\rho' u_i'^2}}{\bar{\rho}} \right) = \bar{k}_t - \frac{1}{2} \frac{\overline{\rho' u_i'^2}}{\bar{\rho}} \quad (2.68)$$

We see thus that the Favre averaged turbulent kinetic energy will be always smaller than the ensemble mean turbulent kinetic energy given by (2.46). We shall return to this result in our analysis of the simulation data.

An expression for the Favre averaged turbulent kinetic energy can be found by subtracting the Favre averaged momentum equation (2.66) from the original momentum equation (2.40), multiplying the result with u_i'' and averaging the result. This leads to the expression

$$\frac{\partial \tilde{k}_t}{\partial t} + \frac{\partial \tilde{k}_t \tilde{u}_j}{\partial x_j} = -\frac{\partial \tilde{k}_t'' u_j''}{\partial x_j} - \overline{u_i'' \frac{\partial p'}{\partial x_i}} - \overline{u_i'' \frac{\partial \bar{p}}{\partial x_i}} + \overline{u_i'' \frac{\partial \tau'_{ij}}{\partial x_j}} + \overline{u_i'' \frac{\partial \bar{\tau}_{ij}}{\partial x_j}}, \quad (2.69)$$

with $k_t'' = \frac{1}{2} \rho u_i''^2$

The fact that Favre averaging leads to equations similar to those in incompressible flow, leads to the application of turbulence models, which have been developed for an incompressible flow. However, when the results of Favre averaging are compared with experiments, one usually assumes that the Favre averaged velocity can be compared direct with e.g. a volume average velocity. In our analysis, we will consider the errors involved in such assumptions.

2.8 Previous work

In this section we will provide a brief overview of the previous work done to model premixed combustion. The first section handles the RANS modelling of premixed combustion, while the second section focusses on LES and DNS simulations of turbulent premixed combustion.

2.8.1 RANS modelling of premixed combustion

Modelling of premixed combustion uses the knowledge that the actual reactive processes occur in thin layers, also called flamelets. These flamelets occur in a turbulent flow field. However since the time scales involved in the chemical reaction are very short, the flow field can be seen as laminar from a chemical point of view. In order to model premixed turbulent combustion, we have to focus on the position and the shape of the flame surface.

We will describe two approaches to model premixed combustion. In the first approach is the classical model for premixed combustion, the Bray-Moss-Libby (BML) model. The second approach is based on the level set approach and used the G -equation, which we have already introduced in section 2.5.

BML model

The BML model, (Bray and Moss, 1997), uses a progress variable c , which is defined as the normalised temperature or the normalised mass fraction in a one step reaction

$$c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_P}{Y_{P,b}}, \quad (2.70)$$

where T_b and T_u are the temperature of the burnt and the unburnt gas. $Y_{P,b}$ is the mass fraction of the product in case the gas is burnt. In the BML model, one assumes the flame to be infinitely thin. Therefore c is a step function that is either 0 in the unburnt gas or 1 in the burnt gas. As a result, the pdf of the progress variable c is given by two delta functions at $c = 0$ and $c = 1$ or

$$P(c, \mathbf{x}, t) = \alpha(\mathbf{x}, t)\delta(c) + \beta(\mathbf{x}, t)\delta(1 - c) \quad \text{with} \quad \alpha(\mathbf{x}, t) + \beta(\mathbf{x}, t) = 1. \quad (2.71)$$

The equation, which describes the evolution of c in time reads

$$\rho \frac{\partial c}{\partial t} + \rho \mathbf{u} \cdot \nabla c = \omega_c, \quad (2.72)$$

where ω_c is a reaction term. Next we introduce an equation for the Favre averaged progress variable $\tilde{c}$ which reads

$$\bar{\rho} \frac{\partial \tilde{c}}{\partial t} + \bar{\rho} \mathbf{u} \cdot \nabla \tilde{c} + \nabla \cdot (\bar{\rho} \widetilde{\mathbf{u}'' c''}) = \bar{\omega}_c, \quad (2.73)$$

where $\bar{\omega}_c$ is the mean reaction term. The turbulent transport term $\widetilde{\mathbf{u}'' c''}$ and the reaction term $\bar{\omega}_c$ need to be modelled. Libby and Bray (1981) showed that the turbulent transport term can be written as

$$\widetilde{u'' c''} = \tilde{c}(1 - \tilde{c})(\bar{u}_b - \bar{u}_u). \quad (2.74)$$

Since the gas expands ($\bar{u}_b - \bar{u}_u$), the difference between the mean velocity of the burnt and the unburnt gas, will be greater than zero and $\widetilde{u'' c''} > 0$. This is in conflict with the gradient transport assumption, often made in incompressible turbulence modelling

$$-\widetilde{u'' c''} = D_t \frac{\partial \tilde{c}}{\partial x}, \quad (2.75)$$

where D_t is the turbulent diffusion coefficient. This assumption requires $\widetilde{u'' c''} < 0$, since $\frac{\partial \tilde{c}}{\partial x} > 0$ if $(\bar{u}_b - \bar{u}_u) > 0$. This phenomenon is called counter gradient

diffusion and has to be taken into account when one wants to model premixed turbulent combustion. Veynante et al. (1997) presented a model to close the turbulent transport term which takes counter gradient transport into account. Counter gradient diffusion is attributed to gas expansion effects, due to heat release. The mean reaction term $\bar{\omega}_c$ also has to be closed. Since the flame front is considered infinitely thin, the BML model can be considered a model for premixed turbulent combustion in the fast chemistry limit. For more information about BML modelling, we refer to Libby and Williams (1994); Bray and Peters (1994).

G-equation modelling

A more recent approach in modelling premixed turbulent combustion is based on the level-set approach, which leads to the *G*-equation, as we have discussed in section 2.5. This approach allows us to take finite rate chemistry into account. We can describe a steady one-dimensional premixed flame with the following equation:

$$\rho s_{fl} \frac{d\psi_i}{dx_n} = \frac{d}{dx_n} \left(\rho D_i \frac{d\psi_i}{dx_n} \right) + \omega_i, \quad (2.76)$$

where ψ_i is a reactive scalar associated with specie i . x_n is the coordinate, normal to the flame front. When we introduce

$$x_n = \frac{G - G_0}{|\nabla G|}, \quad (2.77)$$

we can write

$$\rho s_{fl} |\nabla G| \frac{d\psi_i}{dG} = \frac{d}{dG} \left(\rho D_i |\nabla G|^2 \frac{d\psi_i}{dG} \right) + \omega_i, \quad (2.78)$$

which is a flamelet equation with G as independent variable.

Peters (1992) was one of the first to use the *G*-equation approach to model turbulent combustion in the flamelet regime. He formulated a spectral closure and extended this model to the thin reaction zones regime (Peters, 1999), which resulted in the following expression for the *G*-equation which is valid, both in the corrugated flamelet regime and in the thin reaction zones regime:

$$\rho \frac{\partial G}{\partial t} + \rho \mathbf{u} \cdot \nabla G = (\rho s_{fl}) \sigma - (\rho D) \kappa \sigma, \quad (2.79)$$

with

$$\sigma = |\nabla G|. \quad (2.80)$$

D is a diffusivity coefficient which takes the Markstein effect into account. A model for the G -equation was derived, this time by using Favre averaging, resulting in

$$\bar{\rho} \frac{\partial \tilde{G}}{\partial t} + \rho \tilde{\mathbf{u}} \cdot \tilde{\mathbf{G}} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}'' \tilde{G}'') = -\bar{\rho} D \tilde{\kappa} \tilde{\sigma} + \bar{\rho} s_{fl} \tilde{\sigma} + \bar{\rho} \mathcal{L} \mathbf{n} \cdot \tilde{\nabla} \mathbf{u} \cdot \mathbf{n} \sigma \quad (2.81)$$

and

$$\bar{\rho} \frac{\partial \tilde{G}''^2}{\partial t} + \bar{\rho} \tilde{\mathbf{u}} \cdot \nabla \tilde{G}''^2 \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}}'' \tilde{G}''^2) = -2\bar{\rho} \tilde{\mathbf{u}}'' \tilde{G}'' \cdot \nabla \tilde{G} - \bar{\rho} \tilde{\omega} - \bar{\rho} \tilde{\chi} - \bar{\rho} D \tilde{\kappa} \tilde{\sigma}, \quad (2.82)$$

where $\tilde{\omega} = -2s_{fl}\sigma\tilde{G}''$ accounts for the Favre averaged kinematic restoration. This phenomena causes a wrinkled flame front to smooth by the propagation of the flame front. The term $\tilde{\chi} = 2D(\nabla \tilde{G}'')^2$ denotes the scalar dissipation. Peters presented a closure for these two terms, while he showed that the term $D\tilde{\kappa}\sigma$, which is called the scalar-strain covariance, can be neglected.

Ashurst (1997) studied the influence of gas expansion by superposing a potential flow, caused by the expansion of gas, on top of the regular flow field. This approach has several limitations. The flow does not obey the boundary conditions and vorticity is not generated at the flame front. Nevertheless Ashurst was able to reproduce Darrieus-Landau instabilities, section 2.3 with this approach. Peters et al. (2000) used this approach to incorporate the influence of gas expansion into the G -equation and concluded that gas expansion counter acts kinematic restoration. This effect becomes smaller for higher turbulence intensities and the average flame thickness is considerably increased by gas expansion effects.

2.8.2 DNS of premixed turbulent combustion

While the modelling of the fluid is quite straightforward in direct numerical simulations, there are several approaches to model the chemistry. The first approach is to use complex chemistry. This approach is very demanding in terms of computational resources and therefore only applied in 2-dimensional geometries, (Baum et al., 1994). A simple chemistry approach is more common in 3-dimensional DNS of premixed turbulent combustion. The last approach uses a G -equation and is the approach used in this thesis. In this section, we will give a short overview of the work done on both the simple chemistry and the G -equation approach. For a more extensive discussion on this subject, we refer to the review of Poinso et al. (1996).

Simple chemistry

In the simple chemistry approach, the combustion process is modelled with a single step global reaction.

The reaction rate is determined with the Arrhenius law. Often, the Lewis number is taken equal to unity. This means that the diffusivity of the temperature and the chemical species are equal. As a result, the temperature and the variable to describe the progress of the reaction are equivalent, which leads to the following equation for the temperature T :

$$\frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho \mathbf{u} T) = \frac{1}{Re Pr} \nabla^2 T + \omega_E. \quad (2.84)$$

where the thermal energy produced by the reaction $\dot{\omega}$ is determined with the Arrhenius law

$$\omega_E = B \rho (1 - T) \exp \left(\frac{\beta (1 - T)}{1 - \alpha (1 - T)} \right), \quad (2.85)$$

or

$$\omega_E = B \rho (1 - T) \exp \left(\frac{\beta (\tau - 1) (1 - T)}{\tau T - 1} \right). \quad (2.86)$$

B is a preexponential parameter, β is the activation energy and α is the heat release parameter, defined by $\alpha = \tau / (\tau - 1)$. The parameters B , β and τ are to be determined empirically. The Navier-Stokes equations, together with (2.86) and an equation of state, form a closed system, which can be solved numerically. The smallest chemical length scale has to be resolved on the numerical mesh. In order to determine the requirements of the DNS the Dmkohler number, defined as the ratio between the integral turbulent timescale and the chemical time scale is introduced:

$$Da = \frac{\tau_\ell}{\tau_f} = \frac{\ell s_\eta}{\ell_f u'}, \quad (2.87)$$

where ℓ is the integral turbulent length scale. For the DNS of premixed turbulent combustion, the same limitation in Reynolds number applies as for DNS without combustion

$$Re_\ell^{3/4} < N, \quad (2.88)$$

where N is the number of grid points in a certain direction. Another limitation is the smallest chemical scale. In order to solve the structure of the flame properly, ℓ_f has to span at least a number of grid cells Q , where Q is at least 10 to 20.

When the flame thickness is estimated to be $\ell_f \simeq \nu/s_B$, the product $Re_\ell Da$ can be written as

$$Re_\ell Da = \frac{\ell^2 s_B}{\nu \ell_f} = \left(\frac{\ell}{\ell_f} \right)^2. \quad (2.89)$$

As a result Da can be obtained from

$$Re_\ell Da < \left(\frac{N}{Q} \right)^2. \quad (2.90)$$

given a certain value of Re_ℓ , which has to obey equation (2.88). With $N = 256$ and $Q = 10$, the maximum value of Re_ℓ is about 1600. However this limits Da to a value of 0.4. In order to reach higher values of Da , a lower Re_ℓ has to be chosen. With the same values for N and Q and $Re_\ell = 200$, Da can reach a value of about 3. With values of Da in the order of unity, one can estimate that $\bar{Ka}$, which is the inverse of Da , based on the Kolmogorov scale, will become larger than unity. This means that DNS using the simple chemistry approach is always limited to the thin reaction zones regime. The flamelet regime cannot be modelled this way.

Zhang and Rutland (1995) performed a 3 dimensional simulation using the simple chemistry approach. This DNS is limited to low Reynolds numbers ($Re_\ell = 39$) and rather modest expansion rates ($\tau = 1.5$). Nevertheless it provides very useful information about the turbulent kinetic energy.

Louch and Bray (1998) performed a similar simulation in a 2 dimensional geometry to study the interaction between a flame front and a vortex pair. The same geometry was studied experimentally by Mueller et al. (1998). In both the experiments and the simulation, the destruction and generation of vorticity by the flame front occurs.

Other relevant work has been performed by Chen and Im (1998), who studied the influence of stretch on the propagation of premixed flame in a 2 dimensional geometry.

***G*-equation**

The *G*-equation has been used previously in LES and DNS simulations. Im et al. (1995) and Piana et al. (1996) were the first to study the use of the *G*-equation in a turbulent flow simulation. This resulted in the development of a LES model for the *G*-equation, (Bourlioux et al., 1996; Im et al., 1997). Wenzel (1997); Wenzel and Peters (1998) did apply the *G*-equation in a DNS, but did not include the effect of gas expansion in this simulation. Much effort has been

done to find a way to modify the G -equation itself to account for the effects of gas expansion so that one can continue to calculate with an incompressible flow. Ashurst (1997) has introduced a potential flow field which represents gas expansion as a source of volume. This potential flow field however lacks physical properties like the generation of vorticity at the flame front. Nevertheless, Ashurst (1997) was able to reproduce the Darrieus-Landau instability. Peters et al. (2000) modified the G -equation in the Reynolds Averaged Navier Stokes (RANS) equations to take a potential field into account. Wenzel and Peters (2000) used a modified G -equation in a DNS model and concluded that the effects of gas expansion are only significant for small turbulence intensities.

