Numerical Simulation of Premixed Flames interacting with Obstacles

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Numerical Simulation of Premixed Flames interacting with Obstacles

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With humble determination

(P. A. Paravento)

Italian history is far from lacking variety or vitality, and its course is always swift and rich in unexpected turns. The fact is that resignation, in its Italian form, is never or very rarely despair, or even passivity, but rather an awareness that life must somehow be accepted and must go on, and that there are moments when one must summon all one's resources to keep the machinery turning.

(G. Procacci)
Summary

In this work the modeling of the interaction of a premixed flame with one or more obstacles of different shape is considered.

The challenge of this work was to design a fast numerical tool suitable for a standard personal computer. A tool able to use a simplified chemical model that removes the need to solve a large system of conservation equations. At the same time a stable numerical scheme was needed to model high variations of density generated between the fresh mixture and the burnt gases during the propagation of the flame. Moreover, an efficient strategy was required to model the complex geometry.

Many combustion applications are characterized by low speeds, both for the flow and the flame propagation. In this study we consider systems with typical velocity of the order $O(10^0 - 10^1)$ m/s. Therefore, the flow is described by the Navier-Stokes equations in the low-Mach number limit. This implies that the velocities are much smaller than the speed of sound, so that density variations due to pressure variations can be neglected. In other words, the terms containing the acoustic time scales can be removed from the governing equations.

The reacting nature of the flow is modeled by using a source term in the energy equation which depends on the position of the flame. Energy is released only at the flame front. Hence it is assumed that the combustion takes place in the flamelet regime, i.e. the thickness of the flame is thin enough to be considered a geometric interface. In this case a level set approach can be used to track the position of the flame by using the $G$–equation formulation (Peters 2000). The source term in the energy equation is modeled as function of the zero level of the $G$–equation. This approach removes the need for solving the detailed chemistry because the source term can be thought as the contribution of a single step chemical reaction.

The spatial discretization of the momentum and the continuity equations is a second order finite volume method (Hirsch, 1988) and the time integration is based on a third order Adams-Bashforth scheme (AB3). For the $G$–equation the space discretization is a local third order WENO scheme (Jiang and Peng, 2000), while for its time integration AB3 is used. The same WENO scheme is used for the spatial discretization of the convective term in the temperature equation while the discretization of the diffusive term is carried out using a central difference scheme. An IMEX scheme (‘implicit’ integration of the source and ‘explicit’ integration of the advection-diffusion terms) is used for the time integration of the temperature equation. The IMEX scheme used in this approach was proposed by Pareschi (2001).

The computation of the Navier-Stokes equations is based on a pressure correction algorithm. The main difference between previous pressure correction schemes (i.e. Najm, 1998 or Treumiet, 2002) and the scheme we have introduced here is that in the first cases the time derivative of the density is calculated with a backward discretization whilst in the second case it is computed using the temperature equation and the equation of state. Another important difference in the second case is that the updated value of the density is found by integration of the continuity equation.
The modeling of the complex geometries has been done with an Immersed Boundary Method (IBM) that retains the advantages of numerical accuracy and computational efficiency associated with simple orthogonal grids. On the contrary, conventional numerical models generally use a complex (non-orthogonal) grid structure which requires a substantial computational effort. The IBM can simulate the shape of the part of the computational domain accessible to fluid by locally adding extra forces to the momentum equations. The square or rectangular obstacles considered in this study are aligned with the Cartesian mesh and this allows to apply exactly the forcing at their boundaries. In this method the shear stress on the boundary of the simulated obstacles is replaced in such a way that the no-slip velocity condition for the tangential component is applied at the wall. In conjunction, a non-penetration condition is also applied for the perpendicular velocity components at the boundary.

The heat flux between the boundaries of the obstacles and the flow is well represented with a procedure similar to the stress replacement method used for the momentum equation. This approach keeps the internal region of an obstacle well isolated under different conditions, while the correct heat flux is imposed at the surface of the body.

We have considered several experiments regarding the interaction of a premixed flame with obstacles. In particular, we have simulated the experiment performed by Ibrahim and Masri (2001). This case consists of the evolution of a flame front during deflagration of a air-gas mixture in a rectangular domain. The cases with constant and variable viscosity have been considered. The results obtained are comparable with the experimental data. The flame tip speed and the interaction of the front in the wake are well predicted. We note that the thermal thickness is reduced due to the interaction with the body. This interaction produces also an overpressure. In the case of variable viscosity a higher interaction of the flame front in the recirculation zone beyond the obstacle was found.
Samenvatting

In dit proefschrift wordt de interactie van een van te voorgemengde vlam met een of meer obstakels van verschillende vormen gemodelleerd. Hiervoor wordt directe numerieke simulatie gebruikt.

De uitdaging van dit werk ligt in het ontwikkelen van een snel numeriek numeriek model, dat geschikt is voor een normale PC. Een model dat een simpel chemisch systeem gebruikt waardoor het rekenwerk beperkt blijft. Op hetzelfde moment moet het model numeriek stabiel zijn, gebruikt kunnen worden voor het modelleren van de grote variaties in dichtheid en temperatuur en in complexe geometriën.

Vele verbrandingsapplicaties hebben een lage snelheid. Dit geldt zowel voor de stroming als voor de vlampropagatie. In dit proefschrift kijken we naar systemen met een typische snelheid van $O(10^0 - 10^1)\text{m/s}$. Daarom kunnen we voor de beschrijving van de stroming de Navier-Stokes vergelijkingen in de lage Mach-nummers gebruiken. Dit betekent dat de stroom- en vlamssnelheden veel kleiner zijn dan de snelheid van het geluid. Derhalve kunnen de dichtheidvariaties vanwege drukvariaties verwaarloosd worden. Met andere woorden, de termen waarin de akoestische tijd en de lengteschalen zitten kunnen verwijderd worden van de beschrijvende vergelijkingen en dit kan een aanzienlijke besparing geven in rekentijd.

De respons van de stroming op de chemische reactie wordt gemodelleerd door gebruik te maken van een term die als bron fungeert in de energievergelijking. Deze term is afhankelijk van de positie van de vlam. Energie wordt alleen vrijgelaten op de plaats van de vlam. Als we aannemen dat de vlam voldoende dun is dan kunnen we aannemen dat de vlam beschreven kan worden met een geometrische interface. In dit geval kan een level set methode toegepast worden om de positie van de vlam te volgen door het gebruik van de zogenaamde $G$-vergelijking (Peters 2000). De bronterm in de energie vergelijking wordt gemodelleerd als functie van het nul niveau van de $G$-vergelijking. Deze wijze van oplossen verwijderd de noodzaak tot het oplossen van de gedetailleerde chemie omdat de bronterm als het ware de contributie is van een enkelvoudige chemische reactietap.

De oplossing van de Navier-Stokes vergelijkingen is gebaseerd op een druk correctie algoritme. Het grote verschil tussen eerder gepubliceerde druk correctie schema's (bv. Najm, 1998 of Treurniet, 2002) en het schema dat wij hier geïntroduceerd hebben is dat in de eerste gevallen de tijdsdifferentiaal van de dichtheid wordt berekend met een achterwaardse discretisatie, terwijl het in het tweede geval deze berekening wordt gebruikt te maken van de temperatuur vergelijking en de toestandsvergelijking. Een ander belangrijk verschil in het tweede geval is dat de bijgewerkte waarde voor de dichtheid gevonden wordt door integratie van de continuïteitsvergelijking.

Het modelleren van de complexe geometrieën is gedaan met een Immersed Boundary Methode (IBM) die de voordelen behoudt van een numerieke nauwkeurigheid en computacionele efficiëntie van simpele orthogonale roosters. Daar tegenover staat dat conventionele numerieke modellen over het algemeen een complexe roosterstructuur gebruiken, hetgeen een substantiële rekentijd kost. De IBM kan de vorm van het deel van het rekendomein dat toegankelijk is voor fluidum simuleren door het lokaal toevoegen van extra krachten aan de momentumvergelijking. De beschouwde vierkante of rechthoekige obstakels in deze studie zijn uitgezien met het Cartesische rooster en dit maakt het mogelijk om de forcering op de roostergrens exact toe te passen. Met deze methode wordt de afschuifspanning (stress) op de roostergrens van de gesimuleerde obstakels op een dergelijke manier vervangen dat de no-slip snelheidsconditie voor de tangentiële component wordt toegepast op de wand. Daarbij wordt dan ook nog een niet penetrerbaarheidsvoorwaarde gebruikt voor de loodrechte snelheidscomponenten op de roostergrens.

De warmteflux tussen de roostergrenzen van de obstakels en de stroming wordt goed weergegeven met een vergelijkbare procedure als gebruikt voor de stress vervangingsmethode voor de momentum vergelijking. Deze benadering zorgt er voor dat de interne regio van een obstakel goed geïsoleerd blijft onder verschillende condities, terwijl de correcte warmte flux wordt opgelegd op het oppervlak van het lichaam.

We hebben meerdere experimenten waarbij de interactie van de voor gemengde vlam met obstakels van belang is gesimuleerd. In het bijzonder, hebben we gekeken naar de experimenten uitgevoerd door Ibrahim en Masri (2001). Dit geval bestond uit de evolutie van een vlamfront gedurende de intense verbranding van een lucht-gas mengsel in een rechthoekig domein waarin een dun obstakel is geplaats met een blokkage verhouding van ongeveer 50% ten opzichte van de oppervlakte van het kanaal. De gevallen met een constante en variabele viscositeit zijn bekeken. De resultaten, die hierniet verkregen zijn, zijn vergelijkbaar met de experimentele data. De vlam snelheid en de interactie met het front in het zog achter het obstakel zijn goed voorspeld. We moeten hierbij opmerken dat de thermische dikte is gereduceerd ten gevolge van de interactie met het lichaam. Deze interactie produceert ook een overdruk. In het geval van de variabele viscositeit werd een hogere interactie van het vlamfront in de recirculatiezone voorbij het obstakel gevonden.
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Chapter 1

A tool for premixed combustion

1.1 Outlines, motivations and structure of the thesis

Combustion is a chemical process that releases energy. It consists of an oxidation reaction between a fuel and an oxidant. The fuel can be introduced in the system as solid (e.g., coal), liquid (e.g., oil or gasoline) or gas (e.g., methane) while the oxidant is generally oxygen. In the case of solid-fuel this needs first to be heated up till the flammable temperature when particles start to burn. Also the flammable gases released from the solid will burn. In case of liquid-fuel it is the vapour that burns not the liquid. The gaseous state is the most suitable for atomic and molecular species (radicals) to be formed and take part in a chemical reaction. Other combustion mechanisms exist. They consist of heterogeneous combustion (e.g. liquid droplet combustion, spray combustion or combustion of a fine mixture of crushed coal with oil or water to form slurry mixtures) and catalytic combustion (the oxidation of combustibles on a catalytic surface accompanied by the release of heat). This thesis will focus on combustion mechanisms for mixtures of gas fuel and air.

Two main combustion regimes exist, the non-premixed regime and the premixed regime. A wax candle is an example of non-premixed combustion. The fuel is vaporized into the atmosphere which contains oxygen. The combustion reaction takes place at a specific location that separates the zone of the fuel from the zone of the oxidant. This location is called the flame (the stoichiometric interface). The non-premixed regime is safe because it is not difficult to control the location of the flame sheet and the intensity of the process by controlling the amount of fuel and oxidant introduced into the system and their temperature.

In the case of premixed combustion the reactants are well mixed before entering the combustion chamber. Chemical reactions can occur everywhere and the flame can propagate upstream into the feeding system. This can present some safety issues. Several approaches are used to prevent flash backs and the risk of detonations. One consists of choosing a mixture too rich (more fuel compared to oxidizer) or too poor in order to operate at points close to the flammability limits (the flame cannot easily propagate). Another possibility consists of creating heat losses in those parts of the system where combustion should not occur. For a given thermodynamical state of the mixture (compo-
sition, temperature, pressure), the flame has its own dynamics (speed, heat release, etc). These well defined quantities are convenient to describe the flame characteristics.

Reacting flow models rely on the solution of the Navier-Stokes equations for the flow augmented with the equations for the energy and the conservation of the chemical species. There are three main numerical techniques to compute the Navier-Stokes equations: RANS (Reynolds Averaged Navier-Stokes method), LES (Large Eddy Simulation) and DNS (Direct Numerical Simulation). The latter consists of solving all time and length scales. It is a tool to study turbulent reacting flows and it provides valuable information for improving the other methods, especially with respect to fluid mechanical quantities difficult to measure experimentally. Although DNS of the governing equations offers an alternative to experiments such simulations are limited by available computer resources.

RANS technique consists of averaging the Navier-Stokes equations to describe only the mean flow field. Local fluctuations and turbulent structures are expressed in mean quantities and these structures have no longer to be described in the simulation, hence allowing the use of a coarser grid resolution. The drawback is that unknown terms appear after the averaging procedure and they need to be modeled with turbulence models. The most widely used turbulence model, in industrial applications, is the \( \kappa - \varepsilon \) model which generally gives satisfactory results for many industrial purposes but it is limiting for academy research (Poinset and Veynante, 2001).

The LES approach is a numerical technique with characteristics between DNS and RANS. In LES only the large energetic scales of turbulence are calculated explicitly and the small scales are modeled with a sub-grid scales model (SGS). A commonly used SGS model is the Smagorinsky model that adds an extra viscosity term (eddy viscosity) to the governing equations to take into account the unresolved turbulent scales.

The time scales of the combustion process are in general smaller than the fluid time scales. This wide range of length and time scales should be resolved to completely take into account the effects of the turbulence and of the conservation of the chemical species that react into the flame reaction zone. Hundreds of species are involved which produce thousands of chemical reactions. The aim of this work is to overcome the limitations represented by the complex chemical mechanisms of the premixed combustion process and by the complex geometry. Our model can be considered “a bridge between science and technology”, a tool able to investigate the hydrodynamic characteristics of premixed combustion and, nevertheless, oriented to industrial applications. Our computations use DNS for the resolution of the flow equations, while the reacting part (energy equation with source term) is modeled with a level set approach (\(G\)-equation, Peters 2000). This approach removes the need for solving the detailed chemistry and does not require a model for the turbulence.

This thesis is organized in a first part where the theoretical and numerical aspects are discussed and a second part where results are presented regarding simple and complex flame configurations. Chapter two gives an overview of the problem introducing the governing equations, a discussion on the length and time scales involved, the main aspects of the fluid dynamics of premixed flames and the relations for a level-set based modeling strategy. The derivation of a low Mach number approximation of the Navier-Stokes equations is also described. In chapter three we present a model for premixed flames with realistic density ratios and a strategy to deal with the numerical error generated.
by the computation of the flame stretch. Then our method is applied to some basic fundamental flames and comparisons with other numerical approaches are shown. The immersed boundary method, which is used for complex geometries is discussed in chapter four. This approach allows the fast simulation of complex geometries with the use of very efficient solvers like the Fast Fourier Transform based algorithm. In chapter five we present results for the interaction of a premixed flame with obstacles. In particular, we simulate the experiment performed by Ibrahim (2001) in which the flame tip velocity was measured. A case with variable viscosity is also considered. Finally, concluding remarks summarize the potentialities of the method and indicate further opportunities of investigation.
Chapter 2

Premixed Combustion Theory and Modeling

2.1 Introduction, the combustion process

During the combustion process of gasses many intermediate reactions occur and many species and radicals are produced and consumed. If the reactants are introduced separately into the reaction zone the combustion is called non-premixed combustion. In the case that the reactants are mixed before reacting the flame is called premixed. Energy must be provided (ignition process) to start the combustion phenomenon which then evolves as an exothermic self-sustained reaction.

In this thesis we consider premixed flames of gaseous fuel-air mixtures. A premixed flame is said to be stoichiometric if fuel and oxidizer consume each other completely, forming only carbon dioxide and water. If there is an excess of fuel the system is called fuel-rich and if there is an excess of oxygen it is called fuel-lean. The flame may propagate into the reactants or move with them depending on whether the unburned gas velocity is greater than or less than the flame velocity. If these velocities are equal the flame is stationary in space. Combustion of premixed fuel-oxidizer mixtures can take the form of deflagration if the combustion wave is subsonic or detonation if it is supersonic.

In this study we are interested in the deflagration phenomenon. The typical velocity of deflagration waves in an open tube for hydrocarbon-air mixtures is about 40 cm/s (Glassman, 2000). This velocity is controlled by transport processes, heat conduction and diffusion of radicals. The diffusion of energy in front of the flame heats up the unburned gas until the ignition temperature is reached. According to the definitions given in “Guidelines for evaluating the characteristics of vapor cloud explosions, flash fires, and BLEVEs” (1994) the burning velocity is the velocity of propagation of a flame burning through a flammable gas-air mixture, measured relative to the unburned gases immediately ahead of the flame front. While the flame speed is defined as the speed of a flame burning through a flammable mixture of gas and air measured relative to a fixed observer, that is the sum of the burning and translational velocities of the unburned gases. If we consider to ignite a flammable mixture in a point, the result is an expanding
flame bubble that generates a flow field in its environment. In this expansion flow field, the flame propagation process is enhanced by flame instabilities which wrinkle the flame front surface. Therefore the flame enlarges its reactive area and thereby increases its effective burning speed. The laminar burning speed depends only on the composition of the fresh mixture, while the effective burning speed depends on the turbulence and its scales generated during the propagation.

For a combustion process that takes place adiabatically with no shaft work, the temperature of the products is referred to as the adiabatic flame temperature. This is the maximum temperature that can be achieved for given reactants. Heat transfer, incomplete combustion and dissociation all result in lower temperature. The maximum adiabatic flame temperature for a given fuel and oxidizer combination occurs with a stoichiometric mixture. During the combustion process, heat release, changes in the fluid dynamics of the system and transformation of many chemical species occur, thus the global velocity of the process depends on fluid dynamics, thermodynamics and chemical kinetics aspects. Laminar flame speed does depend on the chemical time scale. However, if we assume chemistry is infinitely fast, a flame development is only limited by mixing on the microscopic scale. It is interesting to note that the laminar flame speed for most hydrocarbon fuels is very similar (around 0.4m/s). This is because all hydrocarbons are quickly pyrolyzed to smaller sized molecules before combustion takes place. Hence for the most part the mixture entering the flame zone is substantially independent of the original fuel (Edwards, 1977).

Many commonly used combustion models rely on the assumption of fast chemistry to de-couple the complex chemistry from the flow-field calculation. As a consequence, in many cases the time evolution of the combustion process is determined by the conditions of the flow and the consequent transport of mass and heat, while the chemical rates of reaction mainly influence the amount of energy released and the thickness of the flame (the size of the reaction zone).

The flow can be laminar or turbulent. Laminar flames are generally slower than turbulent flames and easier to model. In the turbulent case, if the turbulence intensity is high (well stirred reactor regime) the mixing is such that a clear flame interface cannot be seen anymore. This is because the combustion process takes place at the smallest flow scales and in the entire domain.

In this thesis we investigate laminar premixed flames and flames with low level of turbulence intensity. As final goal, we are interested in the simulation of a deflagration evolving in a domain which is the reduced scale version of a real geometry.

### 2.2 Conservation equations

The conservation equations describing chemically reacting flows are the Navier-Stokes equations for variable density flows, augmented with additional equations for the chemical species and energy. Chemical reactions can be very complex and a lot of different species can be involved in the combustion process. For instance, the combustion of methane and oxygen can be described by 125 reactions and 30 different species (Warnatz, 2001).
2.2.1 Species mass fraction equation

The mass fraction of a species $i$ is defined as the ratio between the density of the species and the total density of the mixture as

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

For a system of $n$ species the balance equations for the mass fraction of each species $i$ is

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot [\rho (u + V_i) Y_i] = \dot{\omega}_i \quad (2.2)$$

where $\rho$ is the density of the total gas mixture ($\rho = \sum_{i=1}^{N} \rho_i$, with $N$ the number of species), $u$ its velocity and $V_i$ is the diffusion velocity of the species $i$ that can be derived from the kinetic theory of gases. $V_i$ depends on pressure and thermal diffusion mechanisms of the species $i$ with respect to the others. This is expressed by binary diffusion coefficients. By neglecting pressure diffusion and thermal diffusion effects and further assuming equal binary diffusion coefficients for all pairs of species, a simplified models for $V_i$ can be used like the well known Fick’s law. In this case we can write

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = -\nabla \cdot j_i + \dot{\omega}_i \quad (2.3)$$

always valid with $j_i = \rho V_i Y_i$ where $j_i$ is the diffusive flux and $\dot{\omega}_i$ is the chemical source term or reaction rate which depends on the species concentrations and on the temperature.

Computations of a system with large $N$ are demanding and reduced chemical reaction mechanisms have been introduced. They are derived from the complete mechanisms, e.g. by using steady state and partial equilibrium assumptions. These mechanisms are still too stiff to be used in a turbulent flow simulation. The stiffness arises because of the highly non-linear nature of the source terms which introduces many length and time scales to be captured by the numerical discretization (Tomboulides, 2004). An alternative is the so-called 'simple chemistry approach'. This is a one-step global reaction model which considers a fast reaction between fuel and oxygen resulting in a product,

$$\nu_F F + \nu_{O_2} O_2 \rightarrow \nu_P P$$

where $\nu$ are the stoichiometric coefficients of fuel ($F$), oxygen ($O_2$) and product ($P$). In this model the reaction rate is of Arrhenius type

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

where $A$ is the pre-exponential factor, $n_F$ and $n_{O_2}$ are the orders of the reaction of $F$ and $O_2$, $W$ is the molecular weight, $R$ is the universal gas constant, $E$ the activation energy and $T$ the temperature. All these constants must be found empirically. This approach is too crude to study the chemical details of combustion but it allows for a study of the main fluid dynamical aspects of reacting flows. The simple chemistry approach
generally overestimates the final combustion temperature because heat losses, incomplete combustion and dissociation of radicals are not modeled (Glassman, 2000).

The typical flame structure of a premixed flame with temperature and velocity profiles is depicted in fig. 2.1: $\delta_f$ is the total flame thickness, $l_\delta$ is the thickness of the reaction zone where the main reaction takes place, $l_o$ is the oxidation layer where the final reaction products are formed and $l_p$ is the preheat zone where the fresh gas is heated up by diffusion until the ignition temperature.

### 2.2.2 Governing equations

In this section we introduce the governing equations for the flow. The system of governing equations for fully compressible reacting flow expresses the conservation of mass, species, momentum and energy (Veynante and Verwisch, 2002, Warnatz et. al., 2000, Kuo, 2005).

For the continuity equation we have,

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (2.5)$$

The continuity equation states that combustion does not create mass and the total mass conservation equation is the same compared to non-reacting flows.

The conservation of species, already introduced, reads,

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i u_i) = -\nabla \cdot j_i + \omega_i \quad (2.6)$$

The conservation of momentum can be written as

$$\frac{\partial p u}{\partial t} + \nabla \cdot p u u = -\nabla p + \nabla \cdot \tau + \rho \sum_i Y_i f_i \quad (2.7)$$

where $p$ is the pressure, $f_i$ represents the body forces (e.g. gravity, electromagnetic force if specie $i$ is charged) acting on the species $i$ ($f_i$ will be neglected in this study) and $\tau$ is the stress tensor

$$\tau = \mu \left[ (\nabla u) + (\nabla u)^T \right] - \left( \frac{2}{3} \mu \nabla \cdot u \right) I \quad (2.8)$$

with $I$ the unit tensor.

In reacting flows the momentum equation is strongly coupled to chemistry via the density variations caused by the reaction exothermicity. In addition, heat release alters substantially the dynamic viscosity ($\mu \approx T^{0.8}$, Warnatz, 2000) in real gases and temperature varies by a factor 6 to 10 leading to large variations of the local flow Reynold number.

Multiple forms of the energy conservation equation exist. The most general one is the equation of the total specific energy (chemical + sensible + kinetic energy), $e_t = e + \frac{1}{2} u^2$ where $e$ represents the internal energy (chemical and sensible) and $\frac{1}{2} u^2$ is the kinetic energy. The relation for the total energy reads:

$$\frac{\partial \rho e_t}{\partial t} + \nabla \cdot (\rho e_t u) = -\nabla \cdot q + Q + \nabla \cdot (\tau \cdot u) + \frac{\partial p}{\partial t} + \rho \sum_i Y_i f_i (u_i + V_i) \quad (2.9)$$
where $q$ is the heat flux vector, $Q$ is the heat source term (e.g., radiation) not to be confused with the heat released by combustion, the terms $\nabla \cdot (\tau \cdot u) + \frac{\partial p}{\partial t}$ represent the work done by stresses and $\rho \sum_i Y_i f_i (u_i + V_i)$ represents the work done by body forces.