Chapter 3

Numerical Method

In this chapter the numerical method used for the Direct Numerical Simulation (DNS) in this thesis and the implementation of this method on a parallel computer are described. The basis of the DNS model is given in chapter 2, where the chemistry is modelled, using the G-equation approach, equation (2.18) and the flow is described with the conservation of mass (2.27), the momentum equation (2.28) and an equation of state (2.34). The numerical method consists of a second order accurate finite volume discretisation in space. For the temporal discretisation, an explicit second order accurate predictor-corrector method is. The method is implemented on a parallel computer and the results of the parallel performance shows that the code scales linearly up to 128 CPU's on a parallel computer. This chapter is an adjusted version of the paper, published in the proceedings of Parallel Computing 2001, held on 4 - 7 September 2001 in Naples, Italy

3.1 Introduction

Direct Numerical Simulation (DNS) of turbulence has established itself as an important tool in turbulence research. However, due to the nature of turbulence, which is a three dimensional, time-dependent phenomenon, DNS is restricted to low Reynolds numbers and simple geometries. As we have seen in section 2.8.2 the amount of points needed to resolve all the turbulent length scales, up to the Kolmogorov length scale, scales with $Re^{3/4}$ in each direction, or $Re^{9/4}$ for a full 3-dimensional calculation. With a total amount of grid points in each each

direction in the order of 200, this limits the application of DNS to Reynolds numbers in the order of $10^4 - 10^5$, depending on the definition of the Reynolds number and the flow geometry. This range is below most practical applications, which usually have a Reynolds number of 10^6 or higher.

Although the steady growth in available computing power will not allow us to simulate these practical applications of turbulence any time soon, it does give room to extend DNS to more complicated problems, where turbulence plays an important role. Examples are the influence of turbulence on particles in the flow (van Haarlem, 2000), mixing processes (Brethouwer, 2001) and our application, turbulent combustion.

As we described in section 2.8.2, DNS of premixed turbulent combustion, with a simple chemistry model is only possible for relatively thick flames, since all the chemical length scales have to be resolved on the numerical grid. Zhang and Rutland (1995) use in their DNS a Reynolds number, based in the integral length scale of $Re_\ell = 39$, which is low, compared to DNS simulations without combustion. Brethouwer (2001) performed a DNS of homogeneous isotropic turbulence and used a Reynolds number of $Re_\ell = 314$. A result of the low Reynolds number used by Zhang and Rutland is that the smallest turbulent length scales are relatively large, which increases the Karlovitz number (2.6). The Karlovitz number based on the Taylor micro scale used in this DNS is $Ka_\lambda = 1.27$, which leads to a Karlovitz number as defined in equation (2.6) of $Ka \approx 0.3$, when we assume $\tau \approx 0.4\tau_\lambda$, which is a reasonable, but conservative estimate for Re_ℓ , according to Brethouwer (2001). The laminar flame thickness in the simulation of Zhang and Rutland is approximately 10 grid points, which is the minimum amount needed to resolve the whole flame structure. This shows that even with a low Reynolds number and a minimum flame thickness DNS of the flow, combined with a simple chemistry approach, is only possible when $Ka < 1$ i.e. in the thin reaction zones regime as described in section 2.2. To overcome this limitation and to reach higher Reynolds numbers and thinner flames, we used the G -equation approach, discussed in section 2.5. When we use the G -equation, we do not have to resolve the reaction zone on our numerical grid, but we assume a certain temperature profile, which can be represented on three to four grid points and lead to the possibility to reach higher Karlovitz numbers.

The whole system of equations which we solve numerically is discussed in the sections 2.5 and 2.6, so we will just summarise the system here. The system

consists of the G -equation, (2.18),

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = s_f |\nabla G|. \quad (3.1)$$

conservation of mass, equation (2.27),

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{m} = 0. \quad (3.2)$$

the momentum equations (2.28)

$$\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{m} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (3.3)$$

and an equation of state (2.34)

$$\rho = \frac{1}{T}. \quad (3.4)$$

In section 3.2 the numerical method to solve this set of equations is described. First the temporal discretisation is discussed, followed by the spatial discretisation. In section 3.4 will show us some results of the performance of this model on parallel computers.

3.2 Numerical method

The set of equations (2.27), (2.28) and (2.18) is solved with a second order accurate finite volume method on a staggered grid. For the temporal discretisation, a second order accurate explicit predictor-corrector method is used, which is described in section 3.2.1. The spatial discretisation is described in the sections 3.2.3 and 3.2.5. The numerical method used for the spatial discretisation is the Finite Volume Method (FVM), (Hirsch, 1988). The numerical domain is divided in small control volumes or grid cells, and for each of the cells the conservation and transport equations are applied. This way a lot of physical properties of the problem, like conservation of mass, are maintained in the discrete description and its solution.

3.2.1 Temporal discretisation

Flows with variable density can cause instability in the numerical method. Since an implicit method is too expensive to be applied in a DNS, we used an explicit predictor-corrector time stepping scheme for the integration in time. This

scheme is used by Najm et al. (1998) and has the advantage that it is stable for large values of the heat release parameter τ . A detailed description of this method is given below.

Predictor step

The predicted values on the new time step are denoted with $*$ and are computed with an Adams-Bashfort scheme. So the prediction of G -field reads

$$\frac{G^* - G^n}{\Delta t} = \frac{3}{2} \left. \frac{\partial G}{\partial t} \right|^n - \frac{1}{2} \left. \frac{\partial G}{\partial t} \right|^{n-1}, \quad (3.5)$$

A similar scheme can be written for the momentum equation. However, both after the prediction and correction time step the resulting mass flux $\mathbf{m}$ is only an intermediate value, denoted with $\mathbf{m}'$ for the prediction step and $\mathbf{m}''$ for the correction step. The intermediate value of the predicted mass flux is also obtained with an Adams-Bashfort scheme

$$\frac{\mathbf{m}' - \mathbf{m}^n}{\Delta t} = \frac{3}{2} \left. \frac{\partial \mathbf{m}}{\partial t} \right|^n - \frac{1}{2} \left. \frac{\partial \mathbf{m}}{\partial t} \right|^{n-1} \quad (3.6)$$

A pressure projection step is applied to the intermediate value $\mathbf{m}'$ in order to enforce conservation of mass:

$$\frac{\mathbf{m}^* - \mathbf{m}'}{\Delta t} = -\nabla p^*. \quad (3.7)$$

Taking the divergence of (3.7) together with

$$\left. \frac{\partial \rho}{\partial t} \right|^* + \nabla \cdot \mathbf{m}^* = 0 \quad (3.8)$$

gives

$$\frac{\nabla \cdot \mathbf{m}' + \left. \frac{\partial \rho}{\partial t} \right|^*}{\Delta t} = \nabla^2 p^* \quad (3.9)$$

which has the form of a Poisson equation for the pressure. The solution of this equation will be discussed in section 3.3.3. $\left. \partial \rho / \partial t \right|^*$ cannot be evaluated directly and is given by the following second order backward discretisation in time:

$$\left. \frac{\partial \rho}{\partial t} \right|^* = \frac{1}{2\Delta t} (3\rho^* - 4\rho^n + \rho^{n-1}) \quad (3.10)$$

We solve the system for the pressure and correct the intermediate velocity by using (3.7) which gives us a prediction of the mass flux on the new time $\mathbf{m}^*$. We can compute the velocity from the mass flux and the density.

This is the usual projection method, as is applied in the case of incompressible flows. The predictor step is known to be stable for temperature and density ratios up to 2. Najm et al. (1998). For higher density ratios, a corrector step is needed to stabilise the scheme.

Corrector step

The correction step uses a Crank-Nicolson scheme where the predicted values, denoted with $*$, are used as the values on the new time. This step is also called a quasi Crank-Nicolson step, since the scheme remains explicit, while a Crank-Nicolson scheme is implicit.

The correction step for the G -field reads:

$$\frac{G^{n+1} - G^n}{\Delta t} = \frac{1}{2} \left(\left. \frac{\partial G}{\partial t} \right|^n + \left. \frac{\partial G}{\partial t} \right|^* \right) \quad (3.11)$$

The intermediate mass flux of the correction step $\mathbf{m}''$ is given by

$$\frac{\mathbf{m}'' - \mathbf{m}^n}{\Delta t} = \frac{1}{2} \left(\left. \frac{\partial \mathbf{m}}{\partial t} \right|^n + \left. \frac{\partial \mathbf{m}}{\partial t} \right|^* \right) \quad (3.12)$$

where the estimate of the temporal derivative on the new time step is based on the discretisation of the predicted mass flux and velocity field according to

$$\left. \frac{\partial \mathbf{m}}{\partial t} \right|^* = -\nabla(\mathbf{m}^* \mathbf{u}^*) + \nabla \cdot \boldsymbol{\tau}^* \quad (3.13)$$

with the method described in section 3.2.5. The pressure is now solved, using density on the new time step,

$$\frac{\nabla \cdot \mathbf{m}'' + \left. \frac{\partial \rho}{\partial t} \right|^{n+1}}{\Delta t} = \nabla^2 p^{n+1} \quad (3.14)$$

and corrected with

$$\frac{\mathbf{m}^{n+1} - \mathbf{m}''}{\Delta t} = -\nabla p^{n+1}, \quad (3.15)$$

Figure 3.1: The numerical stability of the Predictor-Corrector (P-C), compared with Adams-Bashfort 2 (AB2). Courtesy of B.J. Boersma

where

$$\left. \frac{\partial \rho}{\partial t} \right|^{n+1} = \frac{1}{2\Delta t} (3\rho^{n+1} - 4\rho^n + \rho^{n-1}). \quad (3.16)$$

In figure 3.1, the stability of the Predictor-Corrector method described above is compared with the stability of the 2nd order Adams-Bashfort method. This figure shows that the Predictor-Corrector method is stable for pure advection equations like the G -equation, i.e. for Eigenvalues which lay on the imaginary axis. The AB 2 method is strictly spoken not stable for pure advection, so the stability is increased considerably by using the Predictor-Corrector method. The time step is determined with

$$\Delta t \leq \frac{C}{\left| \frac{u}{\Delta x} \right| + \left| \frac{v}{\Delta y} \right| + \left| \frac{w}{\Delta z} \right| + \frac{1}{Re} \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)}, \quad (3.17)$$

where the Courant number $C = 0.50$ is used.

Figure 3.2: Control volume of the finite volume discretisation of the G -equation.

3.2.2 Numerical grid

The equations are discretised on an orthogonal staggered spatial grid, which means that different quantities are defined on different positions on the grid, as is shown in figure 3.2. This figure shows that the quantities G and ρ are defined at the centre of the grid cells. The pressure p is defined at this position. The different components of the mass flux and the velocity m_x, m_y, m_z, u, v and w are defined on the different faces of the cell. This has the advantage that spurious pressure oscillations do not occur. The grid cells are indicated with the indices i, j and k in the x, y and z -direction. Due to the fact that a staggered grid is used, interpolation of certain quantities to the position of another quantity during the numerical procedure is needed. In order to indicate that a quantity needs to be interpolated, it will be indicated with the index $\pm 1/2$ in the following section.

In order to increase the numerical resolution in certain areas of the geometry, e.g. in the vicinity of walls and obstacles, grid refinement can be applied. When this is done, the grid spacing is no longer uniform, which means that the position of the cell surface is not exactly in the middle between two cell centres. This results in the following interpolation coefficient, when a quantity which is defined in the cell centre, needs to be interpolated on the cell surface:

$$f_{xi} = \frac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}}, \quad f_{yj} = \frac{\Delta y_{j+1}}{\Delta y_j + \Delta y_{j+1}}, \quad f_{zk} = \frac{\Delta z_{k+1}}{\Delta z_k + \Delta z_{k+1}}. \quad (3.18)$$

In case of a uniform grid, the position of the interpolated value does lay exactly in the middle between the two cell centres, resulting in a value of f_x , f_y and f_z of $1/2$.

3.2.3 Spatial discretisation of the G -equation

The numerical method used for the spatial discretisation is the Finite Volume Method (FVM), which means that the numerical domain is divided in small control volumes or grid cells, (Hirsch, 1988). For each of the cells the conservation and transport equations are applied. In this way many of physical properties of problem, like conservation of mass, are maintained in the discrete problem and in the solution of the discrete problem. Let us now consider the spatial discretisation of the G -equation. The G -equation, equation (2.18) has the form of a hyperbolic differential equation with a source term in the right hand side. This source term has the form of an advection term as

$$s_f |\nabla G| = s_f \frac{(\nabla G)^2}{|\nabla G|} = -s_f \mathbf{n} \cdot \nabla G, \quad (3.19)$$

where $\mathbf{n}$ is the normal vector of an isosurface of G ,

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}. \quad (3.20)$$

The G -equation can now be rewritten as

$$\frac{\partial G}{\partial t} + \mathbf{u}_e \cdot \nabla G = 0, \quad (3.21)$$

where $\mathbf{u}_e$ is the effective velocity, defined by

$$\mathbf{u}_e = \mathbf{u} + s_f \mathbf{n} \quad (3.22)$$

Since a finite volume method is used, it is convenient to write the G -equation in conservative form:

$$\frac{\partial G}{\partial t} + \nabla \cdot (\mathbf{u}_e G) = (\nabla \cdot \mathbf{u}_e) G \quad (3.23)$$

When we look for a numerical solution of this equation, we have to use the effective velocity $\mathbf{u}_e = \mathbf{u} + \mathbf{n} s_f$ instead of $\mathbf{u}$ in our advection scheme, in order to compute the fluxes through the cell faces of the control volume. In figure 3.2, a

sketch of a 2 dimensional control volume is plotted. In order to obtain the rate of change of G on the position i, j , the fluxes $u_e G$ through the cell surface has to be obtained. The values of the different velocity components are located on the cell surfaces of the control volume. The values of G on the cell surface are denoted with the $+$ or $-1/2$. So the value of G at the position of the velocity $u_{i,j}$ is denoted with $G_{i+1/2,j}$ and the value of G at the position of the velocity $v_{i,j-1}$ is denoted with $G_{i,j-1/2}$. Since the values of G are defined in the cell centre, the values of G on the cell surface, or other values which are denoted with the indices $\pm 1/2$ have to be obtained by interpolation.

The numerical approximation of spatial derivatives in (3.23) are obtained with the help of following procedure:

- Compute and store the components of the normal vector $\mathbf{n}$, which are denoted as n_x , n_y and n_z .
- Compute κ with n_x , n_y and n_z , compute S with n_x , n_y , n_z , u , v and w . Use κ and S and ρ to compute s_f and store the value of s_f .
- Compute and store u_e , v_e and w_e by means of s_f , n_x , n_y , n_z , u , v and w .
- Compute the fluxes uG on the cell faces by means of a total variance diminishing (TVD) scheme, based on the Van Leer limiter.
- Compute $\frac{\partial G}{\partial t}$.

Each of these steps are described in the sections below.

The computation of $\mathbf{n}$

The different components of the normal vector $\mathbf{n}$ are obtained with

$$n_{x\ i,j,k} = -\frac{\frac{G_{i+1,j,k} - G_{i,j,k}}{\Delta x h_i}}{\sqrt{(\nabla G)_{i+\frac{1}{2},j,k}^2}}, \quad n_{y\ i,j,k} = -\frac{\frac{G_{i,j,k+1} - G_{i,j,k}}{\Delta y h_j}}{\sqrt{(\nabla G)_{i,j+\frac{1}{2},k}^2}} \quad (3.24)$$

and

$$n_{z\ i,j,k} = -\frac{\frac{G_{i,j+1,k} - G_{i,j,k}}{\Delta z h_k}}{\sqrt{(\nabla G)_{i,j,k+\frac{1}{2}}^2}}.$$

The values of $|\nabla G| = \sqrt{(\nabla G)^2}$ again have to be obtained on each of the cell faces, which means that each of the components of ∇G has to be obtained on each of the cell faces. This results in a rather complicated expression for each of the cell faces:

$$\begin{aligned}
 (\nabla G)_{i+\frac{1}{2},j,k}^2 &= \left(\frac{G_{i+1,j,k} - G_{i,j,k}}{\Delta x h_i} \right)^2 + \\
 &\left(f_{y_j} \frac{G_{i,j+1,k} - G_{i,j-1,k}}{\Delta y h_j + \Delta y h_{j+1}} + (1 - f_{y_j}) \frac{G_{i+1,j+1,k} - G_{i+1,j-1,k}}{\Delta y h_j + \Delta y h_{j+1}} \right)^2 + \\
 &\left(f_{z_k} \frac{G_{i,j,k+1} - G_{i,j,k-1}}{\Delta z h_k + \Delta z h_{k+1}} + (1 - f_{z_k}) \frac{G_{i+1,j,k+1} - G_{i+1,j,k-1}}{\Delta z h_k + \Delta z h_{k+1}} \right)^2 + \\
 (\nabla G)_{i,j+\frac{1}{2},k}^2 &= \\
 &\left(f_{y_j} \frac{G_{i+1,j,k} - G_{i-1,j,k}}{\Delta x h_i + \Delta x h_{i+1}} + (1 - f_{y_j}) \frac{G_{i+1,j+1,k} - G_{i-1,j+1,k}}{\Delta x h_i + \Delta x h_{i+1}} \right)^2 + \\
 &\left(\frac{G_{i,j+1,k} - G_{i,j,k}}{\Delta y h_j} \right)^2 + \\
 &\left(f_{y_j} \frac{G_{i,j,k+1} - G_{i,j,k-1}}{\Delta z h_k + \Delta z h_{k+1}} + (1 - f_{y_j}) \frac{G_{i,j+1,k+1} - G_{i,j+1,k-1}}{\Delta z h_k + \Delta z h_{k+1}} \right)^2 \\
 (\nabla G)_{i,j,k+\frac{1}{2}}^2 &= \\
 &\left(f_{z_k} \frac{G_{i+1,j,k} - G_{i-1,j,k}}{\Delta x h_i + \Delta x h_{i+1}} + (1 - f_{z_k}) \frac{G_{i+1,j,k+1} - G_{i-1,j,k+1}}{\Delta x h_i + \Delta x h_{i+1}} \right)^2 + \\
 &\left(f_{z_k} \frac{G_{i,j+1,k} - G_{i,j-1,k}}{\Delta y h_j + \Delta y h_{j+1}} + (1 - f_{z_k}) \frac{G_{i,j+1,k+1} - G_{i,j-1,k+1}}{\Delta y h_j + \Delta y h_{j+1}} \right)^2 + \\
 &\left(\frac{G_{i,j,k+1} - G_{i,j,k}}{\Delta z h_k} \right)^2. \tag{3.25}
 \end{aligned}$$

Due to the reinitialisation procedure in section 2.5.3, $|\nabla G| \approx 1$. The computation of (3.25) could be discarded if $|\nabla G| = 1$ is assumed. However the reinitialisation procedure is an approximation and there might be a slight deviation from this assumption. This deviation results in an error in the estimation of the propagation velocity of the flame. Therefore it is necessary to compute $|\nabla G|$ with the approximation of equation (3.25).

The discretisation of the flame speed s_f

In order to obtain u_e with equation (3.29), we have to compute the flame speed s_f , which is given by equation (2.25). The numerical values of $s_{f,i,j,k}$ are defined at the cell centre, at the same position of $G_{i,j,k}$. In order to compute $s_{f,i,j,k}$, we first determine $\kappa_{i,j,k}$ with

$$\kappa_{i,j,k} = \frac{n_{xi,j,k} - n_{xi-1,j,k}}{\Delta x_i} + \frac{n_{yi,j,k} - n_{yi,j-1,k}}{\Delta y_j} + \frac{n_{zi,j,k} - n_{zi,j,k-1}}{\Delta z_k}. \quad (3.26)$$

The strain rate S , defined in equation (2.23), is also defined at the same position as $G_{i,j,k}$. The full expression for $S_{i,j,k}$ reads

$$\begin{aligned} S_{i,j,k} = & - \left(n_{xc,i,j,k} \frac{\partial u}{\partial x} \bigg|_{i,j,k} + n_{yc,i,j,k} \frac{\partial u}{\partial y} \bigg|_{i,j,k} + n_{zc,i,j,k} \frac{\partial u}{\partial z} \bigg|_{i,j,k} \right) n_{xc,i,j,k} \\ & - \left(n_{xc,i,j,k} \frac{\partial v}{\partial x} \bigg|_{i,j,k} + n_{yc,i,j,k} \frac{\partial v}{\partial y} \bigg|_{i,j,k} + n_{zc,i,j,k} \frac{\partial v}{\partial z} \bigg|_{i,j,k} \right) n_{yc,i,j,k} \quad (3.27) \\ & - \left(n_{xc,i,j,k} \frac{\partial w}{\partial x} \bigg|_{i,j,k} + n_{yc,i,j,k} \frac{\partial w}{\partial y} \bigg|_{i,j,k} + n_{zc,i,j,k} \frac{\partial w}{\partial z} \bigg|_{i,j,k} \right) n_{zc,i,j,k}, \end{aligned}$$

where the spatial derivatives $\frac{\partial u}{\partial x}$, $\frac{\partial v}{\partial y}$ and $\frac{\partial w}{\partial z}$ are obtained directly, while $\frac{\partial u}{\partial y}$, $\frac{\partial u}{\partial z}$, $\frac{\partial v}{\partial x}$, $\frac{\partial v}{\partial z}$, $\frac{\partial w}{\partial x}$ and $\frac{\partial w}{\partial y}$ are obtained by interpolation. The values of n_{xc} , n_{yc} and n_{zc} on the cell centre are also obtained by a linear interpolation of n_x , n_y and n_z , which are defined at the cell surfaces.

Computation of u_e

The different components of u_e are now obtained with

$$\begin{aligned} u_{e,i,j,k} &= u_{i,j,k} + f_{xi} s_{f,i,j,k} + (1 - f_{xi}) s_{f,i+1,j,k} n_{xi,j,k} \\ v_{e,i,j,k} &= v_{i,j,k} + f_{yj} s_{f,i,j,k} + (1 - f_{yj}) s_{f,i,j+1,k} n_{yi,j,k} \quad (3.28) \\ w_{e,i,j,k} &= w_{i,j,k} + f_{zk} s_{f,i,j,k} + (1 - f_{zk}) s_{f,i,j,k+1} n_{zi,j,k}. \end{aligned}$$

s_f is defined at the position of the cell centre with equation 2.25. In order to obtain the values of s_f in the cell faces, s_f a linear interpolation is applied, where f_x , f_y and f_z are the interpolation coefficients defined by (3.18).

Computation of the advective fluxes $u_e G$

Since equation (3.23) is an advection equation, without diffusion we cannot discretise this equation with a central scheme. Instead of that, the advection terms are discretised with a total variance diminishing (TVD) scheme, (Hirsch, 1988). The advantage of a TVD scheme is, that it preserves monotonicity and does not produce non-physical oscillations. The upwind TVD scheme we used is based on a limiter, which screens the G -field and decides which numerical scheme will be used for the interpolation of the value $G_{i+\frac{1}{2}}$. In smooth regions of G , a higher-order method will be used, while in non-smooth parts, where an higher order method can cause oscillations, a first-order upwind method will be used. When it is assumed that $u_{e,i,j,k} > 0$, this scheme reads

$$G_{i+\frac{1}{2},j,k} = G_{i,j,k} + \frac{1}{2}\phi(r_{i+\frac{1}{2},j,k})(G_{i,j,k} - G_{i-1,j,k}) \quad (3.29)$$

with

$$r_{i+\frac{1}{2},j,k} = \frac{G_{i+1,j,k} - G_{i,j,k}}{G_{i,j,k} - G_{i-1,j,k}}. \quad (3.30)$$

The first term on the right hand side of (3.29) denotes the upwind term, which is known to be diffusive. The second term on the right hand side, containing the flux limiter ϕ , is an anti diffusive term. From the literature, several expressions of ϕ are known (Hirsch, 1988). In our code we used the Van Leer flux limiter, given by:

$$\phi(r) = \frac{r + |r|}{r + 1}. \quad (3.31)$$

As a result of the reinitialisation procedure, described in section 2.5.3, $|\nabla G| = 1$, which means that the G -field is quite smooth. Therefore the limiter will not have to switch to the first-order upwind scheme in order to maintain a smooth solution. We performed some preliminary test, which showed that it is even possible to use a central scheme for the advection, in combination with the reinitialisation procedure. However, due to the fact that there were no visible differences between the structures on the flame between the two methods and the fact that the TVD scheme was more robust, we decided to use the TVD scheme for all the simulations presented in this thesis.

Computation of $\frac{\partial G}{\partial t}$

$\frac{\partial G}{\partial t}$ can now be obtained with

$$\frac{\partial G_{i,j,k}}{\partial t} =$$

$$\begin{aligned}
& \frac{u_{ei-1,j,k}G_{i-\frac{1}{2},j,k} - u_{ei,j,k}G_{i+\frac{1}{2},j,k}}{\Delta x_i} + G_{i,j,k} \frac{u_{ei,j,k} - u_{ei-1,j,k}}{\Delta x_i} \\
& \frac{v_{ei,j-1,k}G_{i,j-\frac{1}{2},k} - v_{ei,j,k}G_{i,j+\frac{1}{2},k}}{\Delta y_j} + G_{i,j,k} \frac{v_{ei,j,k} - v_{ei,j-1,k}}{\Delta y_j} \\
& \frac{w_{ei-1,j,k}G_{i-\frac{1}{2},j,k} - w_{ei,j,k}G_{i,j,k+\frac{1}{2}}}{\Delta z_k} + G_{i,j,k} \frac{w_{ei,j,k} - w_{ei,j,k-1}}{\Delta z_k}.
\end{aligned} \tag{3.32}$$

3.2.4 Reinitialisation of G

As mentioned in section 2.5.3, we apply a reinitialisation procedure, to the G -equation. The procedure is proposed by Sussman et al. (1994) and results in a G -field for which $|\nabla G| = 1$, while the level $G(\mathbf{x}, t) = G_0$ is not changed, i.e. the position of the flame front is not affected. This is achieved by solving equation (2.26), which reads

$$\frac{\partial G}{\partial t} = S(G^0 - G_0) (1 - |\nabla G|), \tag{3.33}$$

until steady state is reached. With G^0 , the initial G -field at the start of the reinitialisation procedure is indicated. $S(\dots)$ is the sign function, which we estimate by

$$S(G) = \frac{G}{\sqrt{G^2 + \epsilon^2}}, \tag{3.34}$$

where ϵ is determined, depending on the grid spacing, with

$$\epsilon = \max(\max(\Delta x), \max(\Delta y), \max(\Delta z)). \tag{3.35}$$

Note that in our case $G_0 = 0$. The time step to solve (2.26) is also determined, depending in the grid spacing with

$$\Delta t = \frac{\epsilon}{10}. \tag{3.36}$$

We use the method, described by Sussman et al., who determine the spatial derivatives in equation (2.26), depending on the value of $G_{i,j,k}$. If $G_{i,j,k} < 0$ than

$$\begin{aligned}
\left. \frac{\partial G}{\partial x} \right|_{i+\frac{1}{2},j,k} &= \max \left(\frac{G_{i+1,j,k} - G_{i,j,k}}{\Delta x h_i}, 0 \right) \\
\left. \frac{\partial G}{\partial x} \right|_{i-\frac{1}{2},j,k} &= \min \left(\frac{G_{i,j,k} - G_{i-1,j,k}}{\Delta x h_{i-1}}, 0 \right)
\end{aligned}$$

$$\begin{aligned}
\left. \frac{\partial G}{\partial y} \right|_{i,j+\frac{1}{2},k} &= \max \left(\frac{G_{i,j+1,k} - G_{i,j,k}}{\Delta y h_j}, 0 \right) \\
\left. \frac{\partial G}{\partial y} \right|_{i,j-\frac{1}{2},k} &= \min \left(\frac{G_{i,j,k} - G_{i,j-1,k}}{\Delta y h_{j-1}}, 0 \right) \\
\left. \frac{\partial G}{\partial z} \right|_{i,j,k+\frac{1}{2}} &= \max \left(\frac{G_{i,j,k+1} - G_{i,j,k}}{\Delta z h_k}, 0 \right) \\
\left. \frac{\partial G}{\partial z} \right|_{i,j,k-\frac{1}{2}} &= \min \left(\frac{G_{i,j,k} - G_{i,j,k-1}}{\Delta z h_{k-1}}, 0 \right)
\end{aligned}$$

and if $G_{i,j,k} > 0$ than

$$\begin{aligned}
\left. \frac{\partial G}{\partial x} \right|_{i+\frac{1}{2},j,k} &= \min \left(\frac{G_{i+1,j,k} - G_{i,j,k}}{\Delta x h_i}, 0 \right) \\
\left. \frac{\partial G}{\partial x} \right|_{i-\frac{1}{2},j,k} &= \max \left(\frac{G_{i,j,k} - G_{i-1,j,k}}{\Delta x h_{i-1}}, 0 \right) \\
\left. \frac{\partial G}{\partial y} \right|_{i,j+\frac{1}{2},k} &= \min \left(\frac{G_{i,j+1,k} - G_{i,j,k}}{\Delta y h_j}, 0 \right) \\
\left. \frac{\partial G}{\partial y} \right|_{i,j-\frac{1}{2},k} &= \max \left(\frac{G_{i,j,k} - G_{i,j-1,k}}{\Delta y h_{j-1}}, 0 \right) \\
\left. \frac{\partial G}{\partial z} \right|_{i,j,k+\frac{1}{2}} &= \min \left(\frac{G_{i,j,k+1} - G_{i,j,k}}{\Delta z h_k}, 0 \right) \\
\left. \frac{\partial G}{\partial z} \right|_{i,j,k-\frac{1}{2}} &= \max \left(\frac{G_{i,j,k} - G_{i,j,k-1}}{\Delta z h_{k-1}}, 0 \right). \tag{3.37}
\end{aligned}$$