Now, an equation for the enthalpy will be derived from the total energy. This is because from the enthalpy equation a temperature equation can be easily derived. For low Mach number numerical codes the temperature equation is often preferred to the enthalpy equation because a direct relation exists between temperature and density through the equation of state. Let us consider the specific enthalpy $h$ that refers to the chemical and sensible energy content of the fuel mixture. It is expressed as

$$h = e + \frac{p_0}{\rho} \quad (2.10)$$

where $p_0$ is the thermodynamic pressure. The contribution of the different fuel mixture components to $h$ is expressed by

$$h = \sum_{i=1}^{N} Y_i h_i \quad (2.11)$$

with

$$h_i = h_i^{ref} + \int_{T^{ref}}^{T} c_{pi}(T')dT' \quad (2.12)$$

$h_i$, $h_i^{ref}$ and $c_{pi}$ are the specific enthalpy, specific enthalpy of formation at reference temperature $T^{ref}$ and specific heat capacity at constant pressure of the species $i$, respectively. Assuming a multiple-component ideal gas, for the specific heat capacity of the mixture it also holds

$$c_p = \sum_{i=1}^{N} Y_i c_{pi} \quad (2.13)$$

It can be shown (Poinso and Veynante, 2001) that by removing the kinetic energy from the total energy and by using the last relations between energy and enthalpy (2.11) the equation for $h$ reads

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho hu) = \nabla \cdot (\tau \cdot u) - \nabla \cdot q + \frac{\partial p}{\partial t} + Q + \rho \sum_i Y_i V_i f_i \quad (2.14)$$

The last two terms in eq. (2.14) drop out if radiation sources and body forces (e.g., gravity, electromagnetic) are neglected. This is assumed for our case. The $q$ vector in the energy equation contains the energy contributions from each species. A common expression for $q$ is (Williams, 1985)

$$q = -\lambda \nabla T + \rho \sum_{i=1}^{N} V_i Y_i h_i \quad (2.15)$$

with $\lambda$ being the thermal conductivity of the mixture.
The ratio of thermal conduction to species diffusion is given by the Lewis numbers defined as

\[ Le_i = \frac{\lambda}{\rho D_{im} c_p} \]  \hspace{1cm} (2.16)

where \( D_{im} \) is the mixture-averaged diffusion coefficient describing the diffusion of species \( i \) in the mixture. By using these Lewis numbers the species diffusion fluxes can be expressed as

\[ \rho V_i Y_i = -\frac{\lambda}{Le_i c_p} \nabla Y_i \]  \hspace{1cm} (2.17)

and the heat flux vector is

\[ q = -\lambda \nabla T - \frac{\lambda}{c_p} \sum_{i=1}^{N} \left( \frac{1}{Le_i} - 1 \right) h_i \nabla Y_i \]  \hspace{1cm} (2.18)

An equation of state for the ideal gas is also used together with the conservation equations,

\[ p_0 = \frac{\rho RT}{\bar{W}} \]  \hspace{1cm} (2.19)

with \( R \) being the universal gas constant and \( \bar{W} \) is the mixture molecular weight

\[ \bar{W} = \frac{1}{\sum_{i=1}^{N} Y_i/W_i} \]  \hspace{1cm} (2.20)

### 2.2.3 Computational issues

The conservation equations introduced above present computational issues. They form a system of partial differential equations (PDEs). To simulate a reactive flow the spatial terms are discretized with an appropriate scheme, resulting in a set of ordinary differential equations (ODEs) in time for all the variables (velocity, density, temperature, species mass fractions etc.). This set of ODE’s is, in general, very large (industrial applications may require millions of points for the spatial discretization). Each of the flow and thermodynamic variables will be described by the same large number of ODEs. We have already mentioned that one of the main problems is represented by the species conservation equations. These form a large system that must be solved. Moreover, for each component of the species the diffusion flux needs to be computed at each grid point of the computational domain.

Another main issue is represented by the non-linear nature of the source terms, \( \omega_i \), in the species conservation equations. The fact that many species and reactions are involved in the combustion process make it difficult to find an exact expression for the source terms since the species are involved in several reactions which all contribute to \( \omega_i \) terms and each \( \omega_i \) is also strongly depending on the temperature.
2.2.4 Assumptions

In order to make the system solvable several assumptions are needed. For clarity we have listed the approximations we have already made below:

a) thermal diffusion (Dufour effect) and pressure diffusion are neglected;

b) the work done by body forces (gravity and electromagnetic forces), the viscous heating and the radiative heating are neglected.

In addition, the following assumptions will be made:

c) the Lewis numbers of the species are assumed to be constant and equal to unity. As a consequence the last term in the heat flux vector drops out;

d) the mixture properties $c_p$, $\mu$ and $\lambda$ are taken constant.

Under these assumptions the governing equations read

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (2.21)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = -\nabla \cdot j_i + \dot{\omega}_i \quad (2.22)$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot \rho uu = -\nabla p + \nabla \cdot \tau \quad (2.23)$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho hu) = \nabla \cdot (\tau \cdot u) + \nabla \cdot (\lambda \nabla T) + \frac{\partial p}{\partial t} \quad (2.24)$$

This system can be further simplified by substituting the species equations with a scalar equation that tracks the position of the flame. An equation for the temperature can be derived from the enthalpy equation and then a source term will account for the energy released by the chemical reactions. This approach will be described later in this chapter.
2.3 Combustion regimes

The governing equations introduced above are suitable to compute laminar premixed flames. However, if we could resolve all flow and chemical length and time scales (with a Direct Numerical Simulation) the same equations could be solved for turbulent combustion without need of closure models for the turbulence and the chemistry. Unfortunately in general this is still far from possible because of computer hardware limitations.

It is important to know under which regime of combustion our system is operating. In a premixed system several non-dimensional parameters become relevant: the turbulent Reynolds, the Damköhler and the Karlovitz numbers. The turbulent Reynolds number is

$$Re_t = \frac{u'L}{\nu}$$

with $u'$ being the turbulence intensity, $L$ some integral length scale related to the flow and $\nu$ the kinematic viscosity. The Damköhler number is defined as the ratio between the turbulent time scale, $\tau_l$, and the chemical time scale, $\tau_f$,

$$Da = \frac{\tau_l}{\tau_f}$$

while the Karlovitz number is defined as the ratio between the chemical time scale and the Kolmogorov time scale, $\tau_\eta$ (where $\eta$ is the Kolmogorov length scale indicating the size of the smallest turbulent eddies),

$$Ka = \frac{\tau_f}{\tau_\eta} = \left( \frac{\delta_f}{\eta} \right)^2$$

with $\delta_f$ the flame thickness.
The structure and propagation characteristics of a laminar or turbulent premixed flame can be represented in a combustion diagram such as the one shown in Fig. 2.2, the so-called Borghi diagram. On the $y$-axis is indicated the ratio between the velocity fluctuation ($u'$) and the laminar burning speed ($s_L$), while on the $x$-axes we have the ratio between the integral length scale and the thermal flame thickness. The regime of particular interest for our study is the flamelet regime (wrinkled and corrugated) that is characterized by $Ka < 1$ and $\delta_f < \eta$: turbulence can only wrinkle or corrugate the flame without affecting its inner structure (flamelet assumption). In the wrinkled regime ($u' < s_L$) the turnover velocity of the eddies is not large enough to compete with the advancement of the flame front with the laminar burning speed $s_L$ and therefore laminar propagation dominates. The corrugated flamelets regime is characterized by $u' > s_L$. In this regime the entire reactive-diffusive flame structure is embedded within eddies of the size of the Kolmogorov scale where the flow is quasi-laminar hence the flame structure is not perturbed by turbulent fluctuations and remains quasi-steady (Peters, 2000). On the other hand, in the distributed reaction regime is $\eta < \delta_f$ and turbulent eddies can penetrate into the flame, thereby modifying the flame structure. Studies by Poinso and Veynante (1991) and Chen and Peters (1996) have suggested that even in the distributed reaction regime the reaction zone is very thin and of the order of the laminar flame thickness. This result is derived from the observations that for large Karlovitz number, Reynolds number and Damköhler number, turbulent eddies can enter the preheat zone and thus, increase turbulent transport of heat and species away from it. This re-distribution can thicken the preheat zone. However, eddies do not penetrate into the reaction zone since they are dissipated by increased viscous dissipation near the flame. Using these results, Peters (2000) has introduced a new boundary into the regimes diagram defined by $l_\delta = \eta$ (where $l_\delta$ is the thickness of the inner layer of the flame) and the distributed reaction regime has been considered as the extended flamelets or the thin-reaction zone regime.
The key implication is that modified versions of models valid for flamelets regime can be used in the thin-reaction-zones regime, as recently described by Peters (2000).

2.4 Estimates of length and time scales involved in premixed combustion

In this paragraph, we want to give order of magnitude estimates of the time and length scales that are generally involved in the combustion processes. After a general overview, we underline those scales that are important for our study of a flame deflagration with obstacles.

The complexity of the combustion phenomenon has to be captured with reasonable accuracy. Most practical combustion systems (for instance a gas turbine or a deflagration in a tunnel) are confined or semi-confined systems where operational design and size constraints define the scale of the device. Moreover instabilities can arise from the interaction between the combustion wave and the acoustic field. Here different phenomena are involved and different length and time scales. Three mechanisms interact between them in a non-linear manner: acoustic fluctuations, fluid motion and combustion heat release. They are characterized as acoustic, vorticity and entropy waves, although only the acoustic field behaves as a wave while both vorticity and entropy ‘waves’ are convected at the local flow velocity (Menon, 2004). If these modes interact in a confined domain, it is clear that there has to be some overlap between their respective time and length scales. In those cases where the acoustic feedback is not dominant with small contribution to the total energy of the system, the acoustic terms in the governing equations can be removed (low Mach number approximation). Using flow velocity and laminar burning speed of \(O(1)\text{m/s}\) and geometry scale \(D\) of \(1\text{m}\), the Reynolds number is estimated around \(O(10^5)\).

We can assume that the integral length scale, \(l\), is of the order of the diameter of the obstacles in the domain, thus of the order \(O(10^{-1} - 10^0)\text{m}\).

The integral scale represents the characteristic ‘energy containing’ eddies that play a major role in energy and scalar transport in shear flows. For the above length scales, the turbulent Reynolds number \(Re_l = u'l/\nu\), is estimated in the range \(10^2 - 10^4\). The higher value reflects the higher level of turbulence in the regions of higher shear. By using inertial range scaling law, \(l/\eta \approx Re^{3/4}\), the Kolmogorov scale \(\eta\) can be estimated to be in the range \(10^{-2} - 10^{-3}\) m. Thus, fluid dynamic length scales characteristic of vortex motion are in the range \(10^{-3} - 10^{-1}\) m. This is a three order of magnitude range in scales of interest. Furthermore, the reaction zone thickness (range of \(10^{-3} - 10^{-5}\) m) is substantially smaller than the effective flame thickness. Moreover, by considering the typical acoustic length scales of interest being in the range of \(10^{-2} - 10^0\) m, then there are at least six decades of scales interacting in a turbulent reacting flow with significant disparity between the characteristic length scales where vortex motion, acoustic fluctuations and heat release respectively dominate. In addition, there are also the time scales to be considered. These are about \(0.1 - 1\) s for the flow and \(O(10^{-6})\) or less for the fastest chemical reactions. This wide range of scales offers a serious challenge to both experimentalists and modelers.

Experimental diagnostic tools and simulation models both have to be refined well enough to capture this wide range of scales accurately. Direct Numerical Simulation tool (DNS) resolves all length (and time) scales from the largest energy containing (integral)
to the smallest dissipative (Kolmogorov) scale. However, even for non-reacting flows, estimates show (Moin, 1998) that the number of grid points required to resolve all the length scales in a 3D domain goes as \( N \sim Re^{9/4} \) which means that even for a moderate Reynolds number of \( Re = 10^4 \) the grid points needed for a DNS is \( N \approx 10^9 \). This requirement along with the fact that to obtain data for statistical analysis sufficient time-evolution of the flow field must be simulated makes DNS of realistic systems (industrial or environmental), even in the case of non-reacting flows, impossible for the foreseeable future (Menon, 2004). Most DNS studies, as a result, are confined to simple flows and to low Re \( (O(10^3)) \) flows. Extension of DNS to reacting flows is even more problematic. In flows of practical interest, the flame structure can be very thin (in the premixed flamelet regime the flame thickness, \( \delta_f \) can be orders of magnitude smaller than smallest turbulent scale, \( \eta \)). Thus, even when the Kolmogorov scale is resolved, thin flames are not resolved. Several approaches have been attempted to circumvent this limitation (J. M. Burgerscentrum combustion course, 2005) and significant insight into flame-turbulence interactions have been obtained using these approaches. Here we mention two widely used approaches: the use of modified chemistry to artificially thicken the flame in order to resolve it (Collin, 2000; Poinsot, 2001) and the use of a thin flame model where the flame front is tracked without resolving it (Williams, 1985). In this thesis we follow an approach similar to the latter one. The non-reactive Navier-Stokes equations are solved directly while the flame structure in the flamelets regime is modeled with a level set method to overcome the stiffness due to the chemistry.

2.5 The Low Mach number approximation

Many combustion applications are characterized by low speed, both for the flow and the flame propagation. Also in our study we consider systems with a typical velocity of the order \( O(10^0 - 10^1) \) m/s. This means that the velocities are much smaller than the speed of sound, so that density variations due to pressure variations can be neglected. This is important from a computational point of view because, as we will show, we can remove the acoustic terms (and therefore the acoustic time and length scales) from the governing equations and save computational time. For these cases the Mach number is small and an approximated version of the Navier-Stokes equations can be derived.

A low Mach number approximation (used for the first time by Relm and Baum, 1978; McMurtry, 1986; Majada, 1991) is suitable to characterize most of deflagration cases with appreciable advantages regarding the computational cost. Now, let us turn to the derivation of this approximation. We consider the continuity, the momentum and the enthalpy equations plus the equation of state for ideal gases. The species conservation equations are not considered because a simplified treatment of the chemistry is used. This treatment consists of deriving a temperature equation from the enthalpy equation. Then a source term, \( \bar{\omega}_s \), in the temperature equation will account for the chemistry. It is convenient to make the governing system of equations non-dimensional by scaling each quantity and operator with reference values (the subscript '0' indicates reference quantities while the superscript '*' denotes dimensional quantities):

\[
\rho = \frac{\rho^*}{\rho_0}, \quad p = \frac{p^*}{\rho_0 RT_0}, \quad u = \frac{u^*}{U_0}, \quad T = \frac{T^*}{T_0}, \quad h = \frac{h^*}{RT_0}, \quad \dot{\omega} = \frac{\dot{\omega}^*}{T_0 RT_0}
\]  \( (2.28) \)
\[
x = \frac{x^*}{L_0}, \quad t = \frac{t^*}{U_0}, \quad \nabla = \frac{\nabla^*}{U_0}, \quad \tau = \frac{\tau^*}{U_0} \\
\mu = \frac{\mu^*}{\mu_0}, \quad \lambda = \frac{\lambda^*}{\lambda_0}
\]  
(2.29)

Some non-dimensional parameters (Reynolds, Prandtl and Mach numbers) are also introduced:

\[
Re_0 = \frac{\rho_0 U_0 L_0}{\mu_0}
\]  
(2.30)

\[
Pr_0 = \frac{c_p \mu_0}{\lambda_0}
\]  
(2.31)

\[
M_0 = \frac{U_0}{\sqrt[\gamma]{RT_0}}
\]  
(2.32)

with \(\gamma\) being the ratio between the specific heats of the mixtures at constant pressure and volume, \(\gamma = \frac{c_p}{c_v}\). The set of non-dimensional equations reads,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0
\]  
(2.33)

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\frac{1}{\gamma M_0^2} \nabla p + \frac{1}{Re_0} \nabla \tau
\]  
(2.34)

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho hu) = \frac{\partial p}{\partial t} + \frac{\gamma M_0^2}{Re_0} \nabla \cdot (\tau \cdot u) + \frac{\gamma}{Re_0 Pr_0 (\gamma - 1)} \nabla \cdot (\lambda \nabla T)
\]  
(2.35)

\[
p_0 = \rho T
\]  
(2.36)

Let us consider the modified Mach number \(\tilde{M} = \sqrt[\gamma]{M_0}\). Following the asymptotic derivation given by Müller (1998) we can identify terms that can be neglected as \(\tilde{M}\) becomes small. Each variable can be expressed in power series of \(\tilde{M}\) (with subscripts \(0, 1, 2\) we indicate the order of the perturbation). This means that each flow variable or term, \(f(x, t)\), is expanded (up to second order) like

\[
f = f_0(t) + \tilde{M}^1 f_1(x, t) + \tilde{M}^2 f_2(x, t)
\]  
(2.37)

To show how this asymptotic derivation works we use an example. We can expand the term \(\rho u\) in two ways: as a single term \((\rho u)\) and as the product of its two expanded variables \((\rho\) and \(u\)),

\[
\rho u = (\rho u)_0 + \tilde{M} (\rho u)_1 + \tilde{M}^2 (\rho u)_2 =
\]

\[
(\rho_0 + \tilde{M} \rho_1 + \tilde{M}^2 \rho_2)(u_0 + \tilde{M} u_1 + \tilde{M}^2 u_2) =
\]
\[ \rho_0 u_0 + \tilde{M}(\rho_0 u_1 + \rho_1 u_0) + \tilde{M}^2(\rho_0 u_2 + \rho_1 u_1 + \rho_2 u_0) \] (2.38)

Between the first and the last side of the previous relation we can sort the terms according to the powers of \( \tilde{M} \):

\[
[(\rho u)_0 - \rho_0 u_0] + [(\rho u)_1 - (\rho_0 u_1 + \rho_1 u_0)]\tilde{M} + \\
[(\rho u)_2 - (\rho_0 u_2 + \rho_1 u_1 + \rho_2 u_0)]\tilde{M}^2 = 0
\] (2.39)

Because the expansions we used are supposed to hold for arbitrary small values of \( \tilde{M} \) then the coefficients of the powers of \( \tilde{M} \) must be zero and we obtain the zeroth, first and second order mass flux:

\[
(\rho u)_0 = \rho_0 u_0 \] (2.40)

\[
(\rho u)_1 = \rho_0 u_1 + \rho_1 u_0 \] (2.41)

\[
(\rho u)_2 = \rho_0 u_2 + \rho_1 u_1 + \rho_2 u_0 \] (2.42)

In a similar way it is possible to expand all the other terms and substitute the zero order terms in the original equations. The pressure in the momentum equations can be expanded as

\[
p = p_0 + \tilde{M} p_1 + \tilde{M}^2 p_2
\] (2.43)

Substituting the previous expression in the momentum equation, expanding all its terms in a similar manner and ordering with the powers of \( \tilde{M} \) we obtain

\[
\tilde{M}^{-2} \nabla p_0 + \tilde{M}^{-1} \nabla p_1 + \nabla p_2 + \frac{\partial \rho_0 u_0}{\partial t} + \nabla \cdot (\rho_0 u_0 u_0) - \frac{1}{Re_0} \nabla \tau_0 = 0
\] (2.44)

which has a form like \([\ldots] \tilde{M}^{-2} + \ldots + [\ldots] \tilde{M} + [\ldots] \tilde{M}^2 = 0 \) requiring the terms in square brackets to vanish. Thus, for the zero and first order pressure terms one has

\[
\tilde{M}^{-2} \nabla p_0 = 0
\] (2.45)

\[
\tilde{M}^{-1} \nabla p_1 = 0
\] (2.46)

Equations (2.45) and (2.46) state that \( p_0 \), which is interpreted as the thermodynamic pressure, and \( p_1 \), which is interpreted as the acoustic pressure, are uniform in space. In case of combustion in an open domain, \( p_0 \) will be fixed to its value of reference which is assumed to be constant in time. Since all the terms with \( \tilde{M}^{-2} \) and \( \tilde{M}^{-1} \) have dropped out from (2.45) and (2.46), the second order momentum equation (with the second order pressure term \( p_2 \)) must be included into the original momentum equation in order to close the system. The momentum becomes

\[
\frac{\partial \rho_0 u_0}{\partial t} + \nabla \cdot (\rho_0 u_0 u_0) + \nabla p_2 = \frac{1}{Re_0} \nabla \cdot \tau_0
\] (2.47)

Here \( p_2 \) is interpreted as the hydrodynamic pressure. We note that the acoustic pressure \( p_1 \) does not appear in any term of the momentum equation. Regarding the total pressure
(static plus dynamic) in the low Mach number context, it can be shown that its non-dimensional form, scaled with the ambient pressure of reference $P_\infty = \rho_0 R T_0$, reads

$$ P_{Tot} = \frac{P_{Tot}^*}{P_\infty} = p_0 + \dot M^2 p_2 + \frac{\rho_0 U_0^2}{P_\infty} \frac{1}{2} \rho u_0^2 $$

(2.48)

Moreover, if we consider the thermodynamic pressure $p_0 = \text{const}$ (for instance for combustion in open domain) the term $\frac{\partial p_0}{\partial t}$ in the lowest order energy equation will drop out.

It can be shown that after the asymptotic analysis we can re-write the system of equations in their zero Mach number limit (the subscripts '0' are removed, the hydrodynamic pressure is indicated with $p$ and the constant thermodynamic pressure with $P$):

$$ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 $$

(2.49)

$$ \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \frac{1}{Re} \nabla \cdot \tau $$

(2.50)

$$ \frac{\partial (\rho h)}{\partial t} + \nabla \cdot [\rho hu] = \frac{\gamma}{(\gamma - 1) Re Pr} \nabla \cdot (\lambda \nabla T) $$

(2.51)

$$ P = \rho T $$

(2.52)

Note that in the energy equation the heating term due to viscous dissipation has dropped out as a result of the approximation.

An equation for the temperature can be derived from the enthalpy equation. At first let us use the definition of enthalpy, $h$, as the sum of the sensible, $h_s$, and the chemical enthalpy

$$ h = h_s + \sum_{i=1}^{N} h_{ref} Y_i $$

(2.53)

By using the last relation it can be shown that the equation for the sensible enthalpy reads

$$ \frac{\partial (\rho h_s)}{\partial t} + \nabla \cdot [\rho h_s u] = \frac{\gamma}{(\gamma - 1) Re Pr} \nabla \cdot (\lambda \nabla T) + \frac{\gamma \rho}{(\gamma - 1)} \dot \omega $$

(2.54)

where the source term $\dot \omega$ contains the contribution of the chemical enthalpy (Poinsoot and Veynante, 2001). A relation between sensible enthalpy, $h_s$ and sensible energy, $e_s$ holds

$$ h_s - \frac{P}{\rho} = e_s $$

(2.55)

with

$$ e_s = \frac{1}{\gamma - 1} T $$

(2.56)
Then, by using the last two relations in the equation for the sensible enthalpy (2.54) it can be easily shown that the temperature equation takes the following form

\[
\frac{\partial T}{\partial t} + u \nabla \cdot T = \frac{1}{\rho \text{RePr}} \nabla \cdot (\lambda \nabla T) + \dot{\omega}
\]  

(2.57)

The source term \( \dot{\omega} \) takes into account the heat released by the combustion process at the flame front and it will be modeled with a level set approach.

2.6 Simplified combustion models based on a level set approach

For a simple one-step irreversible chemical scheme (reactants → products) the flame can be described using a progress variable \( c \) which, for instance, can be defined such that \( c = 0 \) in the fresh gases and \( c = 1 \) in the fully burnt gas:

\[
\frac{\partial (\rho c)}{\partial t} + \nabla \cdot (\rho u c) = \nabla \cdot (\rho D \nabla c) + \dot{\omega}
\]  

(2.58)

\( D \) being a diffusion coefficient. The variable \( c \) can be defined as reduced temperature, \( T_{\text{red}} \),

\[
c = \frac{T - T_0}{T_f - T_0} = T_{\text{red}}
\]  

(2.59)

with \( T \) being the local temperature, \( T_0 \) the temperature of the fresh gases and \( T_f \) the adiabatic flame temperature. If the system is considered as composed only of two species, the burnt and the fresh gases, then the progress variable can also be defined as reduced mass fraction (Veynante, 2002)

\[
c = \frac{Y_f - Y_f^u}{Y_f^b - Y_f^u}
\]  

(2.60)

with \( Y_f \) being the local fuel mass fraction, \( Y_f^u \) the fuel mass fraction in the unburnt gas and \( Y_f^b \) the fuel mass fraction in the fully burnt gas. Now, if we take the Lewis number unity the two definitions of progress variable are equivalent. In this case the temperature and the species equation reduce to the same equation for the evolution of \( c \). This means that we can use the temperature equation with a chemical source term while the species equations can be removed from the system. Now, according to the definition of reduced temperature, eq. (2.59), the reduced local fuel mass fraction left at a certain instant, \( \hat{Y}_f \), is expressed by

\[
\hat{Y}_f = (1 - T_{\text{red}})
\]  

(2.61)

The source in the temperature equation still depends on the heat of each reaction and on the related rate of reaction. Several databases (J. M. Burgerscentrum combustion course, 2005) have been built by solving in advance detailed or reduced chemical mechanisms for combustion problems in one dimension. It is possible to use these databases
during the calculations. Usually, for a certain flame location one can specify the temperature and other properties at one point and then, from the database, the source term is obtained. However, if the flame could be considered as a thin geometric entity (surface) which propagates in the domain and which separates the flow in burnt and unburnt zones, then a simplified source term can be built (based on the one step reaction assumption) such that it is only function of the position of the flame. This approach is possible in the so-called flamelet regime. The flamelet regime holds in premixed laminar or weakly turbulent combustion cases where the flame propagation (thus the flame speed) depends on the characteristics of the fresh mixture and the inner structure of the flame can be considered independent of the flow. In these cases a geometric approach can be used based on a level set scalar function which tracks the flame.