The values of different components of ∇G on the position of the cell centre are now determined with

$$\begin{aligned}
\left(\left. \frac{\partial G}{\partial x} \right|_{i,j,k} \right)^2 &= \max \left(\left. \frac{\partial G}{\partial x} \right|_{i-\frac{1}{2},j,k}^2, \left. \frac{\partial G}{\partial x} \right|_{i+\frac{1}{2},j,k}^2 \right) \\
\left(\left. \frac{\partial G}{\partial y} \right|_{i,j,k} \right)^2 &= \max \left(\left. \frac{\partial G}{\partial y} \right|_{i,j-\frac{1}{2},k}^2, \left. \frac{\partial G}{\partial y} \right|_{i,j+\frac{1}{2},k}^2 \right) \\
\left(\left. \frac{\partial G}{\partial z} \right|_{i,j,k} \right)^2 &= \max \left(\left. \frac{\partial G}{\partial z} \right|_{i,j,k-\frac{1}{2}}^2, \left. \frac{\partial G}{\partial z} \right|_{i,j,k+\frac{1}{2}}^2 \right)
\end{aligned} \tag{3.38}$$

The value of G on the new time $m + 1$ is now determined with

$$G_{i,j,k}^{m+1} = G_{i,j,k}^m - S(G_{i,j,k}^0) \left(1 - \sqrt{\left(\frac{\partial G}{\partial x} \Big|_{i,j,k}^m \right)^2 + \left(\frac{\partial G}{\partial y} \Big|_{i,j,k}^m \right)^2 + \left(\frac{\partial G}{\partial z} \Big|_{i,j,k}^m \right)^2} \right) \Delta t \quad (3.39)$$

Equation (3.39) can be applied, until a certain stopping criterion, e.g. the one proposed by Sussman et al., is reached. However since the time step in our DNS is quite small, we chose to perform only one iteration each time the reinitialisation procedure is applied.

3.2.5 Spatial discretisation of the mass flux m

The mass flux m is also discretised with a second order finite volume method. Only the mass flux in the x -direction, m_x is considered here. The y and z -components, m_y and m_z are treated analog. In figure 3.3 a 2 dimensional control volume of m_x is plotted. The 3 dimensional discretisation is written below. The equation to discretise is equation (2.28), which can also be written as

$$\frac{\partial m}{\partial t} = \nabla \cdot (-\mathbf{u}m + \boldsymbol{\tau}) \quad (3.40)$$

with

$$\boldsymbol{\tau} = \frac{1}{Re} \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right). \quad (3.41)$$

The spatial discretisation of m_x now reads:

$$\begin{aligned} \frac{\partial m_{x i,j,k}}{\partial t} = & - \frac{u_{i+\frac{1}{2},j,k} m_{x i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k} m_{x i-\frac{1}{2},j,k}}{\Delta x h_i} \\ & + \frac{\tau_{xx i+\frac{1}{2},j,k} - \tau_{xx i-\frac{1}{2},j,k}}{\Delta x h_i} \\ & - \frac{v_{i+\frac{1}{2},j,k} m_{x i,j+\frac{1}{2},k} - v_{i+\frac{1}{2},j-1,k} m_{x i,j-\frac{1}{2},k}}{\Delta y_j} \\ & + \frac{\tau_{yx i,j+\frac{1}{2},k} - \tau_{yx i,j-\frac{1}{2},k}}{\Delta y_j} \\ & - \frac{w_{i+\frac{1}{2},j,k} m_{x i,j,k+\frac{1}{2}} - w_{i+\frac{1}{2},j,k-1} m_{x i,j,k-\frac{1}{2}}}{\Delta z_k} \end{aligned} \quad (3.42)$$

Figure 3.3: Control volume of the finite volume discretisation of the momentum equation in 2 dimensions.

$$+ \frac{\tau_{zx_{i,j,k+\frac{1}{2}}} - \tau_{zx_{i,j,k-\frac{1}{2}}}}{\Delta z_k},$$

where the different components of the velocity and mass flux which are indicated with the indices $\pm 1/2$ are obtain by means of linear interpolation. The different components of the stress tensor are obtained with

$$\begin{aligned}\tau_{xx_{i+\frac{1}{2},j,k}} &= \frac{1}{Re} \left(2 \frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x_{i+1}} - \frac{2}{3} \Delta_{i+1,j,k} \right) \\ \tau_{yx_{i,j+\frac{1}{2},k}} &= \frac{1}{Re} \left(\frac{u_{i,j+1,k} - u_{i,j,k}}{\Delta y h_j} + \frac{v_{i+1,j,k} - v_{i,j,k}}{\Delta x h_i} \right) \\ \tau_{zx_{i,j,k+\frac{1}{2}}} &= \frac{1}{Re} \left(\frac{w_{i,j,k+1} - w_{i,j,k}}{\Delta z h_k} + \frac{w_{i+1,j,k} - w_{i,j,k}}{\Delta x h_i} \right),\end{aligned}\quad (3.43)$$

with

$$\Delta_{i,j,k} = \frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x_i} + \frac{v_{i,j+1,k} - v_{i,j,k}}{\Delta y_j} + \frac{w_{i,j,k+1} - w_{i,j,k}}{\Delta z_k} \quad (3.44)$$

3.3 Parallelisation

3.3.1 Division of the grid

The numerical method is parallelised with the Message Passing Interface library using a domain decomposition approach. This means that the computational domain is divided in subdomains, see figure 3.4, and the subdomains are divided over the different nodes of a parallel computer. The method is applied in two different geometries. Geometry 1 is a simple box with periodic boundary conditions in the y - and z -direction. In the x -direction, inflow and outflow boundary conditions are used. This geometry is used to study the interaction of the flame front with homogeneous turbulence, which is described in chapter 4 of this thesis. The upper part of figure 3.4 shows how the numerical grid is divided over a grid of CPU's. The redistribution shown in this figure is only applied to the pressure field and is needed to solve the Poisson equations 3.9 and 3.14 efficiently. This will be discussed in section 3.3.3

Geometry 2 is used to compute the flow and the development of the flame front around a square cylinder. The cylinder axis is in the y -direction. In this direction, periodic boundary conditions are applied. $x = 0$ is a no slip boundary and $x = x_{max}$ is an outflow boundary. At $z = 0$ and $z = z_{max}$ free slip boundary conditions are applied. No redistribution of the pressure is needed in this case, as will be discussed in section 3.3.3.

Figure 3.4: Distributions used to divide the data over the CPU's. The upper distribution is used for geometry 1. A redistribution is needed to allow efficient execution of FFT's in the y - and z -direction to solve the Poisson equation for the pressure. The lower distribution is used for geometry 2. No redistribution is needed when an iterative parallel solver is used to solve the pressure.

3.3.2 Parallel implementation

The method can be implemented on a parallel computer very efficiently, since explicit time stepping is used to compute the intermediate mass fluxes and updating the G -field, which avoids solving global systems of equations. Now only local variables, which are available from the local memory of the node, are needed for computing m' , m'' , G^* and G^{n+1} . The variables ρ^* , ρ^{n+1} , u^* and u^{n+1} are computed from the local variables m and G so there is no communication between the different CPU's involved in computing these variables. The only communication needed to compute these variables is the exchange of the values in the overlaying regions, also called halo regions or ghost cells, at the boundaries of the subdomains.

3.3.3 The Poisson equation for the pressure

The only part of the system which is more complicated to implement on a parallel computer is the solution of the Poisson problems (3.9) and (3.14). Since these are global systems of equations, some communication between the different nodes on a parallel computer is unavoidable.

In geometry 1, a fast direct method can be applied. Since there are periodic

directions in the y - and z -directions, Fourier transforms can be applied in these directions. This reduces the system to a system of uncoupled tridiagonal systems. These can be solved straightforward. After applying the backwards Fourier transform, the desired pressure field is found. In order to perform the FFT's efficiently, all the values of p in the direction of the FFT need to be available on a single CPU performing the FFT. That is why the pressure field needs to be redistributed as shown in figure 3.4. This redistribution is the least efficient part from a parallel computing point of view. However on computers with a fast network, it does not spoil the parallel efficiency as will be shown in section 3.4. Gauss elimination and back substitution, which is needed to solve the tridiagonal systems, spans all the nodes, which means that back substitution is done in a serial way. This means that the back substitution is started on the first node. When this node is finished, an intermediate result is passed to the next node, which start the back substitution, until all the nodes are finished. At first sight one would expect this part of the method to scale very bad. In practise however no scaling problems were observed, when this method is applied.

Another option is to use the distribution in the Poisson solver, which is the second distribution for geometry 1 in figure 3.4 for the whole computation. That way, no redistribution would be needed at all. This distribution however showed to be less efficient for a large number of CPU's, since the halo regions of each CPU becomes relatively large, while for a small amount of CPU's there was hardly any difference between the efficiency of the two distributions.

In geometry 2 the Poisson problem is solved with a different method. First we start by performing a Fourier transform in the periodic y -direction. This results in a 2-dimensional system of equations for each Fourier mode. Because of the cylinder in the geometry, efficient direct methods can no longer be applied. Therefore the remaining 2-dimensional problems are solved using an iterative method. The PETSc library (Balay et al., 2000) is used to solve this problem in parallel. Although no redistribution is needed this way, the iterative method is less efficient than the direct method of geometry 1, since it uses more CPU time and requires more communication. Another way to implement the solver is to redistribute the 2-dimensional problems and let each CPU solve the 2-dimensional systems of one or a few Fourier modes. This might look more efficient, since no communication is needed to solve the 2-dimensional system, but it results in severe load balancing problems. This is due to the fact that the Fourier transform acts as a preconditioner for the 2-dimensional systems. The condition of the systems, associated with the higher Fourier modes is good, but the condition of the lower modes is not much increased. For a large number of CPU's this results in nearly all the CPU's waiting for the first few modes to be

converged. This is very inefficient and reduces the scalability.

3.4 Results

Figure 3.5 shows that the code scales very well for the different geometries on different machines. On a SGI Origin 3800, the code for geometry 1 for small and large grids scales linear or even better, due to cache effects. On a cluster of AMD Athlon 900 MHz PC's, connected with a switched 100 Mb network, the scaling is less, due to latency effects. No scaling data are available for the large grid on the PC cluster, since it did not fit on less than 8 nodes. Although the iterative solver in geometry 2 requires more communication, this geometry still scales very well on a SGI Origin 3800. On the PC cluster, no scaling data are available for this geometry, since the model did not fit on less than 8 nodes. However due to the nature of the communication in the iterative solver, which consist of a lot of relatively small messages, one can expect a less optimal scaling behaviour than for geometry 1 on the PC cluster. The iterative solver takes about 80 percent of the computing time and is 10 to 20 times slower than the direct solver, which takes about 20 percent of the time.

3.5 Conclusions

It is possible to study the interaction between turbulence and premixed combustion in detail with a Direct Numerical Simulations of the flow field, combined with the G -equation to model the flame front. The results confirm the known increase in turbulent flame speed with increasing turbulence intensities. Another interesting phenomenon is the increase in turbulent flame speed with increasing expansion coefficient.

The first results show that the code scales very well on parallel machines, which show promise for higher resolutions, more detailed simulations and more complex geometries.

(a) geometry 1

(b) geometry 2

Figure 3.5: Scaling of the code in the different geometries)

Chapter 4

Premixed Flames in Decaying Turbulence

In this chapter, the DNS model, described in chapter 2 and 3, is used to study a premixed flame in homogeneous isotropic decaying turbulence. This simulation is performed in a box geometry with two homogeneous directions. In the third direction, a realisation of a stationary, homogeneous isotropic turbulent simulation is used as an inflow boundary condition with an uniform inflow velocity U_{in} . In this geometry regions of shear in the mean flow field, which usually occur in the vicinity of walls, are avoided.

The mean position of the flame front is stabilised at a fixed position by adjusting the inflow velocity U_{in} . Such a stable position of the flame front gives us the ability to obtain accurate statistics by averaging in time together with averaging in the two homogeneous directions. The results show that the increase in turbulent flame speed depends on the turbulence intensity, as predicted by Damköhler (1940), but also depends on the expansion rate of the gas. This is due to the hydrodynamic instability process, which is triggered by disturbances on the flame front, caused by the turbulence in the flow. Further, the influence of the flame on the turbulent kinetic energy and enstrophy are presented.

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Figure 4.1: Sketch of the flow geometry.

4.1 Computational domain

The computational geometry is a box with sides L_x , L_y and L_z , with $L_y = L_z$ and $L_x = 4L_y$. A sketch of the geometry is given in figure 4.1. The mean flow is from left to right, while the flame front propagates in the opposite direction. A homogeneous isotropic turbulence field is fed into the channel at $x = 0$ with a velocity U_{in} , which, on average, is the same as the turbulent flame speed s_{ft} . The position of the flame front x_f is defined as

$$x_f = \frac{\int_V (x - G) dV}{V}. \quad (4.1)$$

where V is the total flow volume. This flame position is stabilised around the desired position x_0 by adjusting the inflow velocity U_{in} according to

$$\frac{dU_{in}}{dt} = \frac{d^2 x_f}{dt^2} = c_1(x_f - x_0) - c_2 \frac{dx_f}{dt}. \quad (4.2)$$

The acceleration of the fluid, dU_{in}/dt , and therefore of the flame front, $d^2 x_f/dt^2$, is proportional to the deviation $x_f - x_0$. This would give rise to a harmonic oscillation of x_f around x_0 . Therefore the system is damped by the dx_f/dt term. The parameters c_1 and c_2 determine the characteristics of the system and for $c_2 = 2c_1$ the system is critically damped. This means that the damping is strong enough to avoid unnecessary oscillations around x_0 , but not so strong as to avoid a too quick return to equilibrium. The constant c_1 can be chosen freely and determines the stiffness of the system. In this case we take $c_1 = 10$. With this value the position of the flame is fairly stable and varies no more than 2%

around its equilibrium position, while it gives no additional limitation of the time step.