2.6.1 Level set formulations

A level set or isosurface is a three-dimensional analog of an isoline. It is a surface that represents points of a constant value (e.g., position or temperature) within a volume of space. A level set is also called an implicit curve, emphasizing that such a curve is defined by an implicit function. The G-equation model proposed by Kerstein and Williams (1988) is based on flamelet modeling assumptions and uses a level set method to describe the evolution of the flame front. The level set function \( G \) is a scalar field defined such that the flame front position is at \( G = G_0 \) and that \( G < G_0 \) in the unburned mixture. The \( G \) equation describes the evolution of the front as a level set function that is continuous through the flame front (Pitsch, 2005). An implicit representation of the instantaneous flame surface can be given as

\[
G(x_f, t) - G_0 = 0
\]  

which defines the level set function \( G \). Here, \( t \) is the time and \( x_f \) is the vector of the flame front location. Differentiating the previous equation with respect to time one obtains

\[
\frac{\partial G}{\partial t} + \frac{dx_f}{dt} \cdot \nabla G = 0
\]  

The flame front propagation speed is given by

\[
\frac{dx_f}{dt} = u + s_l n
\]  

where \( u \) is the local flow velocity, \( s_l \) is the laminar burning speed and \( n \) is the flame normal defined to be directed into the unburned mixture and its expression is

\[
n = -\frac{\nabla G}{|\nabla G|}
\]  

The laminar burning speed may be different from the unstrained laminar burning speed (let us call it \( s_l^0 \)) because of the shape of the flame that changes during the propagation forming points where the speed is higher than \( s_l^0 \) due to the effect of the flame stretch.
Fig. 2.3 Flame surface

The definition of stretch was first introduced by Karlovitz (Tomboulides, 2004). In fig. 2.3 a flame surface, $S$, is defined by a constant value of the level set $G = G_0$. $S$ has velocity $U$ while the fluid velocity at the surface is $u$. The definition of the stretch at any location $P$ of the surface is

$$
S_\kappa = \frac{1}{A} \frac{dA}{dt}
$$

(2.66)

with $A$ an infinitesimal area around point $P$. The time derivative here is Lagrangian, i.e. for a reference frame attached to the flame front. The units of $S_\kappa$ are $s^{-1}$. It can be shown mathematically that the Karlovitz definition of the stretch is equivalent to

$$
S_\kappa = \nabla_t \cdot u_t + (U \cdot n) (\nabla_t \cdot n)
$$

(2.67)

where $\nabla_t$ is the gradient on the surface, $\nabla_t = a \frac{\partial}{\partial a} + b \frac{\partial}{\partial b}$ with $a$ and $b$ unit vectors perpendicular to the normal surface vector $n$ and $u_t$ is the component tangential to the surface of the fluid velocity $u$. Moreover, it can be shown that $u_t$ is equivalent to $u_t = n \times (u \times n)$ with '×' denoting the vector cross product. Now, because one has $\nabla = \nabla_t + \nabla_n$, $\nabla_n \cdot u_t = 0$ and $\nabla_n \cdot n = 0$

then the stretch can be written as

$$
S_\kappa = \nabla \cdot u_t + (U \cdot n) (\nabla \cdot n)
$$

(2.68)

Substituting the expression for $u_t$ it becomes

$$
S_\kappa = -n \cdot \nabla \times (u \times n) + (U \cdot n) (\nabla \cdot n)
$$

(2.69)

The first term in the previous expression contains the contribution to the stretch due to the effect of flow non-uniformity via $u$. This term is often called ‘strain’ term. The second term represents the effect of the flame curvature, $\kappa$, defined as
\[ \kappa = \nabla \cdot n \]  

(2.70)

By using the Markstein parameter \( L_M \) and an asymptotic analysis, Pelce and Clavin (1982) gave an expression for \( s_l \) which contains the contribution of the strain and of the curvature:

\[ s_l = s_L^0 - s_L^0 L_M \nabla \cdot n + L_M n \cdot (\nabla u) \cdot n \]  

(2.71)

The Markstein length is of the order of the diffusive flame thickness \( \delta \) which is usually defined in terms of unburned mixture properties,

\[ \delta \sim \lambda/\rho s_l \]  

(2.72)

For a mixture with constant properties, \( L_M \) can be evaluated with (Clavin and Joulin, 1983)

\[ L_M = \frac{T_f}{T_f - T_u} \ln \left( \frac{T_f}{T_u} \delta \right) \]  

(2.73)

where \( T_f \) and \( T_u \) are the flame temperature and the unburnt mixture temperature.

The original equation for the burning speed derived by Pelce and Clavin does not account for the effect of expansion of the burnt gases with respect to the fresh one. This can be taken into account (Piana, 1997) by considering the ratio between the density of the fresh and burnt gases. Then, eq. (2.71) is modified in:

\[ s_l = \left[ s_L^0 - s_L^0 L_M \nabla \cdot n + L_M n \cdot (\nabla u) \cdot n \right] \frac{\rho_u}{\rho} \]  

(2.74)

From the combination of the previous equations the instantaneous \( G \) equation reads

\[ \frac{\partial G}{\partial t} + u \cdot \nabla G = s_l |\nabla G| \]  

(2.75)

which is valid at the flame surface only. The remaining \( G \) field is arbitrary and commonly defined to be a distance function. If \( G \) is a distance function, its value at any position gives always the distance to the flame front. This is possible only if is \( |\nabla G| = 1 \) everywhere. We will see in the next chapter that this constraint can be achieved with a numerical procedure called reinitialization. Once \( G \) is a distance function a direct coupling between the \( G \) field and the temperature of the mixture is possible. One way to do this is by the model proposed by Treurniet (2002). In this approach the temperature is linked directly to the \( G \) equation by a smoothed Heaviside formulation

\[ T = T_u \left( 1 + \frac{\tanh \frac{G - G_0}{\delta_n} + 1}{2} \delta_n \right) \]  

(2.76)

where \( T \) is the local temperature, \( T_u \) is the temperature of the unburnt gas, \( G_0 \) indicates the zero level of the distance function, \( \delta_n \) is an effective thickness (chosen \textit{a priori}) proportional to the flame thickness and \( \tau_h \) is the heat release parameter defined as
$$\tau_h = \frac{T_f - T_u}{T_u} \quad (2.77)$$

This is equivalent to imposing a temperature profile through the flame front with a temperature jump spread over the thickness $\delta_h$. Obviously, the numerical implementation does not allow us to use an infinitely small $\delta_h$ as required by the flamelet assumption, therefore the simulated flame is a thick surface. This is a common limitation for all the G-equation models.

In the approach by Treurniet the energy equation is not solved and the density is coupled to the temperature through the equation of state for the gas mixture. This model gave encouraging results in the simulation of the well known Darrieus-Landau instability and the baroclinic production of vorticity. The last instability is due to the flame front density and pressure gradients not being aligned. Because the energy equation is absent this model does not permit the modeling of heat transfer between the flow and the possible obstacles present in the domain. It was also proved to be a useful tool for understanding the main characteristics of the interaction between turbulence and combustion in the low Mach number limit (Treurniet, 2006).

Another model to couple the temperature $T$ with the scalar $G$ is represented by the 'temperature reconstruction method' (im, 1995, and Kim, Menon and Mongia, 1999). The temperature field is directly estimated from the $G$ field as

$$T = T_u + \frac{Q}{c_p} H(G - G_0) \quad (2.78)$$

where $Q$ is the reaction heat release and $H$ denotes a smoothed Heaviside function. This approach does not require a balance equation for the energy but is not applicable when heat losses or high compressibility effects occur (Veynante and Vervisch, 2002).

Another approach consists of the 'estimate of the heat release rate from the G field' (Piana et al. 1997). $G$ is used to estimate the heat release rate to be incorporated in the balance energy equation as a source term spread on a thickness $\delta$ by a smoothing function. In this way, heat losses and compressibility effects may be included. In the approach followed in this thesis the source term in the energy equation is modeled as function of the G-equation. $G$ tracks the flame and the source releases energy only at the position of the front. Following a similar derivation like the one proposed by Piana (1997) we can write

$$\dot{\omega}(G) = \tau_h \left( \frac{T_f}{T_u} - T \right) \frac{s_l}{\delta} F(G) \quad (2.79)$$

The term $\left( \frac{T_f}{T_u} - T \right)$ is the fuel mass fraction. $F(G)$ is a shape function which spreads the flame over few grid cells. It can be defined in different ways, for instance as a sum of Heaviside functions or a hyperbolic cosine. Here we define $F(G)$ as a Gaussian with a characteristic parameter $\delta$ and the source reads

$$\dot{\omega}(G) = \tau_h \left( \frac{T_f}{T_u} - T \right) \frac{s_l}{\delta} \exp \left( -\frac{G^2}{2\delta^2} \right) \quad (2.80)$$
It is important here to clarify the definition of flame thickness. Following the definitions for simple chemistry given by Poinso and Veynante (2001), we can consider a diffusive flame thickness

\[ \delta = \lambda / \rho c_p s_l \quad (2.81) \]

and a flame thickness obtained by using the temperature profile:

\[ \delta_f = \frac{T_{burnt} - T_0}{\max \left( \left| \frac{dT}{dz} \right| \right)} \quad (2.82) \]

There are correlations to relate these two thicknesses like, for instance, the relationship proposed by Blint (1986) which expresses a linear proportionality between \( \delta \) and \( \delta_f \). Usually \( \delta \) is smaller than \( \delta_f \) by a factor of order 5 (Poinso and Veynante, 2001). For our source with Gaussian distribution, we interpret the parameter \( \delta \) as the diffusion flame thickness chosen such that the full width at half maximum of the distribution is of the order of a grid cell size. As suggested by Poinso and Veynante, \( \delta_f \) can be evaluated with a first flame computation. In our work, once \( \delta_f \) is evaluated with a first preliminary computation, \( \delta \) is chosen according to the profile of \( \delta_f \) and used for a second computation (see chapter five).

There are several advantages for using a \( G \)-equation model rather than numerical simulation with Arrhenius-type chemistry. First, since the flame front is described by a contour of the smooth function \( G \) complex changes in the propagating front can be easily captured. Secondly, since the numerical stiffness due to Arrhenius chemistry with large activation energy is removed in favor of a flamelet whose structure is given \( a \ priori \), the computational cost can be significantly reduced. Furthermore, the modification of the flame structure is accounted for by the flame-speed relation in a parametric manner. The coupling between the hydrodynamic field and the flame is simply taken into account by the Markstein parameter \( L_M \) in eq. (2.74). This is important in validating the existing predictions of turbulent flame speed which are often based on the assumption of constant \( s_l = s^0_L = s_L = \text{const.} \)

The \( G \)-equation is also a useful tool for understanding important issues in turbulent premixed combustion such as the determination of the turbulent flame speed, \( s_T \), as function of flow quantities such as the turbulence intensity \( u' \). The agreement among the various results is far from being satisfactory (Im, 1995). However, there is agreement on the fact that the determination of \( s_T \) in the flamelet regime is based on Damköhler’s idea that the increase in the flame speed is proportional to the area increase which can be related to the turbulent intensity,

\[ \frac{s_T}{s_L} = \frac{A_T}{A_L} \sim 1 + C \left( \frac{u'}{s_L} \right)^q \quad (2.83) \]

where \( A_T \) is the total surface area of the wrinkled front and \( A_L \) the cross section area normal to the direction of propagation. The parameters \( C \) and \( q \) are empirically determined (Im, 1995).

One of the issues in the simulation of such flames is that variable density due to heat release creates large density jumps between burnt and unburnt regions (usually density ratios higher than three). This can often induce instability in the numerical schemes
especially if a low order scheme is used in order to save computational time. We will show a remedy to this common problem in chapter three.

Another specific issue with $G$-equation approaches is that the flame speed depends on the stretch and this term can give large numerical error which can invalidate the simulation. We will discuss this in chapters three and five.
Chapter 3

A Model for Premixed Flames with High Density Ratios

3.1 Introduction

In the previous chapter we have introduced a level set-based model to mimic the chemistry. In this approach there are no species equations to be solved and the computational effort is considerably reduced. However, other numerical difficulties arise when one has to model flames which generate high variations of density between the fresh mixture and the burnt gases. This is because steep gradients of flow quantities and temperature values appear due to the fast heat release. In effect, the dynamics of the energy source term consists of an ignition step during which a strong temperature gradient is introduced in the system until the source reaches the adiabatic condition. During this step the numerical scheme for the governing equations should be able to handle the strong density gradients. Two main issues need to be addressed. One is the time integration of the temperature equation with steep source term. The other issue is the calculation of the time derivative of the density that is used to build the Poisson equation in the pressure correction algorithm.

There exist $G$-equation methods where no heat transfer is considered and no source term has to be integrated. One of these methods is the pure $G$-equation model proposed by Treurniet (2002). In this model there is no energy equation to be solved and therefore no source needs to be ignited. Instead, smooth temperature and density profiles are chosen from the beginning of the calculation. With the pure $G$-equation approach high density ratios between burnt and unburnt regions can be easily handled. Generalizations of this method, for instance to include obstacles with heat release is not feasible. In this work heat transfer is considered and the issues mentioned above are handled as we describe in this chapter. The momentum equation and the energy (temperature) equation are coupled by the equation of state. The source term in the energy equation is a function of the level set variable $G$. The spatial discretization of the momentum and the continuity equations is done with a second order finite volume method (Hirsch, 1988) and the time integration is based on a third order Adams-Bashforth scheme (AB3). For the $G$-equation the space discretization uses a local third order WENO scheme (Jiang and Peng, 2000),
while for its time integration AB3 is used. The same WENO scheme is used for the spatial discretization of the convective term in the temperature equation while the discretization of the diffusive term is carried out using a central difference scheme. An IMEX scheme (‘implicit’ integration of the source and ‘explicit’ integration of the advection-diffusion terms) is used for the time integration of the temperature equation. The IMEX scheme used in this approach was proposed by Pareschi (2001). Implicit-explicit schemes represent a well known numerical technique but they have only recently started to be applied to combustion problems and are under continuous development (Lindblad, 2006).

We will show that the combination of the new pressure correction together with the IMEX scheme is a good candidate for modeling of high density ratios flames. In addition, a strategy is presented to deal with the effect of the numerical error produced during the computation of the stretch term in the propagation velocity of the $G$-equation. This is important because the stretch modifies the propagation flame speed and therefore the shape of the front.

### 3.2 The integration of the energy equation with source term

The temperature equation is given in chapter two, eq. (2.57). For easy of reference it is repeated here,

$$\frac{\partial T}{\partial t} + u \nabla \cdot T = \frac{1}{\rho} \frac{1}{RePr} \nabla \cdot (\lambda \nabla T) + \dot{\omega}$$  \hspace{1cm} (3.1)

with source term $\dot{\omega}$ defined as

$$\dot{\omega} = \tau_h \left( \frac{T_f}{T_u} - T \right) \frac{s_l}{\delta} \exp \left( -\frac{G^2}{2\delta^2} \right)$$  \hspace{1cm} (3.2)

where $T$ is the local temperature, $T_u$ the temperature of the unburnt gas, $T_f$ the adiabatic flame temperature, $s_l$ the flame speed, $\delta$ the diffusive flame thickness, $\tau_h$ the heat release parameter and $G$ the level set variable. The source can be written as

$$\dot{\omega} = \frac{s_l}{\delta} \tau_h \left( \frac{T_f}{T_u} - T \right) \exp \left( -\frac{G^2}{2\delta^2} \right) = \frac{1}{\epsilon} S$$  \hspace{1cm} (3.3)

with $\epsilon = \frac{\delta}{s_l}$ and $S = \tau_h \left( \frac{T_f}{T_u} - T \right) \exp \left( -\frac{G^2}{2\delta^2} \right)$. Now, let us represent the convective and diffusive terms as

$$R(T) = -u \nabla \cdot T + \frac{1}{\rho} \frac{1}{RePr} \nabla \cdot (\lambda \nabla T)$$  \hspace{1cm} (3.4)

Then the temperature equation can be written

$$\frac{\partial T}{\partial t} = R(T) + \frac{S(T)}{\epsilon}$$  \hspace{1cm} (3.5)

$\epsilon$ is a parameter which controls the magnitude of the source term. It represents the time scale of the source. Eq. (3.5) can be seen as a system with relaxation term $(\frac{S(T)}{\epsilon})$. 

26
Methods for such systems have been an active area of research in the past (Lowrie and Morel, 1999) for applications in combustion, multi-phase flows and rarefied gas dynamics.

We integrate the temperature in time with the IMEX scheme proposed by Pareschi (2001). Pareschi’s scheme is a so-called time split scheme. Two implicit steps for the integration of the source, $S$, advance the temperature to two intermediate values $T^*$ and $T^{**}$ while the other terms, $R(T)$, are integrated in three steps with intermediate values for the temperature $T^{(1)}$ and $T^{(2)}$:

$$ T^* = T^n + \frac{\Delta t}{2\alpha - 1} \frac{(\alpha - 1)}{\varepsilon} S(T^*) $$

$$ T^{(1)} = T^n + \Delta t \alpha R(T^*) $$

$$ T^{**} = T^{(1)} + \frac{\Delta t}{\varepsilon} \left[ \xi S(T^*) + (1 - \xi) S(T^{**}) \right] $$

$$ T^{(2)} = T^n + \frac{\Delta t}{2\alpha} \left[ (2\alpha - 1) R(T^*) + R(T^{**}) \right] $$

$$ T^{n+1} = T^{(2)} + \frac{\Delta t}{2\alpha \varepsilon} \left[ (2\alpha - 1) S(T^*) + S(T^{**}) \right] $$

The coefficients $\alpha = 5/3$ and $\xi = 7/10$ result from a stability analysis performed by Pareschi (2001). For the implicit steps we use one iteration per time step.

### 3.3 Comparison of the IMEX scheme with an explicit scheme

In this section we show that the IMEX scheme allows for a larger time step than a conventional explicit scheme. Let us consider also an explicit method (AB3-EF) for the time integration of the energy equation, consisting of a third order Adams-Bashforth scheme for the advection and the diffusion terms (represented by $R$) and an Euler forward scheme for the source ($\dot{\omega}$):

$$ T^{n+1} - T^n = $$

$$ \frac{1}{12} \left[ 23R^n - 16R^{n-1} + 5R^{n-2} \right] \Delta t + \dot{\omega}^n \Delta t $$

(3.11)

To compare the two schemes we consider a simplified 1D model: an advection-diffusion equation with a linear source term $S(T)$. Advection velocity ($U$) and diffusion coefficients ($D$) are considered constant.
3.3.1 Advection-diffusion-source test

In this case we have,

\[
\frac{\partial T}{\partial t} + U \frac{\partial T}{\partial x} = D \frac{\partial^2 T}{\partial x^2} + S(T)
\]  
(3.12)

By using a change of variables, \( x' = x - Ut \) and \( t = t' \), and applying the chain rule, the previous equation can be written in a diffusive form,

\[
\frac{\partial T}{\partial t'} = D \frac{\partial^2 T}{\partial x'^2} + S(T)
\]  
(3.13)

To simplify the problem the source is taken as \( S(T) = \frac{T}{\pi} \). This diffusion equation with linear source has an exact analytical solution whose form is a sum of trigonometric functions weighted with coefficients depending on the initial and boundary conditions:

\[
\begin{align*}
T(x', t) &= \sum_{n=1}^{\infty} D_n e^{-\lambda_n t} \sin \frac{n\pi x'}{L} \\
D_n &= \frac{2}{L} \int_0^L T_n \sin \frac{2\pi x'}{L} dx'
\end{align*}
\]

with \( \lambda_n = \frac{Dn^2 \pi^2}{L^2} - \frac{\pi^2}{4} \) and \( T(0, x') \) initial condition. As boundary conditions we use \( T(t, x' = 0) = T(t, x' = L) = 0 \) with \( L = 0.15 \) being the size of the one dimensional domain and \( N = 100 \) the number of points. These parameters give \( L/N \) the same order of magnitude as \( dx \) used in the 3D computations discussed later in this thesis.

As initial condition we consider an impulsive temperature distribution given by

\[
T(0, x') = \frac{s_t}{\delta} \exp \left( -\frac{(x' - L/2)^2}{2\delta^2} \right)
\]  
(3.14)

with \( \delta = 0.0004 \) and \( s_t = (\epsilon^{-1})\delta \). As discussed in chapter two, \( \delta \) is interpreted as the diffusion flame thickness which is smaller than the thermal flame thickness. \( \delta \) is chosen such that the full width at half maximum of the distribution is of the order of a grid cell size. By increasing the quantity \( \epsilon^{-1} \) the spatial sharpness of the initial distribution increases. In this test we use \( \epsilon = 0.001 \) (which is consistent with the value used in the case of 3D simulations where \( s_t = 0.4 \)).

Eq. (3.12) is solved numerically with IMEX and AB3-EF schemes. An absolute error can be defined between the numerical and the analytical solutions:

\[
err = \frac{1}{N} \sum_{i=1}^{N} |\phi - \phi_{an}|
\]

where \( \phi \) is the numerical solution and \( \phi_{an} \) the analytical solution.

In table 3.1 the errors of the two schemes are shown for the case \( U = 1 \) and \( D = 1 \). The integration is performed from time zero till \( t = 10^{-5} \) with different time steps. In table 3.2 the same quantities are shown for the case \( U = 1 \) and \( D = 0.01 \) and the integration goes from zero to \( t = 10^{-3} \) for different time steps. It can be seen that the AB3-EF scheme diverges when the time step increases to \( 10^{-6} \) and \( 10^{-4} \) respectively (1).

\[1\] It is worth to mention here that we have also performed tests with another scheme based on AB3 for both the diffusive and the source terms. Also in this case we noted exploding calculations.
Table 3.1: Absolute error and maximum values for different time steps. Grid resolution 100 points. \( D = 1, U = 1 \) and \( \epsilon = 0.001 \). Integration until time \( 10^{-5} \).

<table>
<thead>
<tr>
<th>Number of points</th>
<th>( \Delta t )</th>
<th>error IMEX</th>
<th>error AB3-EF</th>
<th>maxval(T) IMEX</th>
<th>maxval(T) AB3-EF</th>
<th>maxval(T) exact</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>( 10^{-5} )</td>
<td>0.251</td>
<td>0.249</td>
<td>259.343</td>
<td>259.281</td>
<td>255.878</td>
</tr>
<tr>
<td>100</td>
<td>( 10^{-4} )</td>
<td>0.252</td>
<td>0.222</td>
<td>259.347</td>
<td>258.722</td>
<td>255.878</td>
</tr>
<tr>
<td>100</td>
<td>( 10^{-6} )</td>
<td>0.379</td>
<td>31197.969</td>
<td>261.400</td>
<td>-</td>
<td>255.878</td>
</tr>
</tbody>
</table>

Table 3.2: Absolute error and maximum values for different time steps. Grid resolution 100 points. \( D = 0.01, U = 1 \) and \( \epsilon = 0.001 \). Integration until time \( 10^{-3} \).

<table>
<thead>
<tr>
<th>Number of points</th>
<th>( \Delta t )</th>
<th>error IMEX</th>
<th>error AB3-EF</th>
<th>maxval(T) IMEX</th>
<th>maxval(T) AB3-EF</th>
<th>maxval(T) exact</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>( 10^{-6} )</td>
<td>9.139</td>
<td>9.135</td>
<td>696.288</td>
<td>696.043</td>
<td>688.627</td>
</tr>
<tr>
<td>100</td>
<td>( 10^{-5} )</td>
<td>9.137</td>
<td>9.095</td>
<td>695.579</td>
<td>692.936</td>
<td>688.627</td>
</tr>
<tr>
<td>100</td>
<td>( 10^{-4} )</td>
<td>8.765</td>
<td>450379.812</td>
<td>684.129</td>
<td>-</td>
<td>688.627</td>
</tr>
</tbody>
</table>

Now, let us consider different spatial resolutions: 25, 50, 100, 200 and 400 points. We consider \( U = 1, D = 0.01 \) and \( \epsilon = 0.001 \). Moreover we define \( \delta = \frac{\Delta x}{3} \) for each resolution. This is because a similar formulation for the diffusive flame thickness will be introduced later in this thesis for the case of realistic combustion simulations. A small time step is chosen (\( \Delta t = 10^{-9} \)) and the equations are integrated for 1000 time steps. In Table 3.3 are reported the errors of IMEX and AB3-EF schemes. With the refinement of the grid the errors reduce drastically. In Figure 3 we plot the L2 integral Root Mean Square (RMS) norm error for the IMEX scheme as function of the number of grid points. The solution is essentially accurate to second order.

Table 3.3: Absolute error for different grid resolutions. \( U = 1, D = 0.01 \) and \( \epsilon = 0.001 \). Integration for 1000 time steps. \( \Delta t = 10^{-9} \).

<table>
<thead>
<tr>
<th>Number of points</th>
<th>( \Delta x )</th>
<th>error IMEX</th>
<th>error AB3-EF</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.006</td>
<td>649.7161</td>
<td>649.7185</td>
</tr>
<tr>
<td>50</td>
<td>0.003</td>
<td>96.7029</td>
<td>96.7029</td>
</tr>
<tr>
<td>100</td>
<td>0.0015</td>
<td>20.9853</td>
<td>20.9854</td>
</tr>
<tr>
<td>200</td>
<td>0.00075</td>
<td>3.7240</td>
<td>3.7242</td>
</tr>
<tr>
<td>400</td>
<td>0.000375</td>
<td>0.3338</td>
<td>0.3339</td>
</tr>
</tbody>
</table>
Figure 3. The L2 (RMS) norm error for the IMEX scheme is shown as function of the grid resolution. The solution is essentially accurate to second order.