In the remainder of this chapter, the length, velocity and time are made dimensionless with the length scale L_y and the laminar flame speed s_{fl} , unless mentioned otherwise.

Four types of simulations, called type I, II, III and IV, have been performed. In the first type we consider spatially decaying incompressible turbulence. A realisation of homogeneous isotropic turbulence in a periodic box, computed with a resolution of 128^3 , is used as an inflow boundary condition at $x = 0$. The inflow velocity at $x = 0$ is fixed to $U_{in} = 1$. The resolution of the type I simulation is $384 \times 128 \times 128$ in the x , y and z -direction, respectively. This simulation can be considered as a reference for decaying turbulence when no combustion effects are present.

The second type of simulation is performed with an imposed gas expansion with $\tau = (\rho_u - \rho_b)/\rho_b = 3$ at a fixed position at $x = 2.66$. As a result of the fixed position of the flame front, the inflow velocity U_{in} needs not to be adjusted to stabilise the flame front, but it remains constant with a value of $U_{in} = 1$. This case is not a realistic combustion simulation, since the flame front is not affected by the turbulence, but remains flat. This simulation is denoted as the 'flat flame' in the graphs.

The third type of simulations is performed to investigate whether the code is able to reproduce the Darrieus-Landau instability of the flame front. This can be considered a test of our code to check whether compressibility effects have been correctly incorporated. The simulations are performed on a two-dimensional geometry and are carried out by using our code with a minimal amount of grid points in the z -direction. We have used a resolution of $256 \times 128 \times 4$ on a domain of $2 \times 1 \times 0.03125$ in the x , y and z -direction. These tests are performed on a PC with on 900 MHz Athlon CPU. Each time step takes about 3 seconds and a run takes 1000 time steps.

In the fourth type of simulations, we carry out the full DNS of a turbulent flow including the interaction between the turbulence and the flame front. These simulations use the same turbulent inflow boundary conditions, as mentioned in the type I simulations. The simulations are performed on a grid in the domain shown in figure 4.1 with a resolution of $384 \times 128 \times 128$ on an SGI O3800 computer. The code is parallelised and runs on 32 nodes. Each time step takes about 5 wall clock CPU seconds. A run takes about 80000 time steps.

The statistical results to be presented below are obtained by taking an ensemble average over at least 50 realisations of the flow field. In order to eliminate the effect of the flame-front stabilisation, mentioned above, on the statistics we

compute the fluctuating quantities with respect to the mean of each realisation and not, as is often done, with respect to the total mean. This has the advantage that the fluctuations in U_{in} , which result from the stabilisation mechanism, and the fluctuations in the pressure gradient, which results from the change in the bulk velocity, give no contribution to the statistics of the velocity fluctuations and the pressure.

The realisation of homogeneous isotropic turbulence, which is applied as inflow boundary condition for the type I, II and IV simulations, is obtained from a pseudo spectral code used before by Brethouwer (2001). This simulation, which we will call the inflow field, has a Reynolds number of $Re_\lambda = 95$, where Re_λ is defined in terms of the rms velocity fluctuation by

$$v' = \sqrt{\frac{u_i^2}{3}}, \quad (4.3)$$

and the Taylor micro scale λ as

$$Re_\lambda = \frac{v'\lambda}{\nu}. \quad (4.4)$$

In this case, $\lambda = 0.0518L$ and the integral length scale $\ell = 0.174L$, where L is the length of the side of the cube, in which the simulation of the homogeneous isotropic turbulent flow field is carried out. The Reynolds number, based on ℓ and v' according to,

$$Re_\ell = \frac{v'\ell}{\nu} = \frac{\ell}{\lambda} Re_\lambda, \quad (4.5)$$

becomes $Re_\ell = 319$. From these data, one can compute the viscosity of the inflow field in order to set the correct parameters for the simulation of the combustion.

An overview of all the simulations of type I, II and IV that we have carried out, is shown in table 4.1. We see that various values for the inflow Reynolds number Re_ℓ have been used. For instance, all the simulation with $v' = 2.35$ have a Reynolds number of $Re_\ell = 818$, which means that the viscosity in the simulation is a factor 2.56 lower than the viscosity in the inflow field, which has a Reynolds number of $Re_\ell = 319$. For $v' = 2.35$, the viscosity is adjusted in order to lower the decay rate of the turbulence, which results in higher turbulence intensities at the position of the flame front. For the cases $v' = 1.17$ and $v' = 0.59$, the velocity of the inflow field is scaled with a factor of 0.5 and 0.25 respectively with respect to the case $v' = 2.35$, while the viscosity is kept

constant. This results in values of the Reynolds number of $Re_\ell = 409$ and $Re_\ell = 205$ as listed in table 4.1. A disadvantage of this approach is that the viscosity of the inflow field and the channel are not equal and the flow field in the channel has to adjust to the different viscosity. However, due to the artificial nature of the inflow boundary condition, the flow in the channel needs to adjust itself anyway, even when the viscosity of the inflow field and the channel match exactly. The effect of this flow adjustment can be seen in figures 4.12 and 4.17 where we show the decay of turbulent kinetic energy and the decay of the enstrophy, respectively. For $\tau = 3$ and $\tau = 5$ the decay of the turbulent kinetic energy is relatively low from $x = 0$ to $x = 0.5$, while in the same region and for the same values of τ , the enstrophy even shows an increase. However after $x = 0.5$, the flow behaves as a fully developed decaying turbulent flow and the effect of the boundary condition at $x = 0$ has disappeared. Therefore, the difference in viscosity between the inflow field and the actual simulation will have no influence at the position of the flame front, i.e. around $x = 2.66$.

4.2 Results of type I simulations (Decay of isotropic turbulence)

As a reference case we have computed the spatial decay of isotropic turbulence, which can be considered as a test of the numerical code. In figure 4.2 the decay of turbulent kinetic energy and its three components are shown as a function of the distance from the inflow boundary. The three components have about the same magnitude during the whole decay, which indicates that the turbulence remains indeed isotropic. By fitting a power law to the computational result, we find that the turbulent kinetic energy decays as x^{-n} with $n = 2.51$. This value is somewhat higher than the value given in e.g. George (1992), who mentions $n \simeq 2.1$.

From this decay, one can estimate the turbulent dissipation ϵ with help of Taylor hypothesis as:

$$\epsilon = -\frac{dk}{dt} = -U_{in} \frac{dk}{dx}. \quad (4.6)$$

The Kolmogorov length scale η , scaled with the size of the domain is then obtained from

$$\frac{\eta}{L_y} = \left(\frac{v'^3}{\ell \epsilon} Re_\ell^{-3} \right)^{\frac{1}{4}} \frac{\ell}{L_y}. \quad (4.7)$$

type	heat release included	heat release parameter τ at $x = 0$	turbulence intensity v'	Reynolds number Re_ℓ	inflow velocity U_{in}	position of flame $\bar{x}_f$	indicated with
I	no	0	2.35	818	1 (fixed)		$\tau = 0, U_{in} = 1$
II	yes	3	2.35	818	1 (fixed)	2.66	flat flame
IV	no	0	0.59	205	1.28	2.70	
IV	no	0	1.17	409	1.34	2.69	
IV	no	0	2.35	818	1.41	2.69	$\tau = 0$
IV	yes	1	2.35	818	1.88	2.62	$\tau = 1$
IV	yes	3	2.35	818	3.38	2.51	$\tau = 3$
IV	yes	5	2.35	818	4.44	2.59	$\tau = 5$

Table 4.1: Overview of the different types of 3D-simulations.

Figure 4.2: The turbulent kinetic energy k_t and its components as a function of x . The total energy is fitted with $k_t = a(x - x_0)^{-n}$, where $a = 1.10$, $x_0 = -0.35$ and $n = 2.51$.

Figure 4.3: The turbulent dissipation ϵ and the corresponding Kolmogorov length η as a function of x . The curves are obtained from the expression of the decay of kinetic energy, determined in figure 4.2, which leads to $\epsilon = 2.75(x + 0.35)^{-3.51}$

The ϵ and η are both plotted in figure 4.3. For $x > 4$ we find $\eta > 0.01$. With the help of the value for η estimated above, we can determine whether our DNS is fully resolved. The grid spacing in the x -direction is 0.0104 and in the y - and z -direction 0.0078 and these values are of the same order as the estimated Kolmogorov length scale. This means that our simulation is can not be regarded as fully resolved up to the Kolmogorov length. Nevertheless we feel that the resolution is sufficient to describe the relevant turbulence dynamics in view of the remarks made by Moin and Mahesh (1998).

4.3 Results of type III simulation (Flame front instability)

Let us now consider the simulation of the hydrodynamic instability discussed in section 2.3. The comparison of this simulation with the theory of section

heat release parameter τ	number of waves $n = L_y/\lambda$	wave number k	flame thickness δ	Figure
1.0	2	4π	0.02	4.5, 4.6 and 4.7
3.0	2	4π	0.02	4.5
5.0	2	4π	0.02	4.5
3.0	1	2π	0.02	4.6
3.0	3	6π	0.02	4.6
3.0	4	8π	0.02	4.6
1.0	2	4π	0.04	4.7
1.0	2	4π	0.1	4.7

Table 4.2: The different values of the parameters τ , k and δ used to study the growth of the disturbances by hydrodynamic instability of the flame front. The initial amplitude is always chosen $A_0 = 0.001$, except for the case $n = 1$, where $A_0 = 0.004$ is used.

2.3 is a check whether compressibility effects are realistically represented by our model and whether these are correctly incorporated in our numerical code. A series of simulations is carried out in the two-dimensional geometry, described in section 4.1. The initial value for the flow field is an undisturbed velocity $\mathbf{u}_0 = (s_f, 0, 0)$. The flame front is put at $x_0 = 1.5$ and on this flame front we impose a small wave-like perturbation with a dimensionless wave length λ and an amplitude A_0 . This leads to a G -field equal to $G = x - x_0 + A_0 \sin(ky)$ where k is the wave number $k = 2\pi/\lambda$. Note that $1/\lambda = n$ is the number of waves in the domain. The initial amplitude is put equal to $A_0 = 0.001$, so that $kA_0 \ll 1$ and $|\nabla G| \approx 1$. The position of the flame front is not stabilised, but $U_{in} = s_f$ is kept constant.

We have varied parameters τ , k and δ in order to study the influence of these parameters on the growth of the disturbances. In table 4.2 the parameters used in the various simulations are given.

In figure 4.4 the evolution of the flame front is plotted for several times after $t = 0$ for the case $\tau = 3$. In the initial stages of the growth, the disturbance keeps its wave-like form, but at later times the shape starts to deviate from a wave due to non-linearity. The flame front develops sharp spikes, pointing in the direction of the burnt gas. This shape is similar to the flame-front pattern that we have shown in figure 2.3 where we have argued that this is due to the Huygens effect which results from the fact that the flame propagates with

Figure 4.4: The evolution of the wave-like disturbance on a flat flame front with $n = 2$ and $A_0 = 0.001$ at $t = 0.05, 0.15, 0.25, 0.35$ and 0.45 . The burnt gas is on the left and the unburnt gas on the right.

Figure 4.5: The normalised amplitude A/A_0 as a function of time for several values of the expansion ratio or heat release parameter, $\tau = 1$, $\tau = 3$ and 5 . In all cases $n = 2$. The dashed line gives the theoretical growth rate.

respect to the unburnt gas in the direction normal to the flame front which is described in section 2.2.2. Therefore, the results shown in figure 4.4 suggest that the instability will be eventually saturated by the flame front restoration process.

Between $t = 0.05$ and $t = 0.15$ the growth of the amplitude $A = (x_{f,max} - x_{f,min})/2$ is small, but thereafter the growth increases in time and becomes exponential as shown in figure 4.5 where we illustrate also the amplitude growth for other values of the expansion ratio or heat release parameter, i.e. $\tau = 1$, and 5 . After the velocity field has developed, figure 4.5 shows that the agreement between the growth rate found from the simulations and the theoretical growth rate is excellent. The results also show the expected increase in growth rate when τ becomes larger. At a later time the growth rate obtained from the simulations levels off and becomes smaller than the theoretical value. This is due to the fact that nonlinear effects like flame front restoration, set in.

Furthermore, we see in figure 4.4 that for $t \geq 0.25$ additional small disturbances appear on the flame front. These disturbances are probably the result

Figure 4.6: The normalised amplitude A/A_0 as a function of time for $n = 1, 2, 3$ and 4 . For all cases $\tau = 3$. The dashed line indicates the theoretical growth rate.

of small discretisation or numerical errors. Namely, it follows from (2.13) that the growth increases with k . Therefore, these errors, which have a large value of k and which are initially very small, become visible in the final stages of the simulation.

According to equation (2.13), the growth rate also depends on the wave length of the disturbance and it increases for larger values of n or $k = 2\pi n$. In figure 4.6 the growth of the disturbance amplitude is plotted for several values of the wave number. For $n = 1$ and $n = 2$ the results show the expected increase with wave number and the agreement between the theory and the actual growth rate is very good as soon as the flow field has established itself. However, for shorter wave lengths, i.e. $n = 3$ and $n = 4$, the computed growth rate deviates from the theory. This is due to the fact that in the theory one assumes that the flame is infinitely thin, but in our calculations this is not the case. The correctness of this explanation becomes more clear in figure 4.7, where the normalised amplitude is plotted as a function of time for one value of n and τ , but for several values of the flame thickness δ . In all the previous graphs.

Figure 4.7: The normalised amplitude A/A_0 as a function of time for several values of the flame thickness $\delta = 0.02, 0.04$ and 0.1 . In all cases $\tau = 3$ and $n = 2$. The dashed line indicates the theoretical growth rate.

the default value of $\delta = 0.02$ has been used. When we use larger values such as $\delta = 0.04$ and 0.1 , figure 4.7 shows that the growth rate decreases. Apparently, the growth rate is only close to the theoretical value (2.13), if $\delta/\lambda \ll 1$. When either δ increases or λ decreases, the actual growth rate becomes lower than the theoretical value, as we have also noticed in figure 4.6.

Although the growth rate increases with increasing wave number, figure 4.6 shows that the final amplitude of disturbances with a short wave length may become smaller than the final amplitude of longer waves. This might be problematic in numerical simulations which use periodic boundary conditions. In that case the largest wave length possible is a wave length equal to the size of the numerical domain. Since a disturbance with this wave length may continue to grow, it might start to dominate the solution, which eventually results in a solution, which is influenced by the size of the numerical domain.

Figure 4.8: The turbulent flame speed s_{ft} as a function of the turbulent intensity u' , together with the expected profile, equation (2.11), with $C = 1$. + indicates the results of simulation without expansion or $\tau = 0$. $\times$ indicates the results of simulations with expansion.

4.4 Results of type IV simulations (Turbulent premixed Combustion)

We now consider the DNS results, in which the full interaction between turbulence and the flame front is taken into account.

Let us first look at the influence of turbulence on the flame front, decoupled from the effect of volume expansion, i.e. without density fluctuations. To this end we have performed three simulations without expansion, i.e. $\tau = 0$, and varying turbulence intensity at the inflow. The resulting turbulent flame speed s_{ft} as a function of the turbulence intensity u' is plotted in figure 4.8 with the + symbols. Here, u' is defined as rms value of the velocity fluctuations at the mean position of the flame front, $\bar{x}_f$, and is given by,

$$u' = \sqrt{\overline{u_i^2}} = \sqrt{2 \frac{k_t}{\rho}}, \quad (4.8)$$

where the latter equality is only valid for this particular case for which $\tau = 0$.

Figure 4.8 shows indeed an increase in flame speed with the level of turbulence as predicted by Damköhler (1940). The relation (2.11) with $C = 1$ agrees reasonably well with data although for the larger values of u' the computed turbulent flame speed seems to fall a little below the linear profile. This latter effect is probably due to the artificial thickness of the flame δ , because for a strongly wrinkled flame, the increase of the flame surface is limited by δ and therefore the flame speed decreases.

Next we have carried out a series of simulations to consider the effect of gas expansion. An example of the instantaneous flame front for the case $\tau = 3$ is shown in figure 4.9. The flame front is strongly deformed and we expect that this will lead to a strong increase of the turbulent flame speed.

The results for the simulations with gas expansion, i.e. $\tau \neq 0$ are also shown in figure 4.8 by the $\times$ symbols. The flame speed has clearly increased. If we assume that this increase results solely from the turbulent distortion of the flame front, the data must fall along the linear line (2.11) discussed above. We see, however, that this is not the case. So it appears that s_{fl} depends also directly on the heat release parameter τ .

Let us assume that (2.11) is still valid approximation for the influence of turbulence on the flame speed in the range of u'/s_{fl} that are found for the cases $\tau \neq 0$. The direct effect on the flame speed by the gas expansion can then be described by plotting the constant C defined as $C = (s_{fl} - s_{fl})/u'$ as function of τ . This is shown in figure 4.10 where we see that increase of the turbulent flame speed grows when the expansion rate becomes larger. The rate of growth of C seems to level off at the higher expansion rates. These results are consistent with the results of Wenzel and Peters (2000), who also observed an additional increase in the turbulent flame speed for higher expansion rates. Their conclusion, that the effect of gas expansion is only important for low turbulence intensities could not be validated here, since u' is low in all our simulations.

The explanation of this dependence of the turbulent flame speed on the gas expansion must be sought in the effect of the hydrodynamic instability. We have seen in section 4.3 that disturbances on the flame front will grow causing an increase in the area of the flame front and therefore an increase in the turbulent flame speed. The results of section 4.3 also indicate that the hydrodynamic instability of the flame front becomes stronger at higher expansion rates in agreement with the behaviour of our data in figures 4.8 and 4.10.

(a) $\tau = 0$ (b) $\tau = 3$

Figure 4.9: An instantaneous picture of the flame front

Figure 4.10: The increase of $C = (s_{ft} - s_{fl})/u'$ as a function of the heat release parameter τ .

Figure 4.11: The probability density of finding the instantaneous flame front at a position x with respect to the mean position $\overline{x_f}$ for several values of the heat release parameter τ .

4.5 The position of the flame front x_f

As can be seen in figure 4.9, the flame front is strongly deformed. As a result, the x -position of the instantaneous flame front, x_f , depends on the y and z coordinate and the time. In figure 4.11, we have plotted the probability density of finding the instantaneous flame front at a certain position x . At $\tau = 0$, i.e. without expansion, the distribution is nearly symmetric with respect to $x_f = \overline{x_f}$. When $\tau \neq 0$ the distribution broadens as a function of τ and at the same time becomes positively skewed. This means that the disturbances on the flame front grow with larger values of τ . This is in agreement with the fact that the growth rate of hydrodynamic instabilities becomes larger when τ increases. The positive skewness, i.e. large excursions of the flame front to the burnt gas side, is in agreement with results of Wirth et al. (1993) and experiments of Plessing et al. (2000). It is due to the fact that the flame develops rounded edges toward the unburnt gas and sharp spikes toward the burnt gas, as e.g. shown in figure 4.4. Another contribution to an increase in the positive skewness

of the pdf follows from the fact that due to the high velocity of the burnt gas, regions of unburnt gas are dragged into the burnt gas region and thus displace the flame front to positive values of x .

4.6 Change of turbulence characteristics across the flame front

Let us now consider how the turbulence changes when the flow passes the flame front. First we consider the turbulent kinetic energy. In figure 4.12 the mean turbulent kinetic energy per unit volume $\bar{k}_t$ defined according to (2.46) is plotted as a function of x for several expansion rates. The initial condition for the turbulence intensity at the inflow is chosen the same for all cases. For the case $\tau = 0$, there is no gas expansion and the development of the turbulence will not be affected in this case, i.e. the decay of turbulence will be similar as found in figures 4.2 for the incompressible case. For the case $\tau = 1$ we see an decrease of the turbulent kinetic energy per unit volume, when the turbulence passes the flame front. However for higher expansion rates, $\tau = 3$ and $\tau = 5$, this turns into an increase in the turbulent kinetic energy.

In order to throw more light on this change of behaviour as function of τ , we also performed a simulation of turbulence passing a flat flame, which is denoted as type II in table 4.1. This means that the gas expands at a fixed flame position and the shape of the flame front is thus not influenced by the turbulence or instability processes. For the expansion rate in case of the flat flame we take $\tau = 3$. We see in figure 4.12 that the kinetic energy strongly decreases when it passes the flat flame front. The conclusion is that the decrease of the kinetic energy across the flame front must be connected to the gas expansion and the increase of kinetic energy must be related to deformation of the flame front which occurs in particular at the higher expansion rates. We shall return to this when we discuss the kinetic energy budget in section 4.7.

In figure 4.13 we have plotted the different components of the turbulent energy for the case $\tau = 3$. Before the flame front the three components are almost equal which implies isotropic conditions. Behind the flame front the x -component of the turbulent energy strongly increases while the other contributions continue to decay. As a result, the turbulence behind the flame front becomes strongly anisotropic and it seems that there is no tendency to return to isotropy further downstream.

The increase of the turbulent kinetic energy is thus solely due to the growth

(a) Normal scale

(b) Log scale

Figure 4.12: The turbulent kinetic energy $\bar{k}_t$ as a function of x for various values of τ . The initial condition at $x = 0$ is the same for all cases. In addition we show the results for the case without combustion and for the simulation with the flat flame front. The flat flame shows a strong suppression of turbulence, while the turbulent kinetic energy is enhanced in case of a wrinkled flame at large values of τ .

Figure 4.13: The different components of the turbulent kinetic energy as a function of x for $\tau = 3$. $k_{tx} = \frac{1}{2}\rho\overline{u'_1u'_1}$, $k_{ty} = \frac{1}{2}\rho\overline{u'_2u'_2}$ and $k_{tz} = \frac{1}{2}\rho\overline{u'_3u'_3}$.

of the velocity fluctuations in the x -direction. This points again in the direction of the hydrodynamic instability as being the cause for this growth because we have seen in section 4.3 that the hydrodynamic instability influences primarily the x -component of the velocity. We shall come back to this issue in the next section when we discuss the kinetic energy budget.

4.7 Turbulent kinetic energy budget

To investigate the background behind the behaviour of the turbulent kinetic energy that we observed in the previous section near the flame front, in more detail, we consider in this section the different terms in the budget for the turbulent kinetic energy as expressed in (2.53). These terms are plotted in figure 4.14 for various values of the expansion parameter τ . The diffusive transport term D_k has been neglected because this term is small since there are no regions of high shear in the mean flow field.

In case of $\tau = 0$, (figure 4.14a), the main balance is between the transport of turbulent kinetic energy by the mean flow, Dk/Dt , and viscous dissipation, ϵ_k . The fluctuations in the Dk/Dt are due to the statistical error in $\bar{k}_t$, which is amplified by the fact that Dk/Dt is computed by taking a spatial derivative of $\bar{k}_t$. The total budget term is not exactly zero in figure 4.14. This is caused by the fluctuations in the Dk/Dt -term and the fact that the stabilisation mechanism to keep the flame front at a fixed position causes a slowly varying mean flow with a long time scale. As a result the statistics converge slowly.

In case of $\tau = 1$, (figure 4.14b), the Dk/Dt and the ϵ_k -term remain important, but contributions of the expansion term E_k and the pressure term Π_k become non-negligible. The Π_k has a positive and negative contribution which seems to cancel each other. The E_k is everywhere negative which we have also observed in relation to (2.53) for this case where $\partial \bar{u}_i / \partial x_i > 0$. Apparently the expansion term E_k accounts for the decrease of turbulent kinetic energy that we observe in figure 4.12 which is consistent with our observation based on the flat-flame results shown in this figure. A decrease of kinetic energy has been also observed in previous studies, e.g. by Lindstedt and Sakthitharan (1998). In that case the decrease of turbulent kinetic energy across a flame front is attributed to an increased viscosity, which accompanies the temperature rise, due to combustion. In our case, the viscosity is taken constant and thus can not play a role. Therefore, our results indicate that the decrease of energy observed may also result from the gas expansion.

At the larger expansion rates $\tau = 3$ and 5, (figure 4.14c and d), the picture

(a) $\tau = 0$ (b) $\tau = 1$

(c) $\tau = 3$ (d) $\tau = 5$

Figure 4.14: Kinetic energy budget for several expansion rates.

Figure 4.15: The different term in the production term P_k of the turbulent kinetic energy as a function of x for $\tau = 3$. $P_{k,1} = -\bar{\rho} u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}$, $P_{k,2} = -\bar{\rho}' u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j}$, $P_{k,3} = -\bar{\rho}' u'_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}$ and $P_{k,tot}$ is the sum of these terms.

changes. Both terms E_k and Π_k remain important, but the production term P_k grows and becomes the dominant term. In the region $x = 2.0 - 2.2$, the terms E_k and Π_k are in balance and Dk/Dt -term almost coincides with the production term P_k . This explains the increase in the kinetic energy that we have observed in figure 4.12 for $\tau = 3$ and 5.

To explain the background of this increase in the production P_k we consider the three terms that contribute to P_k , separately. These are

$$\begin{aligned}
 P_{k,1} &= -\bar{\rho} u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j} \\
 P_{k,2} &= -\bar{\rho}' u'_i u'_j \frac{\partial \bar{u}_i}{\partial x_j} \\
 P_{k,3} &= -\bar{\rho}' u'_i \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j}
 \end{aligned} \tag{4.9}$$

For the case $\tau = 3$ we have plotted these contributions to P_k in figure 4.15. We

Figure 4.16: The different term in the production term Π_k of the turbulent kinetic energy as a function of x for $\tau = 3$. $\Pi_{k,1} = \overline{p' \frac{\partial u'_i}{\partial x_i}}$, $\Pi_{k,2} = -\overline{\frac{\partial p' u'_i}{\partial x_i}}$ and $\Pi_{k,tot}$ is the sum of these terms.

find that the dominant contributions are both $P_{k,1}$ and $P_{k,3}$ with $P_{k,2}$ being much weaker. The $P_{k,1}$ is negative but the $P_{k,3}$ is strongly positive and is therefore responsible for the positive total production P_k .

Given the definition of $P_{k,3}$ in (4.9) and the fact that $\partial \bar{u}_i / \partial x_i > 0$, we find that a positive value can be only result from a negative density transport term $\overline{\rho' u'_i}$. In section 2.3 we found that such a negative density transport is consistent with the deformation of the flame front. Therefore we conclude that the increase of kinetic energy that we have observed at the high expansion rates is the result of the deformation of the flame front. This deformation occurs mainly in the streamwise direction which suggests that only the u'_1 is influenced. This is consistent with the results shown in figure 4.13.

Finally, we consider the pressure contribution Π_k to the kinetic energy budget (2.53) in more detail. This term can be divided in two contributions

$$\Pi_{k,1} = \overline{p' \frac{\partial u'_i}{\partial x_i}}$$

$$\Pi_{k,2} = -\frac{\partial \overline{p'u'_i}}{\partial x_i}, \quad (4.10)$$

where $\Pi_{k,1}$ is called the pressure dilatation and $\Pi_{k,2}$ the pressure transport. These two contributions to Π_k are shown in figure 4.16 for $\tau = 3$. The Π_k seems to be dominated by the pressure transport term. The pressure-dilatation term which behaves with an opposite phase to the pressure transport term, has a maximum value around $x = 2.6$, a value which appears to be somewhat larger than the position where $P_{k,3}$ reaches its maximum. This suggests that this positive contribution of the pressure dilatation term to the kinetic energy budget may depend on another process than the flame-front deformation which, as we have seen above, dominates the $P_{k,3}$. We shall come back to this in the next section.

4.8 Enstrophy budget

Another view on the dynamics of the turbulence in the neighbourhood of the flame front can be obtained by considering the enstrophy. In figure 4.17, we have plotted the enstrophy as a function of x for the same cases as shown in figure 4.12 for the turbulent kinetic energy. The behaviour of the enstrophy follows closely that of the kinetic energy. In case of $\tau = 0$, the enstrophy shows a continuous decay along the x -axis. In case of $\tau = 1$ enstrophy is destroyed at the flame front and in case of $\tau = 3$ and $\tau = 5$ enstrophy is generated. Also the simulation of the flat flame shows the same behaviour as for the kinetic energy, i.e. a strong decrease of the enstrophy at the flame front.

In figure 4.18 we have plotted the contribution of the different vorticity components to the enstrophy for $\tau = 3$. This figure shows that the initially isotropic distribution of the enstrophy over its components becomes anisotropic when it crosses the flame front, i.e. the z and y -components are amplified while the x -component decreases further.

Let us interpret the behaviour of the enstrophy in terms of its budget (2.63). The terms in this budget are shown in figure 4.19 as a function of x , for several values of τ .