### 3.3.2 Stability Analysis

A numerical method whose vector solution at time \( n \) is \( Y_n \), is said absolute stable if there exists a matrix \( C \) of elements \( c_n \) such that

\[
|Y_{n+1}| \leq C |Y_n|
\]

with

\[
0 < c_n < 1 \quad \forall n
\]

For simple Cauchy problems (like \( y' = By \), \( y(0) = y_0 \) with \( y \in R^m \) and \( B \in R^{m \times m} \)) the matrix \( C \) can be easily calculated. Then the radius of the matrix \( C \) of absolute stability can be calculated and the stability region can be represented (more details can be found in Lambert, 1991 or Hirsch, 1988). However, as pointed out by Pareschi and Russo (2007), for a generic linear system \( y' = B_1y + B_2y \) if we want to integrate in time (for example with IMEX) the term \( B_1y \) explicitly and the term \( B_2y \) implicitly, then the stability matrix depends on the two matrices \( B_1 \) and \( B_2 \) and not only on their eigenvalues because in general these matrices do not have the same eigenvectors and they cannot be diagonalized simultaneously.

For simplicity, let us consider the diffusion equation with linear source,

\[
\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2} + \frac{T}{\epsilon}
\]  

\[(3.15)\]
We apply to this equation the Von Neumann analysis to derive the characteristic stability polynomial for the AB3-EF and the IMEX schemes. The fact that we remove the advection for the second case allows us to derive polynomials without complex coefficients. This simplifies the analysis. By considering periodicity in space we apply a Fourier transformation to separate the space from the time dependence by using the substitution $T^n_i = Y_n e^{j i \theta}$ where $n$ indicates the number of time step, $i$ is an integer and indicates the space position, $j = \sqrt{-1}$ is the imaginary unit and $\theta \in [0, 2\pi]$. By using central differences we can discretize eq. (3.15) for AB3-EF scheme as:

$$\frac{(Y_{n+1} - Y_n)}{\Delta t} e^{j i \theta} = \frac{D}{\Delta x^2} \left( \frac{23}{12} R^n - \frac{16}{12} R^{n-1} + \frac{5}{12} R^{n-2} \right) + \frac{Y_n e^{j i \theta}}{\epsilon}$$

with

$$R^n = Y_n e^{j (i+1) \theta} - 2Y_n e^{j i \theta} + Y_n e^{j (i-1) \theta}$$

By using the relation $e^{j i \theta} + e^{-j i \theta} = 2 \cos \theta$ and dividing by $e^{j i \theta}$ we find

$$\frac{Y_{n+1} - Y_n}{\Delta t} = \frac{2D}{\Delta x^2} (\cos \theta - 1) \left( \frac{23}{12} Y_n - \frac{16}{12} Y_{n-1} + \frac{5}{12} Y_{n-2} \right) + \frac{Y_n}{\epsilon}$$

Further, by considering $|Y_n| = |Y_{n-1}| = |Y_{n-2}| = \frac{Y_{n-3}}{\epsilon} = r$ we can write

$$\frac{1}{\Delta t} (r^2 - r) = \frac{2D}{\Delta x^2} (\cos \theta - 1) \left( \frac{23}{12} r - \frac{16}{12} + \frac{5}{12} r \right) + \frac{r}{\epsilon}$$

By rearranging the terms in the last relation the stability polynomial for AB3-EF is

$$r^3 - r^2 \left[ 1 + \frac{23}{12} \frac{2D}{\Delta x^2} (\cos \theta - 1) \Delta t + \frac{\Delta t}{\epsilon} \right] +$$

$$r \left[ \frac{16}{12} \frac{2D}{\Delta x^2} (\cos \theta - 1) \Delta t \right] - \left[ \frac{5}{12} \frac{2D}{\Delta x^2} (\cos \theta - 1) \Delta t \right] = 0$$

The scheme is stable if its polynomial has roots, $r$, such that $|r| \leq 1$.

Applying the same Von Neumann procedure we can find the stability polynomial of the IMEX scheme with root $r$ such that

$$r = \frac{Y_{n+1}}{Y_n} = 1 + \frac{\Delta t (2 \alpha - 1)}{(2 \alpha)} \frac{2D}{\Delta x^2} (\cos \theta - 1) +$$

$$\frac{\Delta t D}{2 \alpha \Delta x^2} \left[ \frac{2 \cos \theta + \frac{\Delta t \alpha}{(2 \alpha - 1) \epsilon} \frac{2D}{\Delta x^2} (1 + \cos 2 \theta - 2 \cos \theta)}{1 - \frac{(1 - \xi) \Delta t}{\epsilon}} \right] +$$

$$\frac{\Delta t \epsilon}{(1 - \frac{(1 - \xi) \Delta t}{\epsilon})} +$$
\[-\frac{\Delta t D}{\alpha \Delta x^2} \left[ 1 + \frac{\Delta t \alpha}{(1 - (\alpha - 1) \Delta t) \Delta x^2} \frac{2D}{\Delta x^2} (\cos \theta - 1) + \frac{\Delta t \xi}{\epsilon} \left( 1 - \frac{1}{(1 - (\alpha - 1) \Delta t) \epsilon} \right) \right] + \]

\[+ \frac{\Delta t (2\alpha - 1)}{2\alpha \epsilon} \left[ 1 - \frac{1}{(1 - (\alpha - 1) \Delta t) \epsilon} \right] + \]

\[+ \frac{\Delta t}{2 \alpha \epsilon} \left[ 1 + \frac{\Delta t \alpha}{(1 - (\alpha - 1) \Delta t) \epsilon(2\alpha - 1)} \frac{2D}{\Delta x^2} (\cos \theta - 1) + \frac{\Delta t \xi}{\epsilon} \left( 1 - \frac{1}{(1 - (\alpha - 1) \Delta t) \epsilon} \right) \right] \]

Now, let us consider the parameters used for the runs in Table 3.1 and Table 3.2 referring to the case when AB3-EF scheme fails. In the first case we considered \( D = 1, \epsilon = 0.001 \) and \( \Delta t = 10^{-6} \), while in the second case the values were \( D = 0.01, \epsilon = 0.001 \) and \( \Delta t = 10^{-4} \). For these two cases the maximum root \( r \) (that can be seen as growth factor for the numerical error) of the stability polynomials for AB3-EF and IMEX schemes are plotted versus \( \theta \) (Figs 3.1-3.3). In both cases only the IMEX scheme satisfies the stability condition \( |r| \leq 1 \).

Figs. 3.1 (left) and 3.2 (right). The advection-diffusion equation with source term is solved with AB3-EF and IMEX schemes for the case with \( D = 1, \epsilon = 0.001 \) and \( \Delta t = 10^{-6} \). The error growth factor for AB3-EF (left figure) is larger than unity meaning an unstable behaviour, while for IMEX (right figure) it is smaller than unity.
Figs. 3.3a (left) and 3.3b (right). The advection-diffusion equation with source term is solved with AB3-EF and IMEX schemes for the case with $D = 0.01, \epsilon = 0.001$ and $\Delta t = 10^{-4}$. The error growth factor for AB3-EF (left figure) is larger than unity meaning an unstable behaviour, while for IMEX (right figure) it is smaller than unity.

In the particular case shown in figs. 3.1 and 3.2 (the same applies to the case in figs. 3.3a and 3.3b), the maximum value of the growth factor curve for the AB3-EF scheme is about 3.2. If now we re-run this case with a time step 3.2 times smaller than in the first run we obtain a growth factor curve which is almost entirely in the stable region (fig. 3.4). Therefore, for this case the IMEX scheme allows for a three times larger time step.

Fig. 3.4. Growth factor curve for the AB3-EF scheme when the computational time step is reduced about 3 times with respect to the IMEX scheme. The other parameters ($D$ and $\epsilon$) are the same like in the case shown in figs. 3.1. In this case the AB3-EF scheme needs a time step three times smaller than for IMEX scheme in order to be stable.

### 3.3.3 Sensitivity analysis

A sensitivity analysis for the IMEX scheme is shown below. Let us consider a stable case defined by the following parameters: $\Delta x = 0.015$, $D = 0.01$ and $\epsilon = 0.001$. The time
step is $\Delta t = 10^{-6}$. This corresponds to the first case reported in table 3.2. Now, if we vary one parameter at a time we can study how the growth factor changes, hence how the stability region of the scheme changes. In particular, if the area subtended between the unity straight line, $|r| = 1$, and the growth factor curve increases then the stability zone increases as well. In fig. 3.5 $D$ has values 0.01, 0.02 and 0.04. The stability region increases when $D$ increases. In fig. 3.6 $\Delta x$ varies with values 0.001, 0.0015 and 0.002. In this case the stability region decreases when the grid gets coarser. In fig. 3.7 we vary $\epsilon$ with values 0.0005, 0.001 and 0.002. In this last case also $\Delta x$ has to change according to $\epsilon$ because we have defined $\delta = \Delta x/3 = s_t \epsilon$ therefore, in order to have a constant flame speed $s_t$, we use $\Delta x = 3s_t \epsilon$. We note that when $\epsilon$ decreases the stability region increases its area.

Because a general stability theory for IMEX schemes is not available yet, the sensitivity analysis shown here is only meant to give an idea of the influence of different parameters on the scheme without pretending to be exhaustive.

Figs. 3.5 Behaviour of the error growth factor for IMEX scheme when the diffusion parameter $D$ has values 0.001, 0.002 and 0.004. The other parameters are $\Delta x = 0.015$ and $\epsilon = 0.001$. The time step is taken $\Delta t = 10^{-6}$. The direction of the arrow indicates increasing value of $D$. 
Figs. 3.6 Behaviour of the error growth factor for IMEX scheme when $\Delta x$ has values 0.001, 0.0015 and 0.002. The other parameters are $D = 0.01$ and $\epsilon = 0.001$. The time step is taken $\Delta t = 10^{-6}$. The direction of the arrow indicates increasing value of $\Delta x$.

Figs. 3.7 Behaviour of the error growth factor for IMEX scheme when the source time scale parameter $\epsilon$ has values 0.0005, 0.001 and 0.002. The other parameters are $\Delta x = 3s_t\epsilon$ and $D = 0.01$. The time step is taken $\Delta t = 10^{-6}$. The direction of the arrow indicates increasing value of $\epsilon$.

3.4 The pressure correction algorithm

The pressure correction scheme in its original formulation, was first introduced by Chorin (1976). In case of constant density it is stable but it fails when a flow with sharp variable density is considered and the density ratio is high (Rauwoens et. al., 2006). In this section we propose a pressure correction scheme that, in combination with the integration of the temperature equation introduced above, represents a suitable model for combustion with
high density ratios. Then, the new algorithm is compared with a scheme derived from the pressure correction used by Treurniet (2002). Let us call this last scheme "classic" to distinguish it from our algorithm (2). The main differences between our algorithm and the one used by Treurniet are the way the time derivative and the update of the density are computed. Now we describe the details of our scheme. Let us consider all quantities at time $n$ (at the beginning of the calculation ($n = 0$) if quantities at times $n-1$ and $n-2$ are required, these are set equal to their values at time $n = 0$). At first the temperature is advanced to an intermediate value $\hat{T}^{n+1}$ with the time integration based on IMEX scheme. Then, the quantity

$$\frac{\partial T^{n+1}}{\partial t} = \frac{T^{n+1} - T^n}{\Delta t}$$  \hspace{1cm} (3.18)

is calculated. Further, the equation of state is used to compute

$$\frac{\partial \rho^{n+1}}{\partial t} = -\frac{P_0}{\left(T^{n+1}\right)^2} \left(\frac{\partial T^{n+1}}{\partial t}\right)$$  \hspace{1cm} (3.19)

Then, the momentum equations is integrated to an intermediate value $\hat{\rho}u$, 

$$\frac{\hat{\rho}u - (\rho u)^n}{\Delta t} =$$

$$= \frac{1}{12} \left[ 23 \left( A_m + D_m \right)^n - 16 \left( A_m + D_m \right)^{n-1} + 5 \left( A_m + D_m \right)^{n-2} \right] - \nabla p^n$$  \hspace{1cm} (3.20)

$A_m$ and $D_m$ stand for the advective and the diffusive terms (their spatial discretization is described in the appendix). Then, with the intermediate level $\hat{\rho}u$ the pressure correction equation is built:

$$\frac{(\rho u)^{n+1} - \hat{\rho}u}{\Delta t} = -\nabla p^*$$  \hspace{1cm} (3.21)

where $p^*$ is the pressure correction. Applying the divergence on both sides gives

$$\frac{\nabla \cdot (\rho u)^{n+1} - \nabla \cdot (\hat{\rho}u)}{\Delta t} = -\nabla^2 p^*$$  \hspace{1cm} (3.22)

From the continuity equation the term $\nabla \cdot (\rho u)^{n+1}$ is computed as

$$\nabla \cdot (\rho u)^{n+1} = -\frac{\partial \rho}{\partial t}$$  \hspace{1cm} (3.23)

\footnote{Treurniet (2002) implemented the pressure correction in a predictor-corrector fashion (similar to the approach of Najm, 1998). The predictor and the corrector parts of the algorithm have the same structure but they differ for the time integration of the momentum (second order Adam Bashforth for the former and quasi Crank Nicolson for the latter). The results shown here are obtained with a pressure correction that is based only on the predictor part of the Treurniet scheme (as described in chapter four). It is worth to mention that, for the classic pressure correction, we have also tested a third order Adam Bashforth scheme for the momentum equations. The original predictor-corrector scheme of Treurniet has been tested as well. In all those cases we obtained the same results (and therefore the same numerical difficulties) shown later in this section.}
where the derivative of the density was calculated with eq. (3.19).
Now substituting (3.23) in (3.22) gives the Poisson equation,

\[
\nabla \cdot \left( \rho \frac{\partial u}{\partial t} + \frac{\partial \rho}{\partial t} u \right) = \nabla^2 p^* \tag{3.24}
\]

Eq. (3.24) is solved with a direct solver based on the Fast Fourier Transform (FFT) algorithm. Once this is solved we can use eq. (3.21) to calculate the mass flux at time level \( n + 1 \):

\[
(\rho u)^{n+1} = \hat{\rho} u - \Delta t \nabla p^* \tag{3.25}
\]

And the pressure is updated adding its calculated correction value:

\[
p^{n+1} = p^n + p^* \tag{3.26}
\]

The continuity equation can now be integrated to calculate the density at the new time level \( \rho^{n+1} \),

\[
\frac{\rho^{n+1} - \rho^n}{\Delta t} = \frac{1}{12} \left[ 23F^n - 16F^{n-1} + 5F^{n-2} \right] \tag{3.27}
\]

with \( F = \nabla \cdot (\rho u) \), (discretized with central differences). Once the new density value has been calculated we can compute the velocity from the mass flux

\[
u^{n+1} = \frac{(\rho u)^{n+1}}{\rho^{n+1}} \tag{3.28}
\]

and the temperature from the equation of state,

\[
T^{n+1} = \frac{P_0}{\rho^{n+1}} \tag{3.29}
\]

Finally the \( G \)–equation is integrated at the new time level also with a third order Adams-Bashforth scheme

\[
G^{n+1} = G^n + \frac{1}{12} \left[ 23 \frac{\partial G^n}{\partial t} - 16 \frac{\partial G^{n-1}}{\partial t} + 5 \frac{\partial G^{n-2}}{\partial t} \right] \Delta t \tag{3.30}
\]

The details for the spatial discretization of \( G \) are contained in appendix A.

### 3.4.1 Comparison with the classic pressure correction

In the previous paragraph we have introduced our pressure correction algorithm and here we are going to compare it with the approach used by Treurniet for the case of a premixed flame. Our approach is in agreement with the statement of Rauwoens (Rauwoens et. al., 2006) mentioning that the two key points in a pressure correction algorithm are the way to determine the density at the new time level and the constraint used to build the Poisson equation. The main difference between the classic scheme and the scheme we have introduced is that in the first case the time derivative of the density is calculated with a backward discretization whilst in the second case it is computed using the temperature
equation and the equation of state. Another important difference in the second case is that the updated value of the density is found by the integration of the continuity equation. In principle more alternatives can be found for this algorithm depending on the correction step. In fact, once the mass flux (or velocity) is calculated in the prediction step (3.20) then, in the correction step (3.25) it is corrected to satisfy the continuity equation or the energy equation or a combination of these two. An interesting study of these algorithms applied to combustion with high density ratios has been done by Rauwoens and al. (2006, 2007). They have shown the limits of the classic approach in the case of variable density and tested several alternatives. They propose a pressure correction algorithm which contains a Poisson equation with variable coefficients. This equation satisfies a constraint that is a combination of the constraints for continuity and energy. In our case we want to avoid the use of a Poisson equation with variable coefficients because the solvers for this kind of equations are very computationally expensive. As we have seen before in our approach the derivative of the density is calculated from the equation of state and a Poisson equation with constant coefficients is built. Once this is solved we obtain an updated value of the mass flux. Finally, we integrate the continuity equation to advance the density to its final value. This enforces mass conservation.

Now, we want to compute the case of a laminar premixed flame ignited in a channel flow. This is done with both pressure correction algorithms and their results are compared. Let us consider a channel flow with domain of size 1x0.32x0.7 in x, y, z directions respectively with number of points 200x64x32. The inlet velocity is $U = 1$. The outflow condition is determined by imposing zero pressure. No-slip conditions for the velocity are applied at the walls of the domain. The laminar burning speed is $s_l = 1.4$ and the time step is chosen $\Delta t = 10^{-7}$. A laminar flat flame is ignited in the channel where it can develop to its adiabatic condition. The flame normal direction is from the right to the left. We solve the continuity, the momentum, the energy, the equation of state and the $G$-equation. This test is calculated with two approaches. In the first case we integrate the temperature with AB3-EF and the classic pressure correction is used. In the second case we use IMEX with the new pressure correction. We want to analyze the behaviour of the time derivative of the density when the density ratio increases. If instabilities in this quantity appear then also the solution of the Poisson equation will be influenced. Errors in the calculation of the pressure field propagate through the whole domain hence influencing the velocity field also far away from the discontinuity generated by the flame (Rauwoens, 2006). Figs 3.8, 3.9 and 3.10 show the temperature profiles and the corresponding $\frac{\partial T}{\partial t}$ profiles at different instants along the $x-$center line of the domain. When the density ratio is low (about 1) the two schemes give the same results. When the density ratio approaches the value of two or more the profile of $\frac{\partial T}{\partial t}$ for the classic pressure correction scheme starts to deviate from the profile of our scheme until oscillations appear which will produce an exploding calculation.
Fig. 3.8 A flame is ignited in a channel flow and simulated with two approaches for the time integration of the momentum and energy equations. (a): instantaneous temperature profiles along the channel. (b) instantaneous $\frac{\partial T}{\partial t}$ profile. The density ratio is about 1.1 and the two solutions coincide.
Fig. 3.9 A flame is ignited in a channel flow and simulated with two approaches for the time integration of the momentum and energy equations. (a): instantaneous temperature profiles along the channel. (b) instantaneous $\frac{\partial \rho}{\partial t}$ profile. The density ratio is about 1.55 and the two solutions starts to be different.
Fig. 3.10 A flame is ignited in a channel flow and simulated with two approaches for the time integration of the momentum and energy equations. (a): instantaneous temperature profiles along the channel. (b) instantaneous $\frac{\partial d}{\partial t}$ profile. The density ratio is higher than 2 and the solution with classic pressure correction and AB3-EF scheme starts to diverge.

### 3.5 Reinitialization of the G-equation

To preserve the level set function $G$ as a distance function a so-called reinitialization procedure must be applied. In this work the method proposed by Van der Pijl (2005) has been used which we now explain briefly. The reason why we use this method is that it achieves a good conservation of the surface area of the level set during the reinitialization.
Let us consider a general level set equation (in the following \( G \) is replaced by the symbol \( \Phi \)),

\[
\frac{\partial \Phi}{\partial t} + U_0 \nabla \Phi = 0 \tag{3.31}
\]

The flame position is initialized as the zero level \( \Phi_0 \) and if \( \Phi \) is a signed distance function then the evolution of the zero level of \( \Phi \) represents the flame interface between burnt and unburnt regions evolving in time. For the level set to be a distance function \( | \nabla \Phi | = 1 \) must hold. Unfortunately during the advection errors are generated and the level set does not necessarily correspond to a distance function anymore. In this case a re-initialization procedure is necessary. One possibility is to apply the algorithm proposed by Sussman (1999) by solving

\[
\frac{\partial \Phi}{\partial t'} - \text{sign}(\Phi_0)(1 - |\nabla \Phi|) = 0 \tag{3.32}
\]

for an artificial time \( t' \) until a steady state is reached. However, the re-initialized interface can shift considerably with respect to the exact solution. As explained below, the density field around the flame can be influenced by the errors generated during the front propagation and the thermal thickness of the flame can change as well. Van der Pijl has proposed an improved re-initialization method that prescribes a maximum band-width within which the level set is re-defined as a signed distance function:

\[
\frac{\Phi^{k+1} - \Phi^k}{\Delta t'} = N_h(\Phi^k, \Phi_0)(1 - q(\Phi_0)) + \frac{\Phi_0 - \Phi^k}{\Delta t'}q(\Phi_0) \tag{3.33}
\]

where \( N_h \) is the spatial discretization of \( U \frac{\partial \Phi}{\partial x} \) and \( q \) is a smooth function which defines the band-width,

\[
q(\Phi_0) = \exp\left(-\left(\frac{\Phi_0}{\sqrt{\frac{3}{2} (\Delta x^2 + \Delta y^2 + \Delta z^2)}}\right)^2\right) \tag{3.34}
\]

In this study we use a stable third order weighted essentially non-oscillatory (WENO) finite volume scheme (Jiang and Peng, 2000) for the spatial discretization of \( \frac{\partial \Phi}{\partial x} \). This WENO scheme is based on a second order ENO scheme obtained following the approach of Osher and Shu (1991). WENO schemes are central schemes in regions where the solution is smooth but emulates ENO schemes near the singularities of the solution. As Jiang and Peng explain in their revealing paper this is achieved by weighting the substencils of the ENO scheme with the weights adapted to the relative smoothness of the solution of these substencils. The authors tested their WENO scheme by computing the curvature of a level set function. They proved that the WENO scheme is much less noisy and more stable than the ENO scheme. In particular for the WENO scheme the amount of noise stabilizes as the iteration continues due to the fact that WENO smoothly weights the candidate stencils in contrast to the ENO scheme which switches from one stencil to another abruptly even in the smooth part of the solution (Jiang and Peng, 2000).
3.6 Numerical error during the level set computation

As mentioned earlier in this thesis, the introduction of the stretch term can create numerical errors in the computation of the level set variable and hence in the propagation of the flame. To study the influence of these errors we have performed a simple 2D numerical experiment for the level set equation without combustion. In this way we can test the quality of the method for the computation of the level set quantities. The domain has dimensions 0.45x0.075 with 450x150 points respectively. We initialize the zero level set ($\Phi = 0$) as a circle of radius $r = 0.01$. In this case the distance function has equation

$$\Phi = \sqrt{(x - x_0)^2 + (z - z_0)^2} - r.$$ 

The circle is initially put close to the inlet of the domain and we move it with constant horizontal velocity, $U = 2$, until it reaches the outlet (figure 3.11). A time step $\Delta t = 10^{-4}$ is chosen for the integration of the level set variable while the pseudo time step used in the reinitialization procedure is of $O(10^{-5})$. We define an absolute error for the level set variable,

$$\epsilon_{LS} = \frac{1}{N} \sum_{i=1}^{N} |\phi - \phi_{ana}|$$

where $\phi$ is the calculated level set value, $\phi_{ana}$ is the value of the analytical distance function (therefore $\phi_{ana} = 0$ at the front) and $N$ indicates a certain amount of points (here we use 10 points) on the circumference of the circle where we compute these quantities every time step. An absolute error for the area of the circle is also considered,

$$\epsilon_{area} = |\text{area}_{computed} - \pi r^2|$$

For the second derivative with respect to the $x$-direction we consider the relative error defined as

$$\epsilon_r = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\phi_{xx} - \phi_{xx}^{ana}}{\phi_{xx}^{ana}} \right|$$

with $\phi_{xx}$ being the computed value of the second derivative in a point and $\phi_{xx}^{ana}$ being the analytical value at the same point. For the second $x-$derivative of the analytical level set we have,

$$\phi_{xx}^{ana} = \frac{(z - z_0)^2}{\left[(x - x_0)^2 + (z - z_0)^2\right]^{3/2}}$$

with $z_0 = l_z/2$ and $x_0 = x_{c0} + Ut$ ($x_{c0}$ is the initial position of the center of the circle).

Figure 3.12a and 3.12b show the absolute error of the level set variable and the relative error of its second derivative versus time. The values of the profiles are taken at each time step. For each step of integration an oscillation appears and this generate oscillatory profiles. This is due to the reinitialization procedure which tries to correct $\Phi$ to be a distance function. We have done the same test with different values for the pseudo time step of the reinitialization and we concluded that this parameter influences the amplitude of the oscillations, generally larger values give smaller amplitudes. Nevertheless, the profiles of the errors remain of the same order of magnitude as shown here. In practice
Fig. 3.11 The advection of a circle in a uniform flow.

Fig. 3.12a The absolute error of the level set variable during the advection test.

Fig. 3.12b The relative error of the second derivative of the level set variable during the advection test.
also the reinitialization itself produces errors and we end up with a well known paradox in the level set community: the reinitialization shifts the interface to bring it at the right position but this shift generates itself an error.