In case of $\tau = 0$ there is a balance between production by vortex stretching S_ω and the viscous dissipation of enstrophy ϵ_ω with a minor contribution by the mean transport term. The fact that the total budget is not zero in any of the graphs of figure 4.19 is due to the fact that ϵ_ω is underestimated. Namely, ϵ_ω is obtained from a spatial derivative of the vorticity fluctuations, which on their turn are obtained from a spatial derivative of the velocity field. In order

(a) Normal scale

(b) Log scale

Figure 4.17: The enstrophy Ω as a function of x for several expansion rates.

Figure 4.18: The contributions of the different vorticity components to the total enstrophy as a function of x for $\tau = 3$. $\Omega_x = \frac{1}{2}\overline{\omega'_1\omega'_1}$, $\Omega_y = \frac{1}{2}\overline{\omega'_2\omega'_2}$ and $\Omega_z = \frac{1}{2}\overline{\omega'_3\omega'_3}$

(a) $\tau = 0$

(b) $\tau = 1$

(c) $\tau = 3$ (d) $\tau = 5$

Figure 4.19: Enstrophy budget for several expansion rates.

to compute these derivatives, the velocity field is interpolated, which smooths the velocity field and introduces an error which causes the higher derivatives, such as the enstrophy, to be underestimated.

In case of $\tau = 1$ the term E_ω becomes more important. This term accounts for the decrease of enstrophy density, due to the expansion in the velocity field. This is the same effect as we saw in the energy budget. In case of the higher expansion rates, i.e. $\tau = 3$ and $\tau = 5$, this term remains important and grows, but the baroclinic production term Π_ω grows even faster, resulting in the production of enstrophy at a position near the flame front.

By comparing figures 4.16 and 4.19 we observe that the maximum of Π_ω appears at the same position where the pressure dilation term $\Pi_{k,2}$ has its maximum. So these two terms seem to describe the same process, i.e. baroclinic production. However, we have seen also in the previous section that the pressure dilation term does not have much influence on the growth of the kinetic energy which is instead dominated by the production term P_k or rather by the flame-front deformation. Therefore, we must conclude that the mechanism for the growth of the kinetic energy and the enstrophy are quite different, despite the fact that their behaviour as a function of x is quite similar as follows from comparing figures 4.12 and 4.17.

We have found that main production mechanism of enstrophy appears to be the baroclinic vorticity production Π_ω . To get a more detailed view of this process we show in figure 4.20a, an instantaneous plot of lines of constant pressure, together with the position of the flame front. This plot shows that the isobars are nearly straight and do not follow the deformation of the flame front. Because the density gradient is perpendicular to the local flame front, the pressure and density gradient are clearly not aligned. This results in baroclinic vorticity production as shown in figure 4.20b. Depending of the orientation of the flame, either positive or negative ω_y vorticity is produced and both contribute to the enstrophy. In case of high expansion rates, this production of vorticity becomes very important and influences the structure of the flow behind the flame front. To illustrate this we plot in figure 4.21 the modulus of the vorticity in an instantaneous xz -slice, which also shows that the vorticity in the flow behind the flame front has a different structure than the vorticity in front of the flame front.

The role of baroclinic vorticity production in the interaction between turbulence and a flame front is consistent with the investigations of Rutland and Ferziger (1991); Mueller et al. (1998) and Louch and Bray (1998), who studied the interaction between vortices and a premixed flame. They found that this results in long regions of vorticity in the streamwise direction, which can be also found in our simulation, as shown in figure 4.21.

(a) Lines of constant pressure

(b) Regions of baroclinic vorticity production. The continuous lines indicate regions of positive ω_y production. The dashed lines indicate regions of negative ω_y production.

Figure 4.20: In both plots the thick solid line indicates the position of the flame front in an instantaneous xz -slice at $\tau = 3$

Figure 4.21: The modulus of the vorticity, $\sqrt{\omega_i^2}$, plotted in an instantaneous slice in the xz -plane. $\tau = 3$

Figure 4.22: The Favre averaged turbulent kinetic energy, compared the the normal averaged turbulent kinetic energy

4.9 Favre averaging

In section 2.7.4, we mentioned that Favre averaging is often used in flows with a varying density. Since all the data, needed to obtain the Favre averaged turbulent kinetic energy (2.67), are available from our DNS data, we can compare the kinetic energy defined in (2.46) with the Favre average turbulent kinetic energy. Both are plotted in figure 4.22 as a function of x . The graphs in this figure have the same shape, but the peak of the Favre averaged energy is about 20% lower, which is consistent with (2.68).

Another view on Favre averaging may be obtained by considering the budget of the Favre averaged kinetic energy $\tilde{k}_t$ defined by (2.67) which reads (Lele, 1994)

$$\frac{\partial \tilde{k}_t}{\partial t} + \frac{\partial \tilde{u}_j \tilde{k}_t}{\partial x_j} = -\frac{\partial \tilde{k}_t'' \tilde{u}_j''}{\partial x_j} - \bar{\rho} \tilde{u}_i'' \tilde{u}_j'' \frac{\partial \tilde{u}_i}{\partial x_j} + \overline{u_i'' \frac{\partial p'}{\partial x_i}} - \overline{u_i'' \frac{\partial \tau'_{ij}}{\partial x_j}} - \overline{u_i'' \frac{\partial \bar{p}}{\partial x_i}} + \overline{u_i'' \frac{\partial \tau_{ij}}{\partial x_j}}, \quad (4.11)$$

with

$$k_t'' = \frac{1}{2} \rho u_i''^2. \quad (4.12)$$

The first four terms on the right-hand side of this equation are the turbulent transport, the shear production, the pressure and the viscous term, respectively. These terms appear also in the budget of kinetic energy for an incompressible flow. The remaining two terms, which have no equivalent in the incompressible energy budget, are a result of the Favre averaging procedure or in particular of the fact that $\overline{u_i''} \neq 0$. Let us consider these two terms in somewhat more detail. With help of the definition

$$\overline{\rho' u_i'} = -\overline{\rho} \overline{u_i''} \quad (4.13)$$

and the momentum equation (2.66) we can write these terms as

$$-\overline{u_i''} \frac{\partial \overline{p}}{\partial x_i} + \overline{u_i''} \frac{\partial \overline{\tau_{ij}}}{\partial x_j} = -\overline{\rho' u_i''} \frac{\partial \tilde{u}_i}{\partial t} - \overline{\rho' u_i''} \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} + \overline{u_i''} \frac{\partial \overline{\rho u_i'' u_j''}}{\partial x_j}. \quad (4.14)$$

This equation shows that, besides a contribution due to a variation of the Reynolds stress, the last two terms in (4.11) are also responsible for the production term $P_{k,3}$ which we have already encountered as part of the production term of the kinetic energy budget (2.53). We have seen that $P_{k,3}$ describes the process of flame-front deformation, which plays an important role in the dynamics of turbulence near the flame front. This means that these terms on the right-hand side of (4.11) can not be neglected and therefore, should be modelled. A model for these terms, however, is far from obvious, so that nevertheless they are usually neglected. In that case we must conclude that the use of Favre averaging will not give a realistic representation of the flame front dynamics for the case studied here.

4.10 Conclusions

We have carried out a Direct Numerical Simulation of a premixed flame in decaying homogeneous turbulence. The simulation includes the effects of gas expansion in a flow at low Mach number. The flame front is modelled by a level set approach. In this way it is possible to perform an efficient simulation, which includes the most important phenomena of premixed turbulent combustion. It is possible to stabilise the mean position of the flame front by adjusting the inflow velocity into our computational domain. This allow us to obtain converged statistics by means of time averaging.

The DNS is able to reproduce hydrodynamic instability of the flame front. The dependency of the growth rate on the expansion rate and on the wave length of the initial wave-like perturbation is in good agreement with the theory. When

the thickness of the flame front increases, the growth rates become lower than the theory because the theory is only valid for infinitely thin flames.

The turbulent flame speed increases with increasing turbulence intensities at the position of the flame front. This is due to the deformation of the flame front by the turbulence with as result that its area increases leading to a larger combustion rate. The rise in flame speed agrees with theoretical and experimental results. Apart from the direct effect of turbulent deformation of the flame front the increase is found to depend also on the heat release. For higher expansion rates the increase of the flame speed grows. This effect is due to the hydrodynamic instability mechanism which results in an amplification of the disturbances that are induced on the flame front by the turbulence.

When passing the flame front the turbulent kinetic energy is distributed over a larger volume as a result of the gas expansion, which accompanies the heat release. This means that turbulent kinetic energy decreases. At the higher expansion rates, however, we find that turbulent kinetic energy can be also produced. The production process is related to flame-front deformation which as a result of the hydrodynamic instability amplifies and produces large velocity fluctuations in the streamwise direction. As a result the total turbulent kinetic energy increases (despite the decay due to the gas expansion). Because the production affects mainly one flow direction the turbulence exhibits an anisotropic structure after the flame front.

Vorticity at the flame front decreases as a result of the same process that we have observed for the kinetic energy, i.e. the distribution over a larger volume due to the gas expansion. Vorticity, however, is also generated at the flame front by baroclinic production which is due to the non-alignment of pressure and density gradients. For high expansion rates, this production will become stronger than the suppression by the gas expansion and this causes the vorticity to increase over the flame front for larger expansion rates. Furthermore, we find that the vorticity after the flame front has an elongated anisotropic structure.

Turbulence in compressible flows as studied here, is frequently treated in terms of so-called Favre averaging. Due to the fact that density fluctuations play an important role in the production of turbulent kinetic energy at the position of the flame front, standard Favre averaging where additional terms in the kinetic energy budget are neglected, fails. To properly model the dynamics of the flame front and the interaction between the flame front and the turbulent flow, these additional terms in the Favre-averaged kinetic energy budget need to be modelled.

Chapter 5

Turbulent Combustion around a square cylinder

Premixed combustion can be strongly enhanced by the interaction between the flame front and obstacles which the flame front encounters when it propagates through a inflammable gas mixture. In this chapter, this phenomena is studied by means of a Direct Numerical Simulation (DNS). To this end, a DNS of the evolution of a flame front around a square cylinder and in the turbulent wake behind that cylinder is carried out. The DNS model, described in chapter 2 and 3 is used. The turbulence in the wake behind the cylinder has a strong influence on the propagation of the flame front. On other phenomena, which strongly influences the propagation of the flame front is the fact that the flame is stretched in the regions of shear in the mean flow field. This results in a strong increase in the area of the flame front and in the total combustion rate.

5.1 Geometry

With the numerical model discussed in the previous sections, we have carried out a simulation of the flow around a square cylinder in a channel as shown in figure 5.1. We use a geometry with a length of 14 times the height of the square cylinder in the x -direction and a height of 6 cylinder heights in the z -direction. The box has a width of 4 cylinder heights in the y -direction. Periodic boundary conditions are applied in the y -direction. At $x = 0$, no slip boundary conditions are applied. At $x = 14$ we use $p = 0$ as boundary condition. On the top and

Figure 5.1: Geometry used in the simulation of the flow around a square cylinder

on the bottom, free slip boundary conditions are applied. All simulations are performed on a grid of $320 \times 96 \times 192$ in the x -, y - and z -direction, respectively. The grid is refined around the square cylinder, resulting in a grid spacing in the x -direction ranging from $\Delta x = 0.012$ to $\Delta x = 0.054$ and in the z -direction from $\Delta z = 0.021$ to $\Delta z = 0.035$. The y -direction is uniform with a grid spacing of $\Delta y = 0.042$.

The simulation of the flow around a square cylinder without combustion takes about 120 CPU hours on a Cray C90, which is about 14 seconds per timestep. Each simulation run with combustion takes about 180 CPU hours on a Cray C90, excluding the simulation to obtain a fully developed turbulent flow field for the initial condition, which is about 80 CPU seconds per timestep.

5.2 Results

5.2.1 Flow field without combustion

First we have carried out a simulation without combustion in order to check the accuracy of the computed flow field. For this simulation we used an inflow boundary condition at $x = 0$ with an inflow velocity equal to one. The Reynolds number, based on the height of the cylinder and the bulk velocity is 1600. Below

Figure 5.2: Contour plot the mean velocity component in the x -direction around the cylinder

we present some results of these simulations.

In the Figures 5.2 and 5.3 we show the contours of the mean stream-wise and wall-normal velocity components, averaged in the periodic y -direction and in time. These plots show a recirculation region with a length of about $1.7h$ behind the cylinder and a small recirculation region on top of the cylinder. This is consistent with the experimental data of Lyn et al. (1995) and Durão et al. (1985). It is also clear that very sharp velocity gradients occur at the leading edge corner of the cylinder. Therefore, a fine grid is needed to resolve these gradients. Our first impression was that our grid was fine enough to resolve these gradients since no visible wiggles are generated at the leading edge of the cylinder. However, figure 5.5 shows that still small wiggles occur. Making the grid even finer is not possible, since the limitation in the time step will then become too severe.

In the regions with a high velocity gradient, a high production of turbulence can be observed, as shown in the contour plots of the rms velocity fluctuations, shown in figures 5.4 and 5.5. As a result, regions of high fluctuations are found on top of the cylinder. Another maximum in the rms velocity fluctuations in the x -direction is found at $x = 5.5$ and $z = 3.7$ while in the same region the rms fluctuations in the z -direction have a maximum around $x = 6.2$. These last two maxima are due to the vortex shedding in the wake behind the cylinder.

In relation with the maxima in the velocity fluctuations we find two extrema in the uw stress as shown in figure 5.6. We find a minimum at $x = 4.0$ and

Figure 5.3: Contour plot of the mean velocity component in the z -direction around the cylinder

Figure 5.4: Contour plot of the rms values of the velocity fluctuations in the x -direction around the cylinder

Figure 5.5: Contour plot of the rms values of the velocity fluctuations in the z -direction around the cylinder

$z = 3.75$, just on top of the cylinder which is due to the instabilities generated at the leading edge of the cylinder. Another minimum is located at $x = 6.0$ and $z = 3.5$. This latter minimum results from the vortex shedding in the instationary wake behind the cylinder.

The simulation has been run for a few cycles of vortex shedding, resulting in a Strouhal number $St = 0.15$. The experiments of Lyn et al. (1995) carried out at a Reynolds number of 21400 and Durão et al. (1985) at a Reynolds number of 14000 produce a Strouhal number of 0.13, which is only slightly lower than the value we found. This difference can be explained by the Reynolds number dependence of the Strouhal number because Davis and More (1982) found an increasing Strouhal number with decreasing Reynolds number and measured a value of about 0.138 for the Reynolds number used in our simulations. This is still a bit lower than the value we found and this is probably due to the fact that we have run our simulation only for a few shedding cycles. Therefore, the data of Davis and More (1982) probably lies within the statistical accuracy of our estimate.