From these results we can see that while the error of the level set variable is small, that one of its second derivative increases until a final error of about 3 - 4% when the circle moves to the outlet. The stretch term depends on the curvature which is proportional to the second derivative, hence this error is also a measure of the error on the stretch. Although in this simple case the error on the second derivative seems to proceed to a limit, we cannot be sure that this error will not increase dramatically in more complex configurations. Moreover, as mentioned earlier in this thesis, the resolution of the grid plays also a role. If we refine the grid by using 900x300 points the error of the second derivative increases dramatically (fig. 3.12c). This is a well known problem (Coyajee et al., 2004) and it can be shown that the discretization error for the second derivative is proportional to the refinement of the grid. Apparently this result discourages the use of the stretch term in the relation for the flame displacement speed. We investigate this point in more detail in chapter five when we explain the influence of the temperature equation on this error and we refine the computational grid. For the following discussion it is important to note here (figure 3.12d) that the area of the circle is well conserved with a very small error of $O(10^{-5})$. Let us imagine that the circle represents a source in the flow (a flame). The energy it releases is proportional to its area. This means that if its area is conserved the amount of energy released is conserved as well.
Fig. 3.12d The absolute error on the total area of the circle during the level set advection test.

3.7 The time step criterion

Due to the low Mach number approximation applied to the flow equations we do not have to resolve the acoustic oscillations. This allows to use a larger time step, $\Delta t$, for the numerical integration. Then, the time step depends on the velocity field and the burning speed for the advection part and on the grid resolution for the diffusion part:

$$\Delta t \leq \frac{C}{\left| \frac{u}{\Delta x} \right| + \left| \frac{v}{\Delta y} \right| + \left| \frac{w}{\Delta z} \right| + \frac{1}{\rho e} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) + \frac{s_1}{\min(\Delta x, \Delta y, \Delta z)}}$$

(3.35)

where $C$ is a parameter chosen equal to 0.3. It is important to note that in our model the characteristic physical time scale, $\tau_{ph}$, is determined by the flame speed $s_l$ and the thickness $\delta$ used for the definition of the source term. Considering $\tau_{ph} = \frac{\delta}{s_l}$ then, the largest time step used for the computation must be smaller than $\tau_{ph}$ to resolve the physical time scales.

3.8 Smoothing of the total stretch for wrinkled flames

In chapter two we introduced the definition of stretch proposed by Karlovitz. Then we showed the relation for the flame speed proposed by Clavin and Joulin based on geometrical arguments and an asymptotic analysis. We write here this relation again:

$$s_l = [s_L^0 - s_L^0 L_M \nabla \cdot n + L_M n \cdot (\nabla u) \cdot n] \frac{\partial u}{\rho}$$

(3.36)

The second and the third terms on the right hand side represent the curvature and the rate of strain. The total stretch reads
\[ K_T = \left( -s^0_L L_M \nabla \cdot n + L_M n \cdot (\nabla u) \cdot n \right) \frac{\rho u}{\rho} \]  

(3.37)

Unfortunately inaccuracies in the computation of the stretch are unavoidable. This is particularly true for the curvature term. As studied recently by Coyajee et al. (2004), the order of the error in the curvature term \( \kappa \) is proportional to \( \frac{1}{h} \) with \( h \) being the mesh width. In other words, this means that the finer the grid the larger is the error on the stretch. This can result in dramatic consequences in cases like the interaction of the flame with the recirculation area produced by a body in a flow. One can apply smoothing of the level set function or on the variation of the curvature term. Some authors (Van der Pijl, 2004) use a diffusion equation for the curvature which contains a filter for the smoothing. This equation is integrated in pseudo time for a certain amount of iterations until the curvature is smooth enough. The disadvantage of this numerical procedure is that the time step and the number of iterations must be empirically tuned with the reinitialization procedure. In effect, if during the reinitialization the curve moves more than a grid cell the smoothing procedure can produce oscillations. In addition, the number of iterations depends on the number of grid points (Van der Pijl, 2004) hence making the procedure dependent on the size of the domain. Furthermore, in our problem the propagation velocity depends not only on the curvature but also on the strain rate. Alternatively, we can extend the entire propagation speed in the neighborhood of the flame with a method described below. In this case the extension process contributes to the smoothing of the interface.

We have also to take into account the fact that each modification of the flame shape will influence the flame speed and hence the mass burning rate, \( \rho s_f \). To better understand this relation we resort to the definition of stretch given by De Goey and Boonkamp (1999), De Goey and Boonkamp (1999) found a relation that expresses the total stretch rate, \( K_t \), as the relative rate of change of the mass \( M(t) \) contained in an infinitesimal Eulerian control volume \( V(t) \) in the flame. The flame moves with velocity \( u_{eff} \)

\[ u_{eff} = u + s_L \cdot n \]  

(3.38)

where \( u \) is the flow velocity, \( s_L \) the flame burning velocity and \( n \) the normal unit vector of the flame element (fig. 3.13).

![Fig. 3.13. Infinitesimal Eulerian control volumes along the flame front.](image)

The mass of the element is defined as
\[ M(t) = \int_{V(t)} \rho dV \]  \hspace{1cm} (3.39)

and the total stretch rate as

\[ K = \frac{1}{M} \frac{dM}{dt} \]  \hspace{1cm} (3.40)

Applying Reynolds’ transport theorem to \( M(t) \) gives the scalar field quantity \( K \),

\[ \rho K = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u_{eff}) \]  \hspace{1cm} (3.41)

Inserting the relation for the effective velocity into the last relation it is possible to rewrite the continuity equation:

\[ \nabla \cdot (\rho s_l \cdot n) = \rho K \]  \hspace{1cm} (3.42)

The effects of flame curvature and flow straining are now taken into account by the term \( \rho K \). This relation states clearly that the local stretch influences the mass burning rate.

Numerical errors in the calculation of the stretch (due to curvature term) can allow that spikes appear on the flame front, hence instability can arise in the flame propagation. Now, we propose to smooth the total stretch along the flame front. This can be done, for instance, with a spline approximation. From the previous relation it is required that the smoothing of \( K \) must be consistent with the values of \( s_l \). We can use eq. (3.37) to have a first guess value of the stretch. Then, we apply a discrete cubic spline to \( K \) at the location of the flame front. Finally we re-calculate the flame speed with eq. (3.36). At this point the flame speed is a smoothed function (the part depending on the stretch) shifted by the term \( s_l \frac{d\rho}{dt} \). The relation (3.42) is still satisfied because \( s_l \) is modified according to \( K \).

Summarizing the details of this procedure, at first we calculate a guessed value of the total stretch from equation (3.37). Then we calculate the positions of the intervals \( \Delta s \) along the flame front. This can be done by calculating a narrow band of points around the flame, for instance with the method proposed by Chunming Li (2005) and then extracting the location of the flame surface. Once we know the location of the flame surface we also know the coordinates of all grid cells that form the flame front. We start to travel from one grid cell to another, on this surface, by using an algorithm that divides the front into curves whose intervals are defined by the minimum distance between two consecutive grid cells containing the front. The original coordinates of these grid points are stored in an array. The stretch is a scalar defined at the center of each cell and we can use a discrete cubic spline (Duris, 1980) to smooth it along the curves we have obtained from the flame surface. Once the stretch on the front has been smoothed we calculate the flame speed from eq. (3.36). This process can be eventually iterated in order to have a better evaluation of the normal vectors.

The correct values of the flame speed, \( s_l \), are only those calculated at the position of the interface. However, our zero level set drives a source which is spread over few grid cells and this modifies the density around the zero level and consequently the flame speed around the flame. As demonstrated by Peng (1999), it is crucial to extend quantities like
the propagation velocity to a neighborhood of the flame along the normal directions at the front. Following Peng we consider the quantity \( s_l \) defined on the front and we extend it away from the interface as a constant along the curve normal to the front,

\[
\frac{\partial s_l}{\partial t} + \text{Sign}(G) \frac{\nabla G}{|\nabla G|} \cdot \nabla s_l = 0 \tag{3.43}
\]

where \( \text{Sign}(G) \) is the sign function of \( G \) defined as

\[
\text{Sign}(G) = \begin{cases} 
-1 & \text{if } G < 0 \\
0 & \text{if } G = 0 \\
1 & \text{if } G > 0 
\end{cases}
\]
3.9 Validation

So far we have described the model proposed in this thesis based on a combination of a pressure correction algorithm with an IMEX scheme for the time integration of the temperature equation. In this section we want to show that our model is able to retain the main characteristics of laminar flames. We have carried out the calculation of three well known cases: a stabilized 1D flat laminar premixed flame in a channel flow, the influence of the gas expansion on the flame surface and the flow field generated by an ozone decomposition flame. In the first case we compare our model with that one proposed by Treurniet (2002) that is based on a pure $G$–equation model without temperature equation and it uses a classic pressure correction algorithm (implemented in a predictor-corrector fashion) for the time integration of the momentum equations. In the second case we reproduce the numerical experiment carried out by Im (1995). This consists of a parametric study of the influence of a small harmonic flow perturbation on the total area of the flame. In the third case we simulate the flow field generated by the well documented ozone decomposition flame (see for instance the work of Rogg, Linan, Rodriguez, Williams, Wichman) and compare our results with the ones of Michaelis and Rogg (2002) who used a detailed chemical model.

3.9.1 1D laminar flame. Comparisons with a pure $G$–equation model

Let us consider a 1D channel flow of length $l_x = 1$ discretized with a grid of 200 points. An inflow velocity, $U$, at the left side of the channel is chosen, while at the outflow a zero pressure condition is applied. A flame is ignited at the center of the domain with normal propagation from the right to the left and laminar burning speed $s_f = 1.4$. A maximum density ratio of 6 is chosen. The flame is stabilized at its initial position by applying an inflow velocity $U = s_f$. We calculate this case with our approach and with the Treurniet model that was described in chapter two. In the latter model there is no energy equation to be solved but a smooth profile of the temperature is imposed at the position of the flame given by the relation (2.76). The spreading parameter $\delta_n$ in (2.76) and the diffusive flame thickness $\delta$ in (2.80) (used in our approach) are chosen of the order of a grid cell. In figures 3.14 and 3.15 the temperature and the velocity profiles for the two models are shown. Our approach allows a steeper jump in the temperature profile. This can also be seen in tables 3.4 and 3.5 which report the positions of the velocity and temperature values through the flame brush. We define the flame brush as the length through the flame where there is a variation of temperature from the 0.1% of $T_0$ to the 99.9% of $T_b$ with $T_0$ being the initial temperature and $T_b$ the maximum one. A small difference between the two models is noted for the velocity profiles in the burnt region (fig. 3.15). For a stabilized flame conservation of mass must hold at the position of the flame:

$$\rho_u u_u = \rho_b u_b$$  \hspace{1cm} (3.44)

where the subscripts $u$ and $b$ refer to unburnt and burnt regions. Because this is a steady state case the $G$–equation in 1D becomes
Fig. 3.14 The temperature profiles for a stabilized 1D laminar flame in a channel flow. Our model is compared with the model by Treurniet (2002).

\[ u_u \cdot \nabla G = s_f |\nabla G| \]

and because \( G \) is a distance function we have

\[ u_u = s_f \]

By substituting the last relation in (3.44) and using the equation of state we have

\[ u_b = s_f T_b / T_0 \]

In this case is \( T_0 = 1 \) and \( T_b = 6 \) therefore for the ideal case it is \( u_b = 1.4 \times 6 = 8.4 \).

Now, by looking at the last row of values in tables 3.4 and 3.5 it is possible to calculate the relative error on the burning velocity \( u_b \) for the pure \( G \)-approach and for our model. In the first case we find an error of 3% while in the second case an error of 1%. This is because the steeper the temperature profile the closer the flame configuration is to the ideal flat flame.
Fig. 3.15 The velocity profiles for a stabilized 1D laminar flame in a channel flow. Our model is compared with the model by Treurniet (2002).

Table 3.4: Values of velocity and temperature through the flame brush for the Treurniet model.

<table>
<thead>
<tr>
<th>Position (x)</th>
<th>Velocity</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.470</td>
<td>1.406</td>
<td>1.001</td>
</tr>
<tr>
<td>0.475</td>
<td>1.423</td>
<td>1.007</td>
</tr>
<tr>
<td>0.480</td>
<td>1.480</td>
<td>1.025</td>
</tr>
<tr>
<td>0.485</td>
<td>1.664</td>
<td>1.087</td>
</tr>
<tr>
<td>0.490</td>
<td>2.188</td>
<td>1.296</td>
</tr>
<tr>
<td>0.495</td>
<td>3.399</td>
<td>1.905</td>
</tr>
<tr>
<td>0.500</td>
<td>5.366</td>
<td>3.153</td>
</tr>
<tr>
<td>0.505</td>
<td>7.158</td>
<td>4.563</td>
</tr>
<tr>
<td>0.510</td>
<td>8.111</td>
<td>5.443</td>
</tr>
<tr>
<td>0.515</td>
<td>8.478</td>
<td>5.812</td>
</tr>
<tr>
<td>0.520</td>
<td>8.602</td>
<td>5.940</td>
</tr>
<tr>
<td>0.525</td>
<td>8.641</td>
<td>5.981</td>
</tr>
<tr>
<td>0.530</td>
<td>8.654</td>
<td>5.994</td>
</tr>
</tbody>
</table>
Table 3.5: Values of velocity and temperature through the flame brush for this thesis model.

<table>
<thead>
<tr>
<th>Position (x)</th>
<th>Velocity</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.490</td>
<td>1.412</td>
<td>1.000</td>
</tr>
<tr>
<td>0.495</td>
<td>1.613</td>
<td>1.018</td>
</tr>
<tr>
<td>0.500</td>
<td>2.492</td>
<td>1.324</td>
</tr>
<tr>
<td>0.505</td>
<td>4.728</td>
<td>2.660</td>
</tr>
<tr>
<td>0.510</td>
<td>7.055</td>
<td>4.502</td>
</tr>
<tr>
<td>0.515</td>
<td>8.126</td>
<td>5.580</td>
</tr>
<tr>
<td>0.520</td>
<td>8.419</td>
<td>5.912</td>
</tr>
<tr>
<td>0.525</td>
<td>8.469</td>
<td>5.974</td>
</tr>
<tr>
<td>0.530</td>
<td>8.476</td>
<td>5.987</td>
</tr>
<tr>
<td>0.535</td>
<td>8.478</td>
<td>5.991</td>
</tr>
</tbody>
</table>

3.9.2 Premixed flame with harmonic inlet velocity flow field

The purpose of this section is to check if our model can qualitatively reproduce the influence of the gas expansion on the flame surface. Following the numerical set up of Im (1995) we consider an initially flat flame ignited in a two-dimensional channel flow with a harmonic horizontal velocity at the inlet.

![Diagram of a channel flow with periodic boundary conditions](image)

Fig. 3.16 Configuration of the domain for the numerical experiment performed by Im (1995). The inlet $x$–velocity consists of an harmonic field. The boundary conditions at the top and the bottom walls and at the outlet are periodic and zero pressure respectively. The flame is ignited at $G = 0$.

The domain is depicted in fig. 3.16. It has dimensions 1x0.7 with number of grid points 300x140 for $x$– and $z$– directions respectively. The boundary conditions are periodic at the top and the bottom boundaries for all quantities and zero pressure condition is applied at the outlet of the domain. The initial vertical velocity is zero. The inlet $x$–velocity profile is
\( u(x = 0) = s_L + u' \cos(2\pi z/l_z) \)  

(3.45)

The laminar flame speed is \( s_L = 0.4 \). The flame is ignited near the outlet of the channel and its position is located where is \( G = 0 \). The flame moves from the right to the left propagating into the fresh mixture. The Reynolds number based on \( s_L \) and \( l_z \) is 2000. The heat release parameter is taken \( \tau_h = \frac{T_f - T_0}{T_0} = 1 \) and the Markstein parameter, \( L_M \), is such that \( L_M/l_z = 0.01 \). According to \( \text{Im} \), the parameter \( u'/s_l \) is considered as an indicator of the strength of the turbulence applied on the flame.

![Graph showing the ratio \( A_T/A_0 \) of the wrinkled flame surface to the initial flat front \( (A_0) \), \( A_T/A_0 \) plotted versus different values of the parameter \( u'/s_L \).](image)

**Fig. 3.17** Ratio \( A_T/A_0 \) of the wrinkled flame surface \( (A_T) \) to the initial flat front \( (A_0) \), \( A_T/A_0 \) plotted versus different values of the parameter \( u'/s_L \). The data from \( \text{Im} \) with zero heat release are also reported. These results confirm what was demonstrated theoretically by Cambray and Joulin (1992) and numerically by \( \text{Im} \) (1995); there is a flame speed and flame surface enhancement due to thermal expansion for weak turbulence \( (u'/s_L < 1) \). Moreover, according to these authors for larger velocity fluctuations (when \( u' = O(s_L) \)) it is expected that the effect of thermal expansion induced self-wrinkling of the front will be less prominent or reduced as the large convective flow field dominates the flame behaviour. However they could not pursue calculations for this case because of numerical difficulties. Our results confirm the theoretical results of Cambray and Joulin. In effect, in fig. 3.17 we can see that the enhancement of the flame area does not increase much anymore when the ratio \( u'/s_L \) is equal to 0.6, instead it decreases when this quantity approaches 1.

### 3.9.3 The ozone flame simulation and comparison

The ozone decomposition flame is one of the simplest premixed flame which was intensively investigated theoretically and experimentally by many authors, in particular Linan and
Rodriguez (1985), Rogg and Wichman (1986) and Rogg, Linan and Williams (1986). Although our simple chemistry model cannot investigate the inner structure of the flame, we are here interested in carrying out a comparison of the velocity profile calculated with our method with respect to the calculation recently performed by Michaelis and Rogg (2002) who used a detailed chemistry model.

The simulation is two dimensional with a domain of 25mm and 5mm in x- and z-directions respectively. No-slip conditions for the velocity are applied at the top and the bottom walls. The walls are adiabatic. The laminar burning speed is \( s_l = 0.283 m/s \). The mixture has an initial fuel mass fraction of 0.25 at ambient temperature. The kinematic viscosity of the mixture is taken \( O(10^{-5}) \). According to these data and to the data found in the works mentioned previously we use a density ratio of 4 for our calculation. Our domain has 300 points in the x-direction and 140 in the z-direction. The flame is ignited at the middle of the channel propagating from the right to the left side into a fresh mixture. In fig. 3.18 we can see the x-velocity profile around the flame plotted along the center line of the channel compared with the numerical data from Michaelis and Rogg. The values we found are generally higher than the results with detailed chemistry in the burnt region. This is in agreement with the limitation of the \( G \)-equation model we use. In effect, as mentioned in chapter two, the coupling between the hydrodynamic field and the flame is simply taken into account by the Markstein parameter \( L_M \) in the relation for the flame speed. This parameter is of the order of the flame thickness \( \delta_f \) which is chosen of \( O(\Delta x) \) in this simulation. In effect, we cannot reproduce an infinitely small \( \delta_f \) as required by the flamelet assumption because we should use a very large number of grid points. As a consequence the simulated flame is a thick surface and also the Markstein parameter is larger than in reality producing a larger influence of the stretch on the flame, hence a higher velocity. In fig. 3.19 the typical 'tulip shape' of this flame is shown.

![Fig. 3.18 Comparison of x-velocity profiles between this work and the computation of Michaelis and Rogg (2002) for an ozone decomposition flame in a channel flow with no-slip conditions.](image-url)
Fig. 3.19 Temperature contour plot of the simulated ozone flame. The flame presents a characteristic tulip shape.

The model we have introduced is intended for fast calculations of premixed flames. In spite of the limitations of a simple chemical model and of a $G$–equation approach which makes the flame thick, this model can reasonably reproduce the correct trend of the interaction between the flame and the hydrodynamic field.
Chapter 4

An approach to handle complex geometries with heat transfer

In this chapter we report the integral version of the paper “An Immersed Boundary Method for Complex Flow and Heat Transfer”, by Paravento, Pourquie and Boersma (2007), which was published in the international journal “Flow, Turbulence and Combustion”. At the end of the chapter, after the journal paper, we illustrate numerical results for the interaction of the immersed boundary method with a reacting flow at low density ratios.

The chapter describes a new Immersed Boundary Method (IBM) used to simulate a geometry consisting of a square body in a flow. The method is applied to flow cases with and without heat transfer. The obstacle simulated in the domain is implemented by local forcing of the flow with a procedure that adjusts locally the shear stress at the position of the object in conjunction with a non-penetration condition on the body walls. This approach has already been successfully applied by Breugem and Boersma (2005). We extend it for the case of heat transfer between body and flow. Comparison with other methods has been carried out as well. However, the proposed method can not be simply extended to immersed boundaries not aligned with the grid. As found by Pourquie (2005), the code is cheaper by a factor of 10 or more per grid point when compared to curvilinear and unstructured codes.

4.1 Introduction

Most of the applications of computational fluid dynamics, heat transfer and combustion require modeling of complex geometries. Conventional numerical models generally use a complex (non-orthogonal) grid structure which requires a substantial computational effort. In order to retain the advantages of numerical accuracy and computational efficiency associated with simple orthogonal grids an Immersed Boundary Method (IBM) can be used. The IBM can simulate the necessary geometry by adding extra forces to the momentum equations locally within the grid. In this way the grid does not have to follow the geometry.
The term 'Immersed Boundary Method' was first used by Peskin (1972) to simulate cardiac mechanics and associated blood flow. However, this method presents severe limitations with respect to numerical stability. Since Peskin introduced his novel procedure, numerous modifications have been proposed and a number of variants of the IBM approach now exist (Mittal, 2005). The first successful improvements to Peskin’s approach, for the case of solid wall treatment, are ascribed to Mohd-Yusof (1997), Verzicco et. al. (2000) and Fadlun et. al. (2000). In these last papers, in order to apply the forcing to the flow equations, only local information is needed for the computation of the body force instead of the complete force distribution over the boundary as in the Peskin approach.

In Fadlun and Verzicco’s methodology, (Fadlun, 2000), this is equivalent to the use of a local interpolation of the velocity directly on the walls and apply no-slip and non-penetration conditions.

Recently, a new method has been used by Breugem and Boersma (2005) for simulation of porous media. In this geometry a grid of cubes mimics a permeable wall with a certain value of porosity. The cubes are aligned with the Cartesian mesh and this allows to apply exactly the forcing at their boundaries. In this method the shear stress on the boundary of the simulated obstacles is replaced in such a way that the no-slip velocity condition for the tangential component is applied at the wall. In conjunction, a non-penetration condition is also applied for the perpendicular velocity components at the boundary.

The main contribution of the present paper is the extension of the Breugem and Boersma method for heat transfer with a low Mach number model and the study of the capability of this approach to keep the internal region of an obstacle well isolated under different conditions. The method is implemented on a simple equidistant grid where a square obstacle is simulated. A preliminary comparison with the data of Franke et al. (1990) is presented and for the same geometry the L2 norm of the vertical velocity component is computed as well. Successively, a two dimensional comparison with the Fadlun and Verzicco approach is carried out, as well as with a conventional method (iterative solver). Afterwards, we test the method for a three dimensional laminar incompressible case with varying inflow velocity. We also perform a three dimensional test for a varying density case with varying heat flux from the cube. In this last case, although combustion is not considered here, we let the temperature vary between the common limits of a premixed combustion flame from the ambient temperature to the adiabatic one (Warnatz, 2000).

This study is intended as a preliminary step before the application of this new IBM to reactive flow cases including combustion. In fact, from preliminary tests on the interaction between a flame front and an obstacle we noted that it is important that the velocity components inside the body remain small to avoid non-physical oscillations of velocity, temperature and density in the surroundings of the body. Therefore, for all tests, we have also looked at the velocity profile inside the body as a measure for the quality of the method.

The paper is organized in three main sections. In the first section the Low Mach number system of flow equations is introduced and the theoretical model for the IBM is presented. The main characteristics of the numerical discretization are summarized as well. In the second section results are shown and discussed. They suggest that this method can be a good candidate for the simulation of flows with or without heat transfer and for combustion cases as well. The last section contains some considerations about
the advantages and limitations of the proposed method and the conclusions.

4.2 Formulation and Numerical Method

Many heat transfer phenomena and reacting flows, such as for instance the burning of natural gas, occur at low Mach numbers. In order to study these cases with Direct Numerical Simulation (DNS), in which all flow scales are resolved, we need a system of equations that allows for large heat release, large temperature and density variations and substantial interaction of the reacting interface with the hydrodynamic flow field, including the effects of turbulence. A low Mach number approximation is suitable to characterize most of deflagration cases with appreciable advantages regarding the computational cost, because we do not have to resolve the acoustic oscillations and the set of equations is similar to the incompressible case, although the density may vary due to heat release (Mc Murtry, 1986). After an asymptotic analysis, used for the first time by Rehm and Baum (1978), the system of equations can be written in non-dimensional form. In the following reference quantities are denoted by the subscript ‘0’, while the superscript ‘*’ denotes dimensional quantities:

\[
\rho = \frac{\rho^*}{\rho_0}, \quad p = \frac{p^*}{\rho_0 R T_0^0}, \quad u = \frac{u^*}{U_0}, \quad T = \frac{T^* - T_0}{T_f - T_0},
\]

\[
x = \frac{x^*}{L_0}, \quad t = \frac{t^*}{T_0}, \quad \nabla = \frac{\nabla^*}{L_0}, \quad \tau = \frac{\tau^*}{T_0}, \quad \mu = \frac{\mu^*}{\mu_0}, \quad \kappa = \frac{\kappa^*}{\kappa_0}
\]

\(T_0\) is the ambient temperature and \(T_f\) is the flame adiabatic temperature.

The non-dimensional set of conservation equations, in conservative form, reads:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{4.2}
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = - \nabla p + \frac{1}{Re} \nabla \cdot \tau \tag{4.3}
\]

\[
\frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho u T) = \frac{1}{Re Pr} \nabla \cdot (\kappa \nabla T) \tag{4.4}
\]

\[p_0 = \rho (1 + \tau_h T) \tag{4.5}\]

with \(\tau_h = \frac{T_f - T_0}{T_0}\) being the specific heat parameter.

We have assumed an open system, thermodynamic pressure, \(p_0\), flow properties and viscosity being constant and we have considered negligible influence of gravity, negligible influence of viscous dissipation in the energy equation and validity of the state equation for the ideal gas.
4.2.1 The Pressure in the low Mach number context

After the asymptotic analysis, once the acoustic effects are neglected, it can be shown that the static pressure can be written as

\[ P = p_0(t) + \tilde{M}^2 p(x, y, z, t) \]  

(4.6)

We can interpret \( p_0 \) as the thermodynamic pressure or as the mean value of the static pressure and the quantity \( p \) is the deviation from the mean pressure (Majada, 1991). \( \tilde{M} \) is the modified Mach number, \( \tilde{M} = \sqrt{\gamma} M_0 \) with \( M_0 = \frac{U_0}{\sqrt{\gamma R T_0}} \). For the 1D case the total pressure (static plus dynamic) in dimensional units is,

\[ P_{T_{\text{tot}}}^* = P^*(t) + \frac{1}{2} \rho^* u^* 2 \]  

(4.7)

making the last equation non-dimensional and using (6) we write the total pressure scaled with the ambient pressure of reference \( P_{\infty} = \rho_0 R T_0 \)

\[ P_{T_{\text{tot}}} = \frac{P_{T_{\text{tot}}}^*}{P_{\infty}} = p_0 + \tilde{M}^2 p + \frac{\rho_0 U_0^2}{P_{\infty}} \frac{1}{2} \rho u^2 \]  

(4.8)

4.2.2 Numerical method

This section gives an outline of the main aspects of the numerical method we used for the time integration of the governing equations treated so far, while the details for the spatial discretization can be found in the appendix. The various quantities are defined on a staggered grid (fig. 4.1).

4.2.2.1 Temporal discretization

Following Treumiet (2002), at first we advance the energy equation (4.4) (which has been put in non-conservative form by using the continuity equation in order to have \( T \) explicit):
\[ T^{n+1} - T^n = \Delta t \left[ \alpha (A_T + D_T)^n - \beta (A_T + D_T)^{n-1} \right] \] (4.9)

where \( \alpha = 1.55 \) and \( \beta = 0.55 \) are modified Adams-Bashforth second order (AB2) coefficients. One can show that the stability region for this scheme is larger than for the classical AB2 and comparable to a second order predictor-corrector scheme used by Treurniet. The operators \( A_T \) and \( D_T \) represent the advective and diffusive terms in equation (4.4).

Subsequently, from the equation of state the density is calculated as:

\[ \rho^{n+1} = \frac{p_0}{(1 + \tau_t T^{n+1})} \] (4.10)

Then we integrate the momentum equations to an intermediate level indicated with \( \hat{\cdot} \):

\[ \frac{(\rho u) - (\rho u)^n}{\Delta t} = \left[ \alpha (A_m + D_m)^n - \beta (A_m + D_m)^{n-1} \right] - \nabla p^n \] (4.11)

Then from the intermediate level \( \hat{\rho u} \) we obtain a divergence free quantity \( (\rho u)^{n+1} \) with the aid of a pressure correction defined by

\[ \frac{(\rho u)^{n+1} - (\hat{\rho u})}{\Delta t} = -\nabla p^* \] (4.12)

Applying the divergence on both sides the last equation becomes

\[ \frac{\nabla \cdot (\rho u)^{n+1} - \nabla \cdot (\hat{\rho u})}{\Delta t} = -\nabla^2 p^* \] (4.13)

Because of conservation of mass we have

\[ \nabla \cdot (\rho u)^{n+1} = -\frac{\partial \rho^{n+1}}{\partial t} \] (4.14)

The derivative of the density is calculated with the following second order backward discretization in time:

\[ \frac{\partial \rho^{n+1}}{\partial t} = \frac{1}{2\Delta t} \left( 3\rho^{n+1} - 4\rho^n + \rho^{n-1} \right) \] (4.15)

Now substituting (4.14) in (4.13) gives the Poisson equation,

\[ \frac{\nabla \cdot (\hat{\rho u}) + \partial \rho^{n+1}}{\Delta t} = \nabla^2 p^* \] (4.16)

The equation (4.16) must be solved.

Once this is solved, equation (4.12) is used to calculate the mass flux at time level \( n + 1 \):

\[ (\rho u)^{n+1} = (\hat{\rho u}) - \Delta t \nabla p^* \] (4.17)

And the pressure is updated by adding its calculated correction value:

\[ p^{n+1} = p^n + p^* \] (4.18)
4.2.3 Immersed Boundary Method

The main computational bottleneck in the numerical procedure outlined above is the solution of equation (4.16). For an arbitrary grid this can be done with an iterative solver, but it is a rather slow procedure, especially in 3D cases. For certain simple grid cases so-called Fast Poisson solvers exist, which are based on the separable nature of the Poisson equation. In this paper we have used a method which allows for complex geometries while still solving a simple Poisson problem. The main idea is to add a force \( f \) to the equation of motion,

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \frac{1}{Re} \nabla \cdot \tau + f
\]

where \( f \) represents the body force. The force \( f \) can be prescribed on a Cartesian mesh so that the efficiency of the solution procedure on simple grids is maintained (Fadlun, 2000).

4.2.4 Fadlun and Verzicco's method

This was one of the first IBMs applied to a combustion problem but in the incompressible case. In Fadlun (2000) a 3D complex geometry is simulated (a IC piston) with moving boundary. Here we applied the method for a simpler configuration with a fixed square body in the flow. Moreover, in the framework of a staggered Cartesian grid, we put the body with one side aligned with the grid. In this way, the normal components of the velocity can be imposed exactly at the boundary of the object. The method computes the velocity value of each point closest to the boundary as linear interpolation between the zero velocity we want to simulate at the wall position and the velocity of a point further into the flow. The interpolation procedure is illustrated in fig. 4.2a. The velocity \( v_{i-1} \) is known and the value \( v_i \) is a linearization between \( v_{i-1} \) and zero. This procedure is equivalent to applying a body force to the momentum equations locally. The use of this method requires particular care for the treatment of the corner points because each of them receives the contribution from two faces (in 2D case) and this must therefore be taken into account in the interpolation procedure.

4.2.5 Breugem and Boersma's stress method

Compared to the method in 4.2.4, this method replaces the stress in the momentum equations (at first solved without body) to ensure that no-slip conditions exist at the boundary of the object. Here we show the main idea for a 2D case by applying the method on one of the walls of a body placed in the flow. In fig. 4.2b a simple case is depicted with a body aligned along the mesh with its sides coinciding with the mesh points where the normal velocities are defined.

We can imagine to apply a force \( f_i \) (see fig. 4.2b) to have no-slip at the position of the cross on the north boundary of the body. In this method three velocity values belonging to the body are involved: \( v_{i,j-1}, v_{i+1,j-1}, u_{i,j-1} \). Looking in the spatial discretization of the momentum (reported in the appendix) we see that these velocity values are involved in the following terms
Fig. 4.2a The Fadlun-Verzicco IB method: the velocity defined one grid point into the flow with respect to the body wall is a linear interpolation which ensures zero tangential velocity at the boundary.

Fig. 4.2b The Breugem-Boersma IB method: at the position of the body the original tangential stress is removed and the new one is added to the momentum in order to impose no-slip at the wall. This is equivalent to applying a force $f_i$ which does not depend on a linear interpolation of velocity values outside the body but depends on the velocities at the boundary and inside it.

Fig. 4.2c temperature treatment for IB methods. The heat flux contained in the diffusive term of the energy equation is replaced with the correct flux we want to impose. This has also consequences for the convective term (par. 4.2.7).
\[ \frac{v_{i+\frac{1}{2},j-1}(\rho u)_{i,j-\frac{1}{2}}}{\Delta y_j} = \]

\[ = \frac{1}{2}(v_{i,j-1} + v_{i+1,j-1}) \cdot \frac{1}{2} \left[ (\rho_{i,j} + \rho_{i+1,j}) u_{i,j} + (\rho_{i,j-1} + \rho_{i+1,j-1}) u_{i,j-1} \right] \]

\[ - \tau_{yx_{i,j-\frac{1}{2}}} = \frac{-\mu}{Re} \left( \frac{u_{i,j} - u_{i,j-1}}{\Delta y h_j} + \frac{v_{i+1,j-1} - v_{i,j-1}}{\Delta x h_i} \right) \]

contained in the advective and diffusive part of the momentum respectively.

These then form the terms which must be modified to make the flow 'feel' the body. In order to have non-penetration at the wall and no-slip condition at the position of the cross (fig. 4.2b) \( v_{i,j-1} = v_{i+1,j-1} = 0 \) and \( u_{i,j-1} = -u_{i,j} \) must hold and the above terms become,

\[ \frac{v_{i+\frac{1}{2},j-1}(\rho u)_{i,j-\frac{1}{2}}}{\Delta y_j} = 0 \]

\[ - \frac{\tau_{yx_{i,j-\frac{1}{2}}}}{\Delta y_j} = - \frac{\mu}{Re} \left( \frac{2u_{i,j}}{\Delta y h_j} \right) \]

The last equation expresses the fact that we update the stress term at the points half a grid cell away from the wall.

This procedure is equivalent to subtracting the old flux term, \( F_{old} = \frac{v_{i+\frac{1}{2},j-1}(\rho u)_{i,j-\frac{1}{2}}}{\Delta y_j} - \frac{\tau_{yx_{i,j-\frac{1}{2}}}}{\Delta y_j} \), from the momentum equations (4.11) and to adding the new flux term \( F_{new} = -\frac{\mu}{Re} \left( \frac{2u_{i,j}}{\Delta y h_j} \right) \). Therefore a force \( f_t \) is applied to the flow,

\[ f_t = -F_{old} + F_{new} = \quad (4.19) \]

\[ = - \left( \frac{v_{i+\frac{1}{2},j-1}(\rho u)_{i,j-\frac{1}{2}}}{\Delta y_j} \right) - \frac{\mu}{Re} \left[ \frac{u_{i,j} + u_{i,j-1}}{\Delta y h_j} - \frac{v_{i+1,j-1} - v_{i,j-1}}{\Delta x h_i} \right] \]

Furthermore, the non-penetration condition at the walls is enforced by imposing a zero value for the normal component of the mass flux at the intermediate time level, \( (\rho u) \), and for the related velocity.

This procedure for the stress is also applied to the inner side of the wall.
4.2.6 Penetration velocity treatment

As it has already been seen in both the IBMs outlined above, the normal component of the velocity at the boundaries must be as close to zero as possible, because we do not want normal penetration at the boundary.

Consider equation (4.17) again,

\[(\rho u)^{n+1} = (\rho u) - \Delta t \nabla p^*\]  \hspace{1cm} (4.20)

What we enforce to be zero is the predicted mass flux \((\rho u)\) and this means that the penetration at the wall is of \(O(-\Delta t \nabla p^*)\). Therefore, it is better to keep both \(\Delta t\) and \(\nabla p^*\) small. However, if the pressure correction does not remain small, for instance due to strong perturbations in the flow, then we have to reduce the time step.

4.2.7 Temperature treatment

When temperature differences are introduced, (for example in the case of a hot body placed in the flow), the heat flux between boundaries and the flow can be well represented with a procedure similar to the stress replacement method for the momentum equation. In practice, we adjust the heat flux on the walls locally by modifying the diffusion and convective terms in the energy equation in such a way to force the correct flux at the boundary. We write the energy equation in non-conservative form,

\[
\frac{\partial T}{\partial t} + u \cdot \nabla T = \frac{1}{\rho} \frac{1}{Re Pr} \nabla \cdot (\kappa \nabla T)
\]

Let us consider the diffusion term at position \(i\) (fig. 4.2c):

\[
\frac{1}{\rho_i} \frac{1}{Re Pr} \nabla \cdot (\kappa \nabla T_i) = \frac{1}{\rho_i} \frac{1}{Re Pr} \kappa \left(\frac{T_{i+1} - T_i}{\Delta x_i}\right) - \kappa \left(\frac{T_i - T_{i-1}}{\Delta x_{i-1}}\right)
\]

We replace the term \(\kappa \left(\frac{T_i - T_{i-1}}{\Delta x_{i-1}}\right)\) with the correct flux we want to impose at the boundary,

\[
\kappa \left(\frac{T_i - T_{wall}}{\Delta x_{i-1}/2}\right)
\]

Similarly one has to replace the flux at \((i - 1)\) as well.

If we use a central differences scheme, we also have to consider the convective term

\[
(u \nabla T)_i = \frac{u_i + u_{i-1}}{2} \left[\frac{T_{i+1} + T_i}{2\Delta x_i} - \frac{T_i + T_{i-1}}{2\Delta x_i}\right]
\]

as at the wall we want \(T = T_{wall}\) then we have to update the convective term in this way,

\[
(u \nabla T)_i = \frac{u_i + u_{i-1}}{2} \left[\frac{T_{i+1} + T_i}{2\Delta x_i} - \frac{T_{wall}}{\Delta x_i}\right]
\]

the same applies to the convective term at the position \((i - 1)\).
This method allows full control of the temperature of a simulated body and it also allows to solve the heat equation inside the body.

4.3 Computational results

Three geometries have been used for the computation of a flow over a square obstacle. The first one (fig. 4.3a) is the same two-dimensional configuration used by Franke (1990) and it has been used for a comparison of the method with validated computational data. The second geometry (fig. 4.3b) is also two-dimensional but is smaller than the first one. It considers a square cylinder placed symmetrically with respect to the height of the channel. The third geometry (fig. 4.3c) is three-dimensional with a cube (representative for example of a motor vehicle in a tunnel) placed four grid cells away from the bottom of the channel. The grid resolutions of these geometries are given in table 4.1.

4.3.1 Comparison with validated computational data

In Franke et al. (1990) the Strouhal number, $St$, and the drag coefficient $C_d$, are computed for different Reynolds numbers. These results are validated with experimental data. The geometry consisting of a square cylinder with diameter $D$ placed in a channel flow is shown in fig. 4.3a. The inflow velocity is unity. Free slip boundary conditions are applied at the walls.

Firstly, for $Re = 10$, we compute the $L_2$-norm (fig. 4.4) of the vertical velocity component in one point along the center-line of the channel at a position $4D$ away from the back of the body. The values are calculated with respect to the number of points in the vertical direction by computing the flow for several grid resolutions, considering the solution on the finest grid as ‘exact’. The method is essentially accurate to the second order.
Fig. 4.3b The 2D geometry used for the comparison between the Fadlun-Verzicco, Breugem-Boersma and iterative solver approaches. The cylinder is located along the central line of the channel. Periodic boundary conditions are applied at the walls.

Fig. 4.3c The geometry for the 3D flow cases. The body is a cube of diameter $D$ located 4 grid cells above the bottom of the channel. No-slip conditions are applied at the walls.
In table 4.2 some values of $St$ and $\overline{Cd}$ for different $Re$ numbers are compared with the data in Franke (1990). The comparison is good. The Strouhal number was calculated by counting the number of periods it takes for the $z$-velocity component to invert its sign at a point located $4D$ past the body along its center line. The drag was calculated by considering the contribution of all the horizontal forces acting on the cylinder.

### 4.3.2 Two dimensional flow: comparison between the IBMs and a standard method

We have performed a 2D simulation of a cylinder in a flow, for the geometry illustrated in fig. 4.3b, by using the methods described in paragraphs 4.2.4-4.2.5. The body is located symmetrically with respect to the $z$ dimension, so that it is exactly aligned with the center line of the channel. In fact, due to the periodic boundary conditions for the flow in $z$-direction the body can have any position along $z$.

For this case, the density is constant. The inflow mass flux in $x$-direction is given (with velocity $u_{in} = 1$). Zero gradient condition for the pressure is used at the inlet. At the outlet the pressure is put to zero (or ambient pressure). The Reynolds number based on the side of the square cylinder is 1400.

Fig. 4.5 shows a comparison between the new IBM, the Fadlun-Verzicco approach and a conventional iterative solver without immersed boundary. The averaged values of the velocity component $u$ along the center line of the cylinder are plotted. The iterative solver was based on the SIP method (Ferziger, 2002) and it used 100 iterations for each time step to get a divergence of $O(10^{-6})$ for the cell at the middle of the front of the body (fig. 4.7). It was found (fig. 4.5) that the results of new IBM and
Table 4.1: Grid resolution for 2D and 3D cases

<table>
<thead>
<tr>
<th></th>
<th>x-points</th>
<th>y-points</th>
<th>z-points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D case</td>
<td>200</td>
<td>2</td>
<td>140</td>
</tr>
<tr>
<td>3D case</td>
<td>200</td>
<td>64</td>
<td>140</td>
</tr>
</tbody>
</table>

Table 4.2: Comparison of St and Cd for different Re numbers for square cylinder with validated data

<table>
<thead>
<tr>
<th>Re</th>
<th>St</th>
<th>Cd</th>
<th>Re</th>
<th>St</th>
<th>Cd</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>0.153</td>
<td>1.61</td>
<td>100(grid:88x76)</td>
<td>0.154</td>
<td>1.61</td>
</tr>
<tr>
<td>150</td>
<td>0.162</td>
<td>1.56</td>
<td>150(grid:88x76)</td>
<td>0.165</td>
<td>1.56</td>
</tr>
<tr>
<td>300</td>
<td>0.138</td>
<td>1.80</td>
<td>300(grid:186x156)</td>
<td>0.130</td>
<td>1.83</td>
</tr>
</tbody>
</table>

iterative solver coincide while for the Fadlun-Verzicco approach the recirculation length is smaller than for the other methods indicating a larger resistance to the flow. The velocity profiles have been averaged over a range of 15 shedding periods between the 25th and the 40th period.

Furthermore, we have checked the new method described in paragraph 4.2.7, for the case with temperature and density coupled by the equation of state. The temperature is set with zero gradient on all boundaries. The body has a small temperature difference $\Delta T = 0.1$ with respect to the flow and the flux replacing method is used. The normal velocity at the wall of the body is of $O(10^{-6} \div 10^{-5})$ with maximum penetration at the corner points and with minimum of $O(10^{-7})$ inside the obstacle (fig. 4.6). In these two dimensional simulations no enforcing of zero velocity has been applied inside the body. By enforcing it the magnitude of the velocity components inside the cylinder can vary between $10^{-7} \div 10^{-9}$.

In these simulations, with time step being $\Delta T = O(10^{-4})$, the shedding appeared earlier for the Fadlun-Verzicco method (around 4300 time steps) than for the stress method (around 40000 time steps). This suggests that the numerical noise produced by the stress method is much smaller than for the case of the Fadlun-Verzicco approach.

4.3.3 Three dimensional flow: body in a laminar flow with periodically varying inflow conditions

In the following all computations were conducted with the new stress IBM described in the paragraphs 4.2.5–7. This case refers to the geometry in fig. 4.3c. The body is a cube of diameter $D$ located symmetrically with respect to the $y$-direction and $0.2D$ (4 grid cells) away from the bottom of the channel. The Reynolds number, based on the height $l_z$ of the box was $Re = 2100$. For this test zero gradient condition for the pressure
Fig. 4.5 2D square cylinder case, averaged $x$-velocity component versus body $x$-center line. Comparison between Fadlun-Verzicco, Breugem-Boersma and Iterative solver approaches. The plots of the last two methods overlap while the Fadlun-Verzicco method gives a smaller recirculation area.

Fig. 4.6 2D case, time-averaged $x$-velocity component versus $x$-center line inside the cylinder for the different IB methods and the standard (iterative) one.
was used at the inlet, while at the outlet the pressure was put to zero. The flow was at constant temperature and a varying inflow velocity was applied defined by

\[ U_{\text{inflow}} = U + 0.1U \cdot \sin(2\pi f \cdot t) \]

with \( U = 1 \). The inflow velocity was varied by 10% of its bulk value with frequency \( f \). This means \( f \) cycles of sinusoidal perturbation occurring in one unit time (of \( O(D/U) \)). We performed tests with three frequencies: 100, 10 and 1. For these three cases, figs. 4.8-4.10 illustrate the \( x \)-mass flux component \( (\rho u)_x \) versus time at the body wall, in the cell adjacent to the center-point of the left body wall (fig. 4.7), on a range of half time unit. The results show that for the frequencies of 1 and 10 the mass flux at the body wall responded with the same frequency, on the contrary this was not the case for the highest frequency of 100. In this case a sort of 'integral' effect is noted and the body reacted like if affected by a global perturbation and the penetration was higher by an order of magnitude: from \( O(10^{-6}) \) for the first two frequency cases to \( O(10^{-5}) \) for the highest frequency case. However, for this case, the penetration was still acceptable. We can expect that for even higher frequencies the reaction time of the new IBM has a limit: for high frequencies it takes longer for the velocity field inside the body to adjust itself. In fact, as we have mentioned above, the penetration velocity depends on both time step
Fig. 4.9 \((\rho u)_x\) versus time at the body wall for the inlet mass flux perturbation of frequency \(f = 10\).

Fig. 4.10 \((\rho u)_x\) versus time at the body wall for the inlet mass flux perturbation of frequency \(f = 100\).

and pressure correction (see eq. (4.20)) and the higher the frequency of the perturbation becomes the higher the pressure correction. Therefore, in this case, we have to reduce the time step if we want small penetration and in particular, if \(f\) is the frequency of the perturbation applied to the system, we must have \(\Delta t \cdot f \ll 1\).

### 4.3.4 Three dimensional flow: body with varying heat flux

We wanted to prove that with the proposed extension for the heat transfer the Breugem-Boersma approach is also suitable for combustion problems. In particular, for premixed flames the interaction of the reacting front with an obstacle produces sharp temperature gradients at the body boundary. The method must be stable under these conditions and for an adiabatic obstacle no transport of energy or mass must take place at the walls to avoid non-physical oscillations of velocity, temperature and density in the surroundings of the body.

For this case the Reynolds number, based on the height \(l_z\) of the box, was \(Re = 2100\) with inflow velocity on the left side of the domain \(u_{in} = 1\). The time step \(\Delta t\) was of
\(O(10^{-4})\). The temperature of the entire body was perturbed with a positive sine profile 
\(T_w = |\sin (2\pi \frac{t_i}{T})|\) where \(i\) represents the progressive number of time steps during the calculation, \(t\) is the time and \(T\) is the period of the oscillations. Two frequencies have been applied \((f = 100 \text{ and } f = 200)\) with periods of oscillations \(T = 0.01\) and \(T = 0.005\) respectively. The flow time scale is of \(O(D/\bar{u}_in) = 0.1\) therefore we apply an intense perturbation of the temperature with respect to the flow.

The positive sine function has the property to go from 0 to 1 that in this model means from the ambient to the adiabatic flame temperature (here the dimensional values are 300K and 1800K respectively, comparable with a premixed air-methane flame). Moreover, after one period its change is sharp enough to check if the central difference scheme suffers of numerical instability for large temperature gradients in time.

The influence of the different frequencies can be seen on several quantities, in particular, velocity, mass flux, pressure and boundary layers. We want to know if we are resolving the momentum and the thermal boundary layers. The ratio of the thickness of these two boundary layers is governed by the Prandtl number. Because in all our laminar simulations the Prandtl number was smaller than unity the thermal boundary layer was thicker than the momentum boundary layer. Therefore we only have to check if we are resolving the momentum boundary layer. We estimated the parameter \(z^+\) and the wall shear stress \(\tau_w\) at the top face of the body with the formulae:

\[
\tau_w = \sqrt{\tau_{xx}^2 + \tau_{xy}^2} \\
z^+ = \frac{\Delta z_p}{\nu} \sqrt{\frac{\tau_w}{\rho}}
\]

where \(\Delta z_p\) is the distance from the wall and \(\nu\) is the kinematic viscosity.

If \(z^+ \leq 5\) we have sufficient grid points to resolve the viscous sublayer (Versteeg, 1995).

The data related to the first frequency case were averaged over 2000 time steps while in the second case over 1000 time steps with \(\Delta t = O(10^{-4})\). In both cases 20 periods were considered. In fig. 4.11 plots of the averaged values of \(z^+\) are compared for the two
heat flux frequencies cases. These pictures are plotted along the $x$-axis center line on the top of the body. We can see that in both cases we have $z^+ \ll 5$.

Fig. 4.12 shows the profiles of the averaged $x$-velocity component, $u$, inside the body along its center line. The order of magnitude of $u$ is between $O(10^{-5})$ and $O(10^{-4})$. Fig. 4.13 shows the $x$-mass flux component $(pu)_x$ versus time at the wall of the body (in the grid cell depicted in fig. 4.7). The mass flux penetration at the wall is of $O(10^{-5}-10^{-4})$ as well.