We have also computed the drag of the cylinder. We can divide the drag in a contribution from the pressure and from viscous stresses. The contribution of the drag, resulting from the mean pressure field is shown in figure 5.7 and it is given in table 5.1 together with the viscous contribution. The negative viscous contribution results from the recirculation zones on top and bottom of the cylinder. Considering statistical error, the total drag coefficient lies reasonably

Figure 5.6: Contours of uw stress around the cylinder

close to the value 2.1 reported by Davis and More (1982).

contribution	C_D
pressure difference between front and back of the cylinder	2.013
friction top	-0.008
friction bottom	-0.009
total	1.997

Table 5.1: Contributions to the drag on the cylinder in the x -direction

5.2.2 Flow field with combustion

Next we consider the simulations with combustion. These are performed on the same grid as the simulations without combustion. The simulation is started from a flow field of the simulation without combustion. The inflow velocity equal to one at the boundary at $x = 0$ is replaced with a no-slip wall and a flat flame is positioned just in front of that wall. The parameters s_{fl} and τ are chosen such that the flow velocity in front of the flame, U_{out} (2.38), is equal to one. With this initial condition we approximate the case that the flame front interacts with a fully developed wake as if the flame has started infinitely far away from the cylinder. With this choice of initial condition we avoid the more difficult interpretation of the data in terms of interaction between turbulence

Figure 5.7: Contour plot of the mean pressure field around the cylinder

and the flame front which occurs when the flame starts close to the cylinder and the wake will not be fully developed.

We have performed two runs with different parameters: one run with the expansion coefficient $\tau = 5$ and $s_{fl} = 0.2$ and one with $\tau = 3$ and $s_{fl} = 0.33$. The Reynolds number which is based on the height of the cylinder and the velocity scale (2.38) and in which viscosity is taken constant, i.e. not dependent on the temperature, is equal to 1600 in both cases. The parameter to adjust the thickness of the flame in (2.36) is set equal to $\delta = 0.1$.

Since the process is instationary, it is not possible to obtain statistics by averaging in time. Due to the amount of CPU time needed for each run, ensemble averaging is also not possible. Therefore, we can obtain averaged values only as an average in the homogeneous y -direction which in our case is not sufficient to obtain stable statistics. As a consequence we will not show in the following statistical data such as mean profiles and rms data.

Figure 5.8 shows the development of the average position of the flame front as a function of time. It shows how the flame is deformed in the wake behind the cylinder and that the area of the flame front is much enlarged in the wake behind the cylinder. This enlargement is caused both by the influence of the mean flow and by the turbulence. The effect of the mean flow field is due to the strong shear on top of the cylinder and behind it as shown in the in figure 5.2. In these regions, the flame front is stretched by the shear and its area much enlarged. The turbulence causes the flame front to wrinkle on a smaller scale as shown in figure 5.9. Both the shear in the mean flow and the turbulence

Figure 5.8: A sequence of plots showing the development of the average position of the flame front $\bar{G} = G_0$ and the turbulent kinetic energy of the turbulent flow field $k = \frac{1}{2}\rho (\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$ in time at $t = 1.19$, $t = 3.51$ and $t = 5.11$. The plots are averaged in the y -direction. $\tau = 3$ and $s_\eta = 0.33$.

Figure 5.9: A 3-dimensional plot of the flame front at $t = 3.6$. $\tau = 5$ and $s_{fl} = 0.2$.

increase the area of the flame but it is not clear how to distinguish between these two phenomena in a quantitative manner.

Another interesting feature of our computations is the tendency to suppress turbulence in burnt gas after the flame front as shown in figure 5.8. For instance the vortex shedding is clearly visible in the structure of the wake before the flame front has arrived. However, when the flame has passed nearly all the turbulent kinetic energy is destroyed. Since an increase of viscosity with temperature has not been taken into account in our computations, this effect must be due to the gas expansion. Such turbulence extinction is also known from the literature (Higuera and Moser, 1994). However, it is often explained there with the increase in viscosity, while our simulation shows that this can not be completely true.

We have also found that when the laminar flame speed s_{fl} is higher, the effect

of enlargement of the flame surface becomes smaller. This is shown in figure 5.10. Here the outflow velocity U_{out} is plotted as a function of time for the two cases that we have computed. The outflow velocity is completely determined by the size of the flame surface and therefore a direct measure for that size. The outflow velocity rises in time. After a small decrease due to the fact that the flame reaches the cylinder, the velocity rises strongly when the flame interacts with the wake behind the cylinder. In case of $\tau = 3$ and $s_{fl} = 0.33$, the outflow velocity reaches a maximum at $t = 5.1$. This is probably due to the fact that the flame tends to restore itself again to a flat surface and thus must return to its initial value. This effect is called kinematic restoration (Peters, 2000). The computational domain is too short to observe this restoring effect in the case of $\tau = 5$ and $s_{fl} = 0.2$. We find that the outflow velocity and therefore the size of the flame surface in the wake region, increases slower for the case $\tau = 3$ and $s_{fl} = 0.33$. This indicates that flames with a higher laminar flame speed have a tendency to restore quicker to a flat shape and to be less influenced by shear and turbulence.

5.3 Concluding remarks

We have presented a numerical method that is well suited to perform DNS simulation of turbulent premixed combustion including the effect of gas expansion.

Based on the computation with this method we find that the flame front is enlarged in the wake of an obstacle. This enlargement is due to shear in the mean flow field and the turbulence in the wake behind the obstacle. As an additional effect of this enlargement of the flame front and the resulting acceleration of the flow we expect an increase in the turbulence levels in the wakes behind other subsequent obstacles. It is, therefore, interesting to study the same effects on an array of obstacles.

The turbulent kinetic energy is strongly suppressed by the passing of the flame front. This is due solely to the expansion of the gas at the flame front and it can not be explained by the usual argument found in the literature, i.e. the increase in viscosity with the temperature, since this effect is not taken into account in our study.

We have argued that it is very difficult to obtain quantitative statistics from our simulations due to the instationary nature of the problem. Therefore, to gain more insight in the interaction between turbulence and premixed combustion, a different approach is needed. It is for instance better to look at the interaction between homogeneous turbulence and combustion in a flow condition where the

Figure 5.10: Mean velocity at outflow as a function of time

flame can be stabilised at a given position. This will be addressed in a future simulation.

Chapter 6

Conclusions

In this chapter, we summarise the results and conclusions, which are presented in this thesis

6.1 Numerical Method

- The numerical method, presented in chapter 3, is an efficient method to perform Direct Numerical Simulations of flows with large density gradients and a low Mach-number, as the occur in combustion processes.
- The results show that the code scales very well on parallel machines, which show promise for higher resolutions, more detailed simulations and more complex geometries.

6.2 Premixed flames in decaying turbulence

- The DNS is able to reproduce hydrodynamic instability of the flame front. The dependency of the growth rate on the expansion rate and on the wavelength of the initial wave-like perturbation is in good agreement with the theory. When the thickness of the flame front increases, the growth rates become lower than the theory. However, the theory is derived for infinitely thin flames and is no longer valid for these flames.
- The turbulent flame speed increases with increasing turbulence intensities at the position of the flame front. This is due to the deformation of the

flame front by the turbulence with as result that its area increases leading to a larger combustion rate. The rise in flame speed agrees with theoretical and experimental results. Apart from the direct effect of turbulent deformation of the flame front the increase is found to depend also on the heat release. For higher expansion rates the increase of the flame speed grows. This effect is due to the hydrodynamic instability mechanism which results in an amplification of the disturbances that are induced on the flame front by the turbulence.

- When passing the flame front the turbulent kinetic energy is distributed over a larger volume as a result of the gas expansion, which accompanies the heat release. This means that turbulent kinetic energy decreases. At the higher expansion rates, however, we find that turbulent kinetic energy can be also produced. The production process is related to flame-front deformation which as a result of the hydrodynamic instability amplifies and produces large velocity fluctuations in the streamwise direction. As a result the total turbulent kinetic energy increases (despite the decay due to the gas expansion). Because the production affects mainly one flow direction the turbulence exhibits an anisotropic structure after the flame front.
- Vorticity at the flame front decreases as a result of the same process that we have observed for the kinetic energy, i.e. the distribution over a larger volume due to the gas expansion. Vorticity, however, is also generated at the flame front by baroclinic production which is due to the non-alignment of pressure and density gradients. For high expansion rates, this production will become stronger than the suppression by the gas expansion and this causes the vorticity to increase over the flame front for larger expansion rates. Furthermore, we find that the vorticity after the flame front has an elongated anisotropic structure.
- Turbulence in compressible flows as studied here, is frequently treated in terms of so-called Favre averaging. Due to the fact that density fluctuations play an important role in the production of turbulent kinetic energy at the position of the flame front, standard Favre averaging where additional terms in the kinetic energy budget are neglected, fails. To properly model the dynamics of the flame front and the interaction between the flame front and the turbulent flow, these additional terms in the Favre-averaged kinetic energy budget need to be modelled.

6.3 Combustion around a square cylinder

- Based on the computation with this method we find that the flame front is enlarged in the wake of an obstacle. This enlargement is due to shear in the mean flow field and the turbulence in the wake behind the obstacle. As an additional effect of this enlargement of the flame front and the resulting acceleration of the flow we expect an increase in the turbulence levels in the wakes behind other subsequent obstacles. It is, therefore, interesting to study the same effects on an array of obstacles.
- The turbulent kinetic energy is strongly suppressed by the passing of the flame front. This is due solely to the expansion of the gas at the flame front and it can not be explained by the usual argument found in the literature, i.e. the increase in viscosity with the temperature, since this effect is not taken into account in our study.

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Nomenclature

symbol	description	unit
<i>normal symbols</i>		
c_p	specific heat at constant pressure	$J\,kg^{-1}K^{-1}$
c_s	speed of sound	ms^{-1}
Da	Damköhler number	—
E	activation energy	J
E_k	expansion term in $\overline{k}_t$ budget	Wm^{-3}
E_ω	expansion term in enstrophy budget	s^{-3}
k	kinetic energy	Jm^{-3}
k_m	kinetic energy of mean flow	Jm^{-3}
k_t	turbulent kinetic energy	Jm^{-3}
Ka	Karlovitz number	—
ℓ	integral length scale	m
ℓ_f	flame thickness	m
ℓ_o	thickness of oxidation layer	m
ℓ_G	Gibson length scale	m
ℓ_δ	thickness of the inner reaction zone	m
$\mathcal{L}$	Markstein length	m
m_i	mass flux ρu_i (tensor notation)	$kg\,m^{-2}s^{-1}$
$\mathbf{m}$	mass flux $\rho \mathbf{u}$ (vector notation)	$kg\,m^{-2}s^{-1}$
m_x, m_y, m_z	mass flux $\rho u, \rho v, \rho w$ (separate components)	$kg\,m^{-2}s^{-1}$
R	universal gas constant	$J\,kg^{-1}K^{-1}$
Re	Renolds number	—

symbol	description	unit
<i>normal symbols (continued)</i>		
p	pressure	Nm^{-2}
P_k	production term in $\bar{k}_t$ budget	W
s_f	flame speed	ms^{-1}
s_{fl}	laminar flame speed	ms^{-1}
s_{ft}	turbulent flame speed	ms^{-1}
t	time	s
T	temperature	K
T_b	temperature of the burnt gas	K
T_u	temperature of the unburnt gas	K
u_i	velocity (tensor notation)	ms^{-1}
$\mathbf{u}$	velocity (vector notation)	ms^{-1}
u, v, w	velocity (seperate components)	ms^{-1}
u'	rms velocity $\sqrt{u_i'^2}$	ms^{-1}
v'	rms velocity $\sqrt{u_i'^2/3}$	ms^{-1}
w	reaction rate	$kg\ m^{-3}s^{-1}$
x_i	Cartesian coordinates (tensor notation)	m
x, y, z	Cartesian coordinates (seperate components)	m
W	molecular weight	$kg\ mole^{-1}$
Y	mass fraction	—

symbol	description	unit
<i>Greek symbols</i>		
ϵ	dissipation rate	Wm^{-3}
ϵ_k	dissipation of turbulent kinetic energy	Wm^{-3}
ϵ_ω	dissipation of enstrophy	s^{-3}
λ	thermal conductivity	$Wm^{-1}K^{-1}$
λ	Taylor micro length scale	ms^{-1}
κ	curvature of the flame front	m^{-1}
ν	stoichiometric coefficient	—
ν	kinematic viscosity	m^2s^{-1}
ω_i	vorticity (tensor notation)	s^{-1}
ω	vorticity (vector notation)	s^{-1}
$\omega_x, \omega_y, \omega_z$	vorticity (separate components)	s^{-1}
Π_k	pressure term in the k_t budget	W
Π_ω	baroclinic enstrophy production	s^{-3}
ρ	density	kgm^3
ρ_b	density of the burnt gas	kgm^3
ρ_u	density of the unburnt gas	kgm^3
S_ω		s^{-3}
τ	heat release parameter	—
τ_{ij}	viscous stress (tensor notation)	Nm^{-2}
τ	viscous stress (vector notation)	Nm^{-2}
τ_f	chemical time scale	ms^{-1}
τ_η	Kolmogorov time scale	ms^{-1}

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Theo.

Curriculum vitea

Theo Treurniet is geboren op 20 maart 1974 te Berkel en Rodenrijs. Na de basisschool volgde hij zijn middelbare schoolopleiding aan de Gereformeerde Scholengemeenschap te Rotterdam, waar hij in 1992 zijn VWO diploma haalde.

Van 1992 tot 1997 studeerde hij Technisch Natuurkunde aan de Technische Universiteit in Delft. Zijn afstudeerwerk is verricht aan het Laboratorium voor Aero- en Hydrodynamica en ging over het gedrag van deeltjes in een turbulente stroming.

Na zijn afstuderen begon hij in december 1997 aan zijn promotieonderzoek aan het Laboratorium voor Aero- en Hydrodynamica van de Technische Universiteit Delft. Het onderwerp van dit promotieonderzoek, waarvan dit proefschrift verslag doet, is *Direct Numerical Simulation of Premixed Turbulent Combustion* en is uitgevoerd onder supervisie van prof.dr.ir. F.T.M. Nieuwstadt.

Sinds januari 2002 is hij werkzaam bij Philips Lighting als Development Engineer.

In oktober 2000 is hij getrouwd met Jolien Boxman.