In fig. 4.14 a time interval of an instantaneous plot of the total pressure (eq. (4.8)) is shown as function of time. The values are taken at the $yz$ plane which was $0.6l_x$ away from the inlet and $0.2l_x$ from the right side of the cube ($l_x$ being the $x$-size of the channel). The second frequency value for the perturbation of $T_w$ was used in this case. We note periodic oscillations of the pressure with frequency of $O(100)$ that is half of the frequency of the imposed heat flux. The picture shows the peaks of pressure oscillations corresponding to the minimum values of body temperature (when the sine profile starts a new cycle) but the oscillations do not create instabilities.
Fig. 4.14 Sample of total pressure versus time at a location 2 diameters past the body.
The peaks correspond to the moment when the sinusoidal perturbation starts a new cycle.

4.4 Final considerations and conclusions

We summarize here the main advantages and limitations of the proposed method.

Our code uses a pressure-correction method. The solution of the momentum and mass balance equations is satisfied in two steps. First the momentum balance is satisfied using the pressure at the old time level. Next the velocity is corrected to satisfy the mass balance. Correction is done with an update of the pressure for which we have to solve a Poisson equation. The boundary conditions are enforced by addition of extra momentum sources. This is done before the pressure-correction and is independent of it. As a result we can use so-called fast Poisson solvers which only work on a separable domain. Inclusion of obstacles makes the Poisson problem non-separable for a traditional approach and we have to resort to slower iterative solvers (Pourquie, 2005). Therefore, as first advantage, the method we use is faster than traditional methods (like iterative solvers). The speedup with respect to Cartesian codes which do not use a direct solver is in general a factor of 2.5 or more (which of course depends on the divergence required and on the resolution) (Pourquie, 2005). The code is cheaper by a factor of 10 or more per grid point when compared to curvilinear and unstructured codes (Pourquie, 2005).

Our IBM has been specifically designed for square geometries and to consider complicated geometries including many obstacles. In fact, by aligning a square body with the grid lines it is possible to apply almost exactly the non-penetration conditions for the vertical components of the velocity. Velocity interpolations are also avoided near the wall both for the non-penetration and the no-slip conditions. This is the second advantage.

For non-aligned bodies or for curvilinear geometries our method can still be applied but its implementation becomes complicated because interpolations are required. In this case it loses the third advantage which is its simplicity to be implemented and to add as many square bodies as required which can be included independently of one another, or removed (Breugem, 2005). In conclusion, for non-aligned or curved obstacles the Fadlun-Verzicco method is certainly more suitable. However, it has higher wall normal leakage of the order of $10^{-3}$ of the bulk velocity (Pourquie, 2005). In both methods the near wall quantities can not be well represented out of the sub-viscous layer, however in Pourquie (2005) has been shown that in this case the Fadlun-Verzicco approach presents larger
errors due to its linear interpolation into the flow.

In conclusion, we have performed calculations with an Immersed Boundary Method for the case of a hot or insulated square body located in a box-domain open at the two faces perpendicular to the main stream direction. Two geometries have been used, a 2D geometry with few grid cells in the span direction and a fully 3D geometry. The object has been simulated with a new Immersed Boundary Method. Several tests have been carried out by using different conditions for the inflow velocity and the heat flux from the body. Initially we have made a two dimensional simulation of a cold and hot body in a laminar channel flow with constant inflow conditions and comparison with a previous IBM and an iterative solver has been performed. The new IBM shows a very good agreement with respect to the results of an iterative solver. For the three dimensional geometry, at first we have simulated laminar cases with perturbation of the inflow mass flux for different frequencies. Secondly, we have studied the case of a laminar flow with a hot body whose heat flux and internal temperature can vary within the temperature limits of a common air-methane premixed flame. For this last case two tests have been done with different frequencies of the temperature oscillations.

The results show good behaviour of the stress IBM in all conditions considered with a velocity at the body walls and inside the object of an order of magnitude varying between $10^{-9}$ and $10^{-4}$ depending on the magnitude and the frequency of the disturbances applied. The method is able to adjust the velocity field inside the obstacle also for high frequency of mass or heat flux perturbations. We conclude that this new immersed boundary method is easy to implement, it requires less computational resources than standard methods, it has accuracy comparable with that one of an iterative solver approach and it is suited for heat transfer and combustion problems.

4.4.1 References


4.5 IBM with reacting flows at low density ratios

In this chapter we have introduced an immersed boundary method (IBM) and we have given numerical results for non-reacting flows with and without heat transfer. In this section we prove the capability of our IBM to reproduce complex geometries in the case of reacting flows with low density ratios between the fresh and the burnt regions of the flow (applications of IBM for realistic flames like deflagrations in tunnels with one or more obstacles will be covered in the next chapter).

For the IBM with reactive flow case, a 'reconstruction temperature method' (eq. (2.78)) is used in conjunction with the G-equation (eq. (2.75) ). Then, two extra equations have to be solved:

\[
\frac{\partial G}{\partial t} + u \cdot \nabla G = s_l |\nabla G| \tag{4.21}
\]
\[ T_{\text{updated}} = T + \frac{Q}{c_p} H(G) = T + \frac{c_p(T_{\text{burnt}} - T)}{c_p} H(G) = T + (1 - T) e^{-\frac{Q^2}{2\delta}} \] (4.22)

\( T_{\text{updated}} \) indicates the new value of the local temperature and \( T \) the last value. The quantity \( s_l \) in (4.21) is calculated with the relation (2.74) in chapter two. The \( G \)-equation tracks the flame and combustion heat is released where is \( G = 0 \). In this approach the mixture is completely burnt once the front has passed, hence at the position of the flame the temperature rises till the adiabatic flame temperature value. The temperature equation does not contain an explicit source term but after advection and diffusion it is reconstructed at the flame position to have the adiabatic value. In case of interaction with a solid body, the energy equation is treated as described above to have zero heat flux from the body walls. The reconstruction temperature approach has been found stable and efficient only for low density ratios between the burnt and unburnt regions (Kim, 1999).

Nevertheless, we can imagine to have combustion of preheated gases which undergo a smaller jump in density during the combustion process. This artifice is often used in combustion calculations to avoid the numerical difficulties of high density ratios.

We consider the same geometry of the non-reacting case (geometry “c” in fig. 4.3c) with a body placed few grid cells away from the bottom of the channel which has no-slip conditions at its walls. The tunnel has the inflow at the left side and the outflow at the right side. A reactive surface, ignited near the outflow, moves in the direction of the body (to the left side) with laminar flame speed \( s_l = 1.5 \). The fresh mixture is supplied at the inflow with velocity equal to 0.416 and constant temperature. A low density ratio, \( \rho_u/\rho = 2 \), between fresh and burnt gases is chosen. The resolution used consists of 200\( \times \)64\( \times \)140 points. Figs 4.15a and b show contour plots of temperature and \( x \)-velocity, at a certain instant in the plane \( xz \).
Fig. 4.15: (a) Instantaneous temperature contours plot and (b) $x$-velocity contours plot. Low density ratio flame ($\rho_u/\rho = 2$) approaching a square cube from the right with laminar flame speed $s_1 = 1.5$. To keep the body adiabatic only the diffusion term of the energy equation has been 'forced' as described earlier in this chapter.
Fig. 4.16: Temperature 'leakage'. The flame moves from the right to the left of the domain. Low density ratio flame ($\rho_u/\rho = 2$) at an instant after its interaction with the body. The temperature contours plot shows a leakage due to the fact that the advective term of the energy equation has not been adjusted according to the zero flux at the body.

The flame starts to propagate faster along the boundaries where no-slip conditions are applied. After a while the flame starts to assume a characteristic spike shape toward the burnt region (fig. 4.16). The body is considered adiabatic but only the diffusive term of the energy equation has been treated. We note that after the flame has passed the body a 'leakage' of temperature appears (fig. 4.16).
Figs. 4.17: (a) Instantaneous temperature contours plot when the flame has passed the body (flame moves from the right to the left); (b) body centerline $x$-velocity profile at an instant when the flame is over the body. The “forcing” of the heat flux has been applied on both the diffusive and the convective terms at the same time. The body is now perfectly insulated without temperature leakage.

Only by adjusting the convective term in the energy equation in conjunction with the imposed heat flux in the diffusive term we can have a perfectly insulated body without heat or mass transport through the boundaries \(^1\). An example is shown in figs. 4.17. In fig. 4.18 a 3D representation of the flame reaching the body is depicted. At this instant we note from fig. 4.17b that the penetration velocity along the centerline of the body is

\(^1\)As illustrated in fig. 4.2c and already shown in this chapter, we replace the old heat flux in the
reasonably very small when the flame is passing over it.

![Diagram of 3D temperature contour plot]

Fig. 4.18: Instantaneous 3D temperature contour plot. In this picture the $x$-axes is directed to the left side of the domain, therefore here we see a flame propagating from the left to the right. The body is placed 4 grid cells away from the bottom of the domain. Its left side is at the position $x = 0.4$. The lower part of the flame front has just reached the cube.

diffusive term with the correct flux $\phi^{new}$ at the boundary. Then, the wall temperature must be

$$T_{wall} = T_i - \phi^{new} \frac{\Delta x_{i-1}}{2\kappa}$$

which leads to a modification of the convective term as well,

$$(u\nabla T)_i = \frac{u_i + u_{i-1}}{2} \left[ \frac{T_{i+1} + T_i}{2\Delta x_i} - \frac{T_{wall}}{\Delta x_i} \right]$$

For the adiabatic case it is $\phi^{new} = 0$ and $T_{wall} = T_i$ hence the convective term becomes

$$(u\nabla T)_i = \frac{u_i}{2\Delta x_i} \left[ \frac{T_{i+1} - T_i}{2} \right]$$
Chapter 5

Numerical Results (interaction flame-obstacles)

5.1 Introduction

The subject of this chapter is the interaction of a flame front with obstacles. We consider the interaction taking place into a rectangular domain filled with a stoichiometric mixture of methane and air. The domain is semi-confined with solid boundaries on all but one side (outlet). The fuel mixture at rest is ignited by a spark plug at one side of the domain and an initially hemispheric flame front starts to develop (fig. 5.1, flame front contour at \( t = 0 \)). Then, the flame propagates along the domain where an obstacle is set. For this mixture a constant laminar burning speed, \( s_i \), of the unstrained flame front is assumed equal to 0.4\( m/s \) and a density ratio of 6 is considered. It is well understood that if the area of the flame surface increases then also the burning ratio increases. During the interaction flame/obstacle the flame surface is indeed stretched and its area increases. In addition, turbulence in the flammable mixture is produced which can wrinkle the propagating flame front. Therefore, at different times \( t \), several phenomena are observed (an oversimplified sketch of the main steps is given in fig. 5.1):

- the flammable gas flow is accelerated and eddies are produced at the edges of the obstacle;
- the interaction with the obstacle enhances the burning rate and hence the flame speed;
- the level of turbulence starts to increase when the flame reaches the obstacle and the turbulence contributes to wrinkle the flame front;
- when the flame reaches the obstacle the pressure reaches a peak;
- the blockage of the channel flow due to the obstacle causes local acceleration of the flame front in the form of jetting;
Fig. 5.1 Evolution of the flame front during deflagration of air-gas mixture in a rectangular domain. At time $t = 0$ the front is ignited as hemispherical surface. At time $t_1$ the front increases its area with an almost constant velocity of its tip. Afterwards, $t_2$, the flame has interacted with the obstacle and it propagates through the free space between the body and the walls of the domain with a jet-like behaviour. Since the first instants the flammable flow is accelerated and eddies form at the edges of the obstacle. Once the flame reaches the recirculation zone pockets of fresh fuel are trapped ($t_3$). After the recirculation zone, $t_4$, the flame tip speed increases again.

- in the recirculation zone that is formed behind the body, the flame is wrapped on itself (wake/flame interaction) and the flame speed reduces. Pockets of fuel can be trapped;
- after the recirculation zone the flammable flow velocity and the level of turbulence have raised such that the velocity of the flame front increases again.

The overpressures generated during the interaction flames/obstacles are of interest. For instance, in an offshore facility, the increase in burning rate can enhance the local explosion (hence its overpressure) and intensify the hazard with consequent domino effects. Masri et al. (2000), Ibrahim and Masri (2001) and Hargrave, Jarvis and Williams (2002) performed laboratory-scale experiments with obstacles in a domain where a premixed air-methane flame was ignited. They found that the shape of the obstacles and their blockage ratios have influence on the flame speed and on the overpressure.

We focus on two geometries studied by Ibrahim and Masri and Hargrave et. al. The first one consists of a rectangular domain of size $0.45x0.15x0.075m^3$ in $x, y, z$ direction respectively. The domain is closed at the left side where a flame is ignited and open at the right side (figure 5.2). A sealing membrane at the outlet keeps the gas inside the domain and the bursting time is unknown in the experiment and will not be considered in our simulations. A rectangular cylinder with thickness of 0.012$m$ and a side 0.04$m$ is placed with its center line 0.150$m$ away from the left closed side of the domain. The blockage ratio of the obstacle with respect to the $yz-$cross section is 53%. The second geometry
differs from the first one only with respect to the shape of the obstacle which is now a square cylinder with a side 0.04m (Fig. 5.3).

The first geometry described here was studied numerically by Patel et al. (2003) who used a numerical model based on a RANS approach for the solution of the flow field and a flame surface density approach (FSD) for the combustion modeling. With the method described earlier in this thesis we present the simulation of these two geometries and a comparison with Patel's results. For an equidistant Cartesian grid, several different mesh sizes have been used to check grid convergence. The flame is ignited as an hemisphere with radius of 5mm at the center of the left closed side of the domain. No-slip and non-penetration conditions for the velocity are applied at the walls of the channel, zero pressure is set at the outflow and a zero gradient condition is chosen for all scalar quantities at the walls including the temperature. The obstacles are considered adiabatic. The Reynolds number is $Re = \frac{\rho_0 s_l^0 l_{body}}{\mu_0} = 1600$. It is important to underline that the characteristic physical time scale, $\tau_{ph}$, of our model is defined by the laminar burning speed, $s_l^0$, and the thermal flame thickness, $\delta_f$. Considering, for the first two configurations, $s_l^0 = O(0.4) m/s$.
and \( \delta_f = O(0.001)m \) it is found \( \tau_{ph} = \delta_f/s_1^0 = 0.0024s \). The largest time step used in the computations is \( O(10^{-5})s \) therefore the physical time scales are resolved.

### 5.2 Calculation for the optimization of the diffusion flame thickness \( \delta \) and the influence of the Markstein parameter \( L_M \)

In chapter two we have introduced the definitions of diffusive, \( \delta \), and thermal flame thicknesses, \( \delta_f \), and also a relation for the Markstein parameter (Clavin and Joulin, 1983), \( L_M \). Usually \( \delta \) is smaller than \( \delta_f \) by a factor of order 5 (Poinset and Veynante, 2001). We re-write here the relations 2.82 and 2.73,

\[
\delta_f = \frac{T_{burnt} - T_0}{\max (|\frac{dT}{dn}|)} \\
L_M = \frac{T_{burnt}}{T_{burnt} - T_0} \ln \left( \frac{T_{burnt}}{T_0} \right) \delta
\]

where \( \frac{dT}{dn} \) is the derivative of the temperature in the normal direction of the flame front.

In our approach we apply two types of optimizations. The first optimization is based on numerical experiments: how small can the diffusion parameter \( \delta \) be such that the front is as steep and thin as possible. The second optimization is physical: diffusion thickness \( \delta \) and thermal thickness \( \delta_f \) are linearly related (Blint, 1986) and because during the interaction with an obstacle the thermal thickness changes then also the diffusion thickness can be expected to follow the same trend. We have mentioned in chapter two that in this study we assume the diffusive parameter of the Gaussian source term (eq. 2.80) to be the diffusive flame thickness \( \delta \). In this way the diffusive thickness can be calculated by a relation for the full width at half maximum of the distribution (FWHM):

\[
FWHM = 2\sqrt{2\ln 2}\delta = \frac{\Delta x}{3} \tag{5.1}
\]

where we have set the last equality based on optimization by numerical experiments in order to have a flame as thin as possible (first optimization) while the maximum value of the source term (dependent on \( \delta \)) is released at each grid cell containing the zero level set. This relationship makes sure that 90% of the source is distributed over a range never less than at least two grid cells. The idea we follow here is to estimate \( \delta_f \) with a first computation by using a constant \( \delta \) calculated by (5.1). After this first calculation we know how the profile of \( \delta_f \) changes, that is the information we could not guess in advance. Then, we can make \( \delta \) changing with the same trend (the same percentage of change during the propagation) because as we know from chapter two \( \delta \) is linearly related to \( \delta_f \) (second optimization). Moreover, because the Markstein parameter is function of \( \delta \) also \( L_M \) needs to be optimized according to the profile of \( \delta_f \). In fact, \( L_M \) has a direct influence on the flame speed (eq. 3.36). In the following we want at first to show the influence of different values of the Markstein parameter on the flame speed.

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Fig. 5.4 Flame tip speed profile along the main length of the domain for the case with 
$L_M = 0$ (no stretch effects). The computation is stopped at the early stage of the interaction 
with the body.

Let us consider the first geometry with a rectangular cylinder as obstacle. A grid of 
450x64x150 points in $x$, $y$, $z$ directions respectively is used. The Courant number is 
$C = 0.3$. Initially the Markstein parameter is set equal to zero ($L_M = 0$) hence no stretch 
effects on the flame front are included. Let us consider the flame tip speed (that is the 
quantity measured in the experiments). At each instant the tip is the furthest point of 
the flame in the main direction of propagation. In fig. 5.4 the velocity of the tip is plotted 
versus the distance from the ignition point and the calculation is stopped at the early 
stage of the interaction of the flame with the wake behind the obstacle. We can see that 
the tip speed increases slowly until 0.1$m$ when a small decrease occurs just before the 
front reaches the body. Then, the speed increases about five times once the flame has 
reached the obstacle. Snap shots of these stages are shown in fig. 5.5.

Now let us consider the effect of $L_M$ on the flame tip speed. The Markstein parameter, 
$L_M$, is a prefactor for the stretch in the relation for the displacement speed (eq. 3.36) 
. It is of the order of the diffusive flame thickness, $\delta$, and, as discussed in chapter two, 
it can be evaluated with the relation proposed by Clavin and Joulin, (1983). By using 
a maximum density ratio of about 6 between burnt and fresh regions we find that the 
Markstein parameter is of $O(L_M) = 2\delta$. In figure 5.6 we plot the flame tip speed for 
different values of $L_M$. The larger $L_M$ the higher the value of the tip speed. This is 
because the contribution of the stretch increases the flame area.

At this point we can run the preliminary calculation that will be used to optimize the 
profile of $\delta$ and $L_M$ with respect to the trend of $\delta_f$. It is assumed $L_M = 2\delta$ where $\delta$ is 
calculated from eq. (5.1). In figures 5.7a and 5.7b are plotted versus time the original 
profile of the thermal thickness, $\delta_f$, and its polynomial fit obtained with a Bezier spline 
interpolation (over a time-range when the flame is around the position of the obstacle).

It can be seen that $\delta_f$ decreases when the flame starts to interact with the obstacle (at a 
time between 0.025 - 0.03s). The acceleration of the tip flame can be noted also in figure
Fig. 5.5 2D snap shots of the flame front at different instants during its propagation until the early stage of interaction with a rectangular cylinder. a) at 0.022 s; b) at 0.027 s; c) at 0.03 s.
Fig. 5.6 The flame tip speed for different values of the Markstein parameter $L_M$.

Fig. 5.7a Thermal thickness versus time for the first calculation.
Fig. 5.7b Thermal thickness versus time for the first calculation (polynomial fit over a time-range when the flame is around the position of the obstacle).

<table>
<thead>
<tr>
<th>x-intervals along the channel (m)</th>
<th>% var of ( \delta_f ) with respect to ( \delta_f(t = 0.02s) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.14-0.14</td>
<td>7%</td>
</tr>
<tr>
<td>0.14-0.28</td>
<td>14%</td>
</tr>
<tr>
<td>0.28-0.32</td>
<td>15%</td>
</tr>
<tr>
<td>0.32-0.35</td>
<td>47%</td>
</tr>
</tbody>
</table>

5.7c where the position of the flame tip in time is shown: at a time of \( \approx 0.025 - 0.03s \) the slope of the curve increases. This is due to the stretching of the flame. It is interesting to note that in the temporal range of about \( 0.018 - 0.027s \) the flame thickness shows an almost constant profile. This range corresponds to the period of time when the flame is approaching the obstacle and its shape changes: from a spherical shape the front assumes at first a flat shape in front of the object (its speed slightly decreases at about \( x = 0.12m \), see fig. 5.5) and then, at about 0.03s it propagates in the space between the block and the walls of the channel.

As discussed in chapter two, \( \delta \) and \( \delta_f \) are linearly related so that after a preliminary computation of the latter a better profile for the former can be found (Poinset and Veynante, 2001). By using the previous figures it is possible to build the table 5.1 which gives the percentage variation of the thickness (with respect to its value at \( t = 0.02s \)) along the channel. According to the Clavin and Joulin relation between \( L_M \) and \( \delta \), \( L_M \) should also change in the same way according to the stretching of the flame near the obstacle (1).

---

1 The following approach can be used to obtain a smooth profile of a quantity in a given interval. Let us assume we have an interval \( \Delta L \) composed of \( N \) points each one indicated by the index \( i \). A quantity \( q \) is defined in \( \Delta L \) with initial value \( q_0 \) and final value \( q_L \). Then a profile of \( q(i) \) in \( \Delta L \) can be computed as \( q(i) = q_0 \cdot \left( \frac{q_L}{q_0} \right)^{1/N} \) with \( i = 1, \ldots, N \).
5.3 Grid refinement in the main directions and boundary layer

Now that we have the optimized profile for $\delta$ and $L_M$ we can check the influence of the grid refinement on the numerical solution for the first geometry case. The quantity we are interested in is still the flame tip speed. We refine the grid in one direction at a time. In fig. 5.8 the flame tip speed is shown for three grid resolutions refined in $x$-direction: $450 \times 64 \times 150$, $525 \times 64 \times 150$ (16% finer) and $600 \times 64 \times 150$ (33% finer). The results for the finer resolutions in $x$ are close to that one obtained with the coarsest resolution. The flame speed at the relative maximum and minimum points has a difference of less than $2m/s$ if we compare the coarsest and the intermediate resolutions and less than $1m/s$ if we compare the intermediate and the finest resolutions. This suggests that convergence can be achieved by refinement of the grid. However the computational time increases. For the grid with 450 points in $x$-direction the computation takes 102788 CPU seconds (on a AMD 2GHz processor with 8GB of RAM), while for the cases with 525 points and 600 points it takes respectively 192% and 259% more time than for the coarsest case. In fig. 5.9 we show the case of grid refinement in $y$-direction (resolutions $275 \times 32 \times 150$, $275 \times 64 \times 150$ and $275 \times 128 \times 150$). Also in this case the computation converges.

Now, we investigate the refinement of the grid in vertical direction, $z$, and its effect on the boundary layer formed at the top of the rectangular cylinder (the quantities of interest shown below are calculated in the area circled in fig. 5.10). We use three grid resolutions refined in $z$-direction, $300 \times 64 \times 150$, $300 \times 64 \times 210$ and $275 \times 64 \times 300$ points respectively (in these cases the $z$-length of the domain has been reduced to 0.3 and 0.275$m$ respectively). The same time step is used: $\Delta t = 6 \times 10^{-7}$. In effect, our DNS must have enough points to be able to reproduce the boundary layer that develops around the obstacle. A first approximation of the boundary layer thickness can be done in the following way. From the previous simulations we know that before the flame interacts with the obstacle its speed slightly decreases and the thermal thickness assumes an almost constant profile in
Fig. 5.8 Calculation of the flame speed for three grid resolutions refined in x-direction in the case of the Ibrahim setup (rectangular cylinder as obstacle).

Fig. 5.9 Calculation of the flame speed for three grid resolutions refined in y-direction in the case of the Ibrahim setup (rectangular cylinder as obstacle).
a short temporal range starting at 0.02s (fig.s 5.5 and 5.7a). At this instant we take the mean value of the flow velocity (in \(x\)-direction), which is about 2.1m/s, as mean stream velocity \(U\). Then, by means of the Blasius relation we calculate an estimate for the thickness of the boundary layer at the top on the cylinder:

\[
\delta_L = \frac{5L}{\sqrt{UL/\nu}} = 0.00122
\]

(with \(L\) the thickness of the cylinder). The ratio \(\frac{\delta_L}{\Delta z}\) for the three grid resolutions is 2.5, 3.3 and 5 respectively. In fig. 5.11 we note the convergence of the boundary layer profiles. The finest grid has 6 points in the boundary layer.

Another quantity of interest is the total kinetic energy, \(k_T\). Because we do not have periodic directions in our configuration, we calculate an estimate of this quantity by first averaging the velocity components in the \(y\)-direction and then subtracting these averages from the instantaneous values to have an estimate of the fluctuating components. In fig. 5.12 we show the total kinetic energy for the three grid resolutions before the flame approaches the body (at \(t = 0.044s\)). In figures 5.13 the estimate of the kinetic energy is plotted at the instant \(t = 0.024s\) when the flame is close to the body but does not touch it yet. The value of \(k_T\) is still small. Fig. 5.14 shows the instant (\(t = 0.03s\)) when the flame is over the body. In this case \(k_T\) reaches its maximum value at the top and bottom surface of the body. The flame interacts with the obstacle and its propagation starts to be non-symmetric. This effect is prominent for the case of the coarsest grid. This phenomenon is influenced by the ‘turbulence’ produced during the interaction and in particular we paid attention to the shear stress produced at the top of the body. The shear stress generates a force (\(F\)) over the top face (\(A\)) of the obstacle. This force, normalized by the viscosity \(\mu\) is given by \(\frac{F}{\mu} = \int \frac{\partial u}{\partial z} dA\). In fig. 5.15 this quantity is plotted in time for the finest and the coarsest resolutions. We note a difference in the shear force for the two
Fig. 5.11 Boundary layer for different grid resolutions in vertical direction: $x-$velocity profiles around the top of the cylinder (circled area in fig. 5.10).

Fig. 5.12 An estimate of the total kinetic energy $(k_T = \frac{1}{2} \rho (u'^2 + v'^2 + w'^2))$ for the three grid resolutions at an instant $t = 0.004s$ before the flame reaches the body. The profiles are plotted along the $z-$center line of the body as indicated in fig. 5.10.
Fig. 5.13 An estimate of the total kinetic energy \( k_T = \frac{1}{2} \rho (u'^2 + v'^2 + w'^2) \) for the three grid resolutions at an instant \( t = 0.024 \) s before the flame reaches the body. The profiles are plotted along the \( z \)-center line of the body as indicated in fig. 5.10.

Resolutions in a short time interval around the values \( t = 0.03 \) when the flame is over the body. In this interval, in the case of the coarsest grid, the absolute value of the shear force is the smallest one. For this resolution one would expect the flow in principle to accelerate more because of the smaller shear. Instead this case presents the lowest peak in the kinetic energy, hence the interaction flame/body is not well captured resulting in a weaker propagation of the flame. In other words, for a poorly resolved boundary layer the stretching of the flame is not reproduced completely and therefore the enhancement of the flame speed, which is related to the increase in flame surface, is less intense.
Fig. 5.14 An estimate of the total kinetic energy \( k_T = \frac{1}{2} \rho (u'^2 + v'^2 + w'^2) \) for the three grid resolutions at \( t = 0.03s \) when the flame has reached the body. The profiles are plotted along the \( z \)-center line of the body as indicated in fig. 5.10. The kinetic energy undergoes a strong increase.

Fig. 5.15 The normalized force \( \frac{F}{\mu} = \int \frac{\partial u}{\partial z} dA \) generated by the shear stress at the top of the body plotted versus time for the finest and coarsest grid resolutions.

In fig. 5.16 the flame tip speed along the \( x \)-direction is plotted. The grid refinement shows converging calculations.
Fig. 5.16 Calculation of the flame speed for three grid resolutions. The domain is shortened to 0.3 m in x-direction. In the case of the coarsest grid the profile is lower and the recirculation zone is slightly shifted to the right with respect to the other resolutions.

Moreover, in the case of coarsest grid the profile is lower and the recirculation zone is slightly shifted to the right.

5.4 Simulation of the Ibrahim and Masri experiments

Once the profiles of $\delta$ and $L_M$ have been optimized we calculate the cases of the two geometries described above with rectangular (Ibrahim set-up) and square (Masri set-up) cylinders as obstacles placed in a deflagration tunnel. For the computational results shown in this section we have used a grid with resolution 450x64x150 points in $x$, $y$, $z$ directions respectively. We believe this choice is a reasonable compromise between computational time and accuracy if compared to the other resolutions used in the grid refinement study of the previous section.

In the case of the Ibrahim set-up at first we analyze the characteristics of the front at the early stage of the interaction with the wake. In figure 5.17a the interaction of the flame front in the wake past the corners of the body is shown by plotting the temperature field with the fluid particles trajectories. This picture is an enlargement of the upper part of the obstacle. A recirculation area is created by the object. In figure 5.17b the modulus of the vorticity ($\sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$) is plotted together with the zero $G$–level. The vorticity decreases at the position of the flame due to the thermal expansion while it increases at the edge of the flame due to the baroclinic production mechanism (fig. 5.18). The vorticity also increases after the body due to the friction of the accelerated flow with the body and the walls.

Hargrave et. al. (2002) repeated the same experiment of Ibrahim and they used PIV technique to measure the displacement speed, the strain and the curvature terms of the flame front at the early stages of the interaction with the wake formed behind the obstacle. However, these authors report that the measurements close to the walls were inaccurate
Fig. 5.17a Temperature isocontour and fluid particles trajectories at the early stages of the interaction of the flame with the body. The picture refers to the zone between the upper part of the body and the wall of the channel.

Fig. 5.17b The vorticity modulus and the zero level set plotted at the early stages of the interaction of the flame with the body. The flame position is indicated by the continuous line. This picture refers to the zone between the upper part of the body and the wall of the channel.
Fig. 5.18 The maximum absolute values of the baroclinic production term $\left| \nabla \frac{1}{\rho} \times \nabla p \right|$. Vorticity production is maximum when the gradients of the pressure and of the density are not aligned. This is the case along the flame front as shown in this figure.

since the rate of change of the flow velocity was very high with significant variation during the time over which the flame speed was calculated. Moreover, we do not know the exact position and time interval used by Hargrave et. al. for taking these measurements. Therefore, here we are only interested in comparing the order of magnitude of calculated instantaneous values of the strain and the curvature terms with the order of magnitude of the experimental results. This comparison is shown in fig.s 5.19a and 5.19b. The values are plotted at an instantaneous position of the flame (different for the calculated and the measured values) over a range of 20mm. The calculated values are averaged in the span wise direction $y$. Despite the fact that the inner flame structure is not resolved and the thermal thickness spreads over a maximum range of about 6-8 cells, their order of magnitude is not too different from the experimental data. In figure 5.20 the total stretch of the front at a certain instant past the corner of the body is also shown. The two profiles correspond to the case with and without smoothing of the stretch. The smoothed profile is obtained with a high level of smoothing (see Duris algorithm, 1980, for more details). The fact that we smooth the stretch means that we redistribute the energy contribution due to the enhancement of the flame surface but still keeping the total surface conserved. The flame tip speed is shown in figure 5.21. This picture compares our results with the experimental data of Ibrahim (repeated also by Hargrave et. al.) and with the simulation of Patel et al. (2003) that, at our present knowledge, is the most recent attempt of such a calculation. In Patel et al. a RANS approach is used with a $\kappa - \varepsilon$ model for
Fig. 5.19a An instantaneous plot of the strain around the flame (experimental data and calculated profile). The calculated and measured values are not taken at the same time and position therefore this graph is intended for comparing only their orders of magnitude.

Fig. 5.19b An instantaneous plot of the radius of curvature around the flame (experimental data and calculated profile). The calculated and measured values are not taken at the same time and position therefore this graph is intended for comparing only their orders of magnitude.
Fig. 5.20 An instantaneous plot of the total stretch of the flame past the corner of the body in the case with high and low smoothing.

Fig. 5.21 Flame tip speed comparison with experimental data and numerical calculations.
the turbulence. For the combustion modeling they use a flame surface density approach (FSD) that assumes the mean rate of reaction as function of a transport equation for the flamelet surface density. Our results are in good agreement with the experiment, the relative maximum value of the flame speed is well predicted and also the part of the profile in the recirculation area is well captured although the minimum in the recirculation area is higher than the experimental data. The isocontours of the temperature (figure 5.22) show that the time evolution of our calculation is qualitatively correct. In figure 5.23 the over-pressure (spatially averaged in the whole domain) calculated in time is shown and compared with the experimental values. There are two main peaks in the experimental data while in our work we have only one peak predicted. As explained by Patel et al. (2003) the first pressure peak is due to the disposable sealing membrane which holds the flammable mixture prior to ignition and insufficient information is available on the time scale of the bursting of this membrane. This effect is not included in our approach.
Fig. 5.23 Comparison of calculated overpressure with experimental data for the interaction flame/rectangular obstacle. The first peak of the experimental results is due to the bursting of the disposable membrane that keeps the gas into the tunnel. This phenomenon is not included in the numerical simulation.

Nevertheless, the predicted peak is close to the second peak in the experiment. Although we have to take into account that when the flame acceleration is such that the local Mach number becomes too large our low Mach number model loses its applicability and the calculated values of the overpressure are questionable.

In figure 5.24 we plot the computed flame tip speed for the first and the second geometries together with the experimental values. The second configuration (square cylinder as obstacle) was studied experimentally by Masri. Hargrave et. al. repeated this experiment and measured the flame tip speed. We can see that the calculated profile for the square cylinder is close to the experimental data by Hargrave et al. We find the same behaviour as Hargrave et al. (2002) that for the rectangular body, after the interaction, the flame front undergoes a higher acceleration resulting in a tip speed higher than for the square obstacle. In fig. 5.25 we can see that for the rectangular cylinder the flame front has tendency to wrap itself after the body, therefore, trapping more flammable mixture in the recirculation zone with respect to the square cylinder. As explained by Hargrave, this trapped mixture will be rapidly burnt generating more vorticity and a highly wrinkled flame front. This suggests that during the interaction with the flame, the rectangular shape creates more turbulence in the recirculation zone that enhances the flame speed.
Fig. 5.24 Comparison of the flame tip speeds between the cases of square and rectangular obstacles. The calculated and the experimental values are shown.

Fig. 5.25 Particles velocity vectors and flame isocontours for the cases of the square (fig. a) and the rectangular (fig. b) obstacles. For the rectangular cylinder case, the flame front has tendency to wrap more on itself and to trap a larger amount of flammable mixture in the recirculation zone.
5.5 The importance of the temperature equation

Let us consider a simulation of the interaction flame/rectangular body with a pure G-equation model (no temperature equation used, the temperature is directly linked to the G-equation, see Treumiet for details). Because the temperature is directly linked to G and the level set suffers of numerical errors during the calculation of the curvature in the stretch term, then, it is expected that the flame is very sensitive to the stretch. We want to verify if our model gives a better prediction of the flame propagation with respect to a pure G-equation model. It can be seen in figure 5.26 that for the pure G-equation approach the propagation of the front after the body is very different from the experimental case (fig. 5.22a): the trapped mixture in the recirculation zone is consumed faster than in the experiment and the interaction into the recirculation zone is not captured correctly. These results suggest that in our model the numerical error of the stretch is somehow mitigated. In a previous section, we have also observed that our model shows a convergent solution for the flame tip speed by the refinement of the computational grid.

A possible explanation is that while in the pure G model there is only the level set variable to drive the flow (so that the calculation is very susceptible to errors on G and its derivatives) in our model the effect of G is contained in the source term which is diffused by the temperature equation. In addition, the model used in this thesis ensures that the energy released by the source is conserved as far as the total area of the flame is conserved during the reinitialization procedure and matches with the burning rate. The fact that the temperature equation contains a source term which depends on the stretch is a key point of the model. In effect, the stretch term contained in the chemical source influences
the amount of energy produced by the flame. When the stretch is smoothed the value of the flame speed is updated such that the relation 3.42 between the burning rate and the stretch term continues to be satisfied and hence the energy released by the source is conserved.

5.6 Variable viscosity case

In this paragraph we want to consider the case of variable viscosity for the Ibrahim configuration with rectangular obstacle studied in the previous sections. If we remove the assumption of constant viscosity then the flammable gas mixture viscosity will be a function of the temperature. It will increase with the temperature. In principle, also the diffusion flame thickness would be influenced. Let us consider the relation

\[ \frac{\delta s_L}{a} = \text{const} \] (Veynante, 2002)

where is \(\delta\) the diffusive flame thickness, \(s_L\) the laminar flame speed and \(a\) the thermal diffusivity,

\[ a = \frac{\lambda}{\rho c_p} = \frac{\nu}{P_T} \]

Taking the Prandtl number constant we have

\[ \delta = \text{const} \cdot \nu = \text{const'} \cdot \mu \]

hence

\[ \frac{\delta}{\delta_0} = \frac{\mu}{\mu_0} \] (5.2)

where the under script '0' stands for the case with constant viscosity \(\mu_0\). With this simple dimensional consideration we see that the thickness is influenced by a variable viscosity. For the variable viscosity case we use the Sutherland law:

\[ \mu = \mu_0 \left( \frac{T}{T_0} \right)^{3/2} \frac{T_0 + S}{T + S} \]

where \(S\) is a constant (taken here equal to 0.368).

As described earlier in this chapter, in our model the diffusive thickness is optimized according to the thermal flame thickness profile. Now, considering a variable viscosity \(\mu\), \(\delta\) should be re-optimized every time the viscosity changes. However, in this way it could be difficult to distinguish between the effect on the solution due to a variable viscosity and the effect due to a variable thickness. Here, we are interested in the influence of a variable viscosity, hence we make an approximation: by using the Sutherland law we calculate the ratio \(\frac{\mu}{\mu_0}\) for \(T = T_0\) and \(T = T_{\text{adiabatic}}\), then we take its mean value and from the relation (5.2) we calculate a constant value for \(\delta\) that is used in the computation. It results that the diffusive thickness, \(\delta\), to be used for the variable viscosity case is twice the thickness of the constant viscosity case.

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For the computation a grid resolution of 300x64x210 points in x,y,z directions respectively is used. In Fig. 5.27 the flame tip speed is plotted for the two cases with constant and variable viscosity. The profile of the variable viscosity case is higher than the constant viscosity case in the initial part until the interaction with the body. Then it becomes slightly lower in the recirculation zone after the object and finally it increases again more than the profile of the constant viscosity case.

Fig. 5.27 Flame tip speed profiles for the two cases of constant and variable viscosity.
Fig. 5.28 Vorticity isocontour at an instant before the flame front reaches the obstacle. Fig. (a) refers to the constant viscosity case. Fig. (b) refers to the variable viscosity case. (Dashed lines indicate negative values).

The size of the eddies produced at the flame front in the case of variable viscosity is larger than in the case of constant viscosity as we can see in fig. 5.28 from the isocontour plot of the vorticity. During the laminar propagation these vortices increase the area of the flame and hence its speed. Once the flame fingers between the body and the channel walls pass over the body these larger vortices interact more with the recirculation zone behind the body and the flame is wrapped more than in the case of constant viscosity (figs. 5.29 and 5.30).
Fig. 5.29 Vorticity isocontour at an instant when the flame is passing over the obstacle. Fig. (a) refers to the constant viscosity case. Fig. (b) refers to the variable viscosity case. (Dashed lines indicate negative values).
Fig. 5.30 Vorticity isocontour at a later instant when the flame is interacting with the recirculation zone after the obstacle. Fig (a) refers to the constant viscosity case. Fig. (b) refers to the variable viscosity case. (Dashed lines indicate negative values).

This interaction slows down the flame tip speed. Then, after the recirculation zone the flame can enhance again its area and therefore its speed (fig. 5.27).

5.7 Simulation of a deflagration in a tunnel with multiple blocks

In this paragraph we show results for the case of a deflagration in a tunnel with multiple obstacles. This case shows the limit for our low Mach number model when the flame front undergoes such a large acceleration that the local Mach number becomes larger than unity. The geometry under investigation is described in figure 5.31 (in $xy$-plane). It consists of a domain of size $2x0.5x0.25m^3$ open at the right side. It contains eight rectangular blocks of size $0.24x0.1x0.0925m^3$ each one, placed at $0.025m$ away from the bottom ($z = 0$) of the tunnel and $0.125m$ from the left closed side. The blocks are distributed symmetrically with respect to the $y$-direction. A flat flame is ignited at the closed side. An equidistant Cartesian grid of $400x100x100$ points in $x$, $y$ and $z$ directions is used. This is a very coarse
resolution but it is considered enough to give an indication of the limits of the model for this configuration. No-slip and non-penetration conditions for the velocity are applied at the walls of the channel, zero pressure is set at the outflow and a zero gradient condition is chosen for all scalar quantities at the walls. The blocks are adiabatic. Viscosity is taken constant and laminar burning speed is $s_l = 0.4m/s$. The Reynolds number is

$$Re = \frac{\rho_0 s_l l_{body}}{\mu_0} = 3700.$$  

The flame is ignited as flat surface at the closed side of the domain. In the series of figures 5.32 and 5.33 the temperature isocontours at different instants are shown. They are taken in the planes $xy$ (at $z = l_z/2$) and $xz$ (with $y$ at the center line of the first row of blocks) respectively. The evolution of the flow presents an acceleration and an increase of vorticity produced during the interaction with the rows of bodies. As we can see from the plot of the flame tip speed in figure 5.34 there is an acceleration each time the flame reaches a row of obstacles. Unfortunately, for this configuration no experimental data were available for the temperature and the velocity fields. We were also not able to predict physical values of overpressure for this case. The reason is that the acceleration of the flow during the flame propagation gets so high that the validity of the low Mach number approximation is questionable. In figure 5.35 the local Mach number is plotted along the channel at an instant when the flame is close to the outlet. Its value is of order $O(1)$.
Fig. 5.32 Temperature isocontour plots at different instants along the channel. The plots are taken in the plane $xy$ with $z = l_z/2$.

Fig. 5.33 Temperature isocontour plots at different instants along the channel. The plots are taken in the plane $xz$ along the $y$–center line of the first row of obstacles.
Fig. 5.34 The flame tip speed along the tunnel with eight obstacles.

Fig. 5.35 The local Mach number along the tunnel at an instant when the flame is reaching the outlet.
Chapter 6

Conclusions and Future Work

The main scope of this study has been to introduce a new model for the simulation of low Mach number premixed flames. In this approach the energy equation contains a source term which depends on a level set variable ($G$-equation). The method has been applied in the case of high density ratios between burnt and fresh mixture. The numerical model is based on a new pressure correction algorithm for the time integration of the flow equations and on an implicit/explicit (IMEX) Runge-Kutta scheme for the energy equation. This approach has proved to be stable for high density ratios and appears a promising tool for further computations of combustion problems. A second aim has been to simulate the interaction of a premixed flame with obstacles. In particular, we have simulated the experiment performed by Ibrahim and Masri (2001) where a flame was ignited in a domain with a rectangular obstacle. The geometry was mimicked with an immersed boundary method (IBM) particularly suitable for the simulation of square and rectangular bodies. The IBM presented here is easy to implement, it requires less computational resources than standard methods, it has accuracy comparable with that one of an iterative solver approach and it is suited for heat transfer and combustion problems.

We have also investigated the influence of the flame stretch term on the propagation of the front. In our model the total stretch is smoothed in order to limit the effects of its numerical error. The temperature equation smears out the energy released at the position of the flame and this appears as a mechanism that stabilizes the calculation.

The results obtained are comparable with the experimental data. The flame tip speed and the interaction of the front in the wake are well predicted. We note that the thermal thickness is reduced due to the interaction with the body. This interaction produces also an overpressure. Only if the low Mach number approximation is valid we can obtain meaningful values of overpressure. In effect, when the local Mach number becomes large the method cannot be applied anymore and one should consider the possibility of using a fully compressible model. This limitation is underlined in the simulation of a deflagration in a tunnel with eight blocks. The local Mach number increases along the channel with local peaks every time the flame front hits a new row of obstacles. At the end of the domain the low Mach number approximation does not hold anymore. Nevertheless, for this geometry the code is able to predict the flame speed profile. A validation of this case with experimental data appears necessary for future work.
We have also considered a simple variable viscosity model (Sutherland's law). An approximation for this case has been applied by considering the diffusive flame thickness still constant. The results show a higher interaction of the flame front in the recirculation zone beyond the obstacle in the case of variable viscosity.

In this study we have used a uniform and fixed Cartesian grid. For future work a suitable stretched grid could save computational time. Our model can be considered an intermediate approach between DNS and LES. In effect, we do not solve the chemistry and we assume a flame much thicker than in reality. A full LES approach could be easily derived from this model for a future study of a case with high turbulence intensity.

With the use of the $G$-equation we got rid of the stiffness of the chemistry, however examples of models which implement detailed chemistry in a $G$-equation approach are available in the literature (Liang et. al., 2006). Therefore, an extension of the method elaborated in this thesis with a more sophisticated model for the chemistry can in principle be achieved. It could be useful to test a parallel computer version of the code on a supercomputer, especially if a detailed chemistry model will be implemented. In fact, the use of chemistry database can require large computer memory. Single personal computers have very finite memory resources. For large problems, using the memories of multiple computers may overcome this obstacle.
Appendix A: spatial discretization

The spatial discretization (second order finite volume) is outlined here, for pure central differences scheme of the terms $A$ (advection) and $D$ (diffusion) for the $x$-components of the energy, momentum and $G$ equations. In the other directions the procedure is similar.

For the energy equation (in non-conservative form) we have:

$$A_T = - \left[ \frac{1}{2} \left( u_{i-1,j,k} + u_{i,j,k} \right) \frac{1}{2} \left( T_{i+1,j,k} - T_{i-1,j,k} \right) \right]$$

$$D_T = \left[ \frac{1}{\rho_{i,j,k}} \frac{1}{RePr} \frac{1}{\Delta x_i} \lambda \frac{1}{2} \left( T_{i+1,j,k} + T_{i-1,j,k} - 2T_{i,j,k} \right) \right]$$

For the $x$-component of the momentum considering $u$ as the $x$-component of the velocity it is:

$$A_m = \nabla \cdot (-u(\rho u))_{i,j,k} = - \frac{u_{i+\frac{1}{2},j,k} (\rho u)_{i+\frac{1}{2},j,k} - u_{i-\frac{1}{2},j,k} (\rho u)_{i-\frac{1}{2},j,k}}{\Delta x_i} +$$

$$- \frac{v_{i+\frac{1}{2},j,k} (\rho u)_{i+\frac{1}{2},j,k} - v_{i-\frac{1}{2},j,k-1} (\rho u)_{i-\frac{1}{2},j,k}}{\Delta y_j} +$$

$$- \frac{w_{i+\frac{1}{2},j,k} (\rho u)_{i+\frac{1}{2},j,k} - w_{i+\frac{1}{2},j,k-1} (\rho u)_{i+\frac{1}{2},j,k-1}}{\Delta z_k}$$

$$D_m = \frac{\tau_{xx_{i+\frac{1}{2},j,k}} - \tau_{xx_{i-\frac{1}{2},j,k}}}{\Delta x h_i} + \frac{\tau_{yx_{i+\frac{1}{2},j,k}} - \tau_{yx_{i-\frac{1}{2},j,k}}}{\Delta y_j} + \frac{\tau_{zx_{i+\frac{1}{2},j,k}} - \tau_{zx_{i-\frac{1}{2},j,k}}}{\Delta z_k}$$

with,

$$\tau_{xx_{i+\frac{1}{2},j,k}} = \frac{\mu}{Re} \left( 2 \frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x_{i+1}} - \frac{2}{3} \Delta i+1,j,k \right)$$

$$\tau_{yx_{i+\frac{1}{2},j,k}} = \frac{\mu}{Re} \left( \frac{u_{i,j+1,k} - u_{i,j,k}}{\Delta y_{j+1}} + \frac{v_{i+1,j,k} - v_{i,j,k}}{\Delta x_{i+1}} \right)$$

$$\tau_{zx_{i+\frac{1}{2},j,k}} = \frac{\mu}{Re} \left( \frac{u_{i,j,k+1} - u_{i,j,k}}{\Delta z_{k+1}} + \frac{w_{i+1,j,k} - w_{i,j,k}}{\Delta x_{i+1}} \right)$$

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and

\[ \Delta_{i,j,k} = \frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x_i} + \frac{v_{i,j+1,k} - v_{i,j,k}}{\Delta y_j} + \frac{w_{i,j,k+1} - w_{i,j,k}}{\Delta z_k} \]

**For the G-equation** there are no diffusion terms, \( D = 0 \). The G-equation is a hyperbolic differential equation with a source term on the right hand side:

\[ \frac{\partial G}{\partial t} + u \cdot \nabla G = s_L |\nabla G| \]

At first, it can be re-casted in pure advective form,

\[ \frac{\partial G}{\partial t} + u_e \cdot \nabla G = 0 \]

with the effective velocity \( u_e \) being

\[ u_e = u + s_L \cdot n \]

where \( n \) is the normal defined in chapter two. The x-component of \( n \) on the face of the cell is defined as

\[ n_{x,i,j,k} = -\frac{G_{i+1,j,k} - G_{i,j,k}}{\Delta x_i} \]

\( (\nabla G)_{i+\frac{1}{2},j,k} \) must also be calculated on the cell faces. More details can be found in Treurniet (2002). Then, in conservative form the G-equation reads,

\[ \frac{\partial G}{\partial t} + \nabla \cdot (u_e G) = (\nabla \cdot u_e)G \]

Because \( G \) is defined at the center of the cells, its values and the values of its normal vectors on the cells surface are obtained by interpolation. The term \( u_e G \) is computed with a third order WENO scheme (Jiang and Peng, 2000) while the term on the right hand side with central differences.
Bibliography


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- Fabio was born on 15-03-1975 in Salerno, Italy, spending a wonderful childhood and youth in the stunning scenario of the Amalfi Coast.


- 1994-2002: engineering studies at University of Rome “La Sapienza”, student kind of sporadic jobs and support to a social voluntary organization.

- November 2002-December 2003: stage as master student at the Nuclear Engineering Laboratory (LKT) of the Swiss Federal Institute of Technology – ETHZ, Zurich. Main task: stability analysis and modeling of a nuclear boiling water reactor.

- July 2003: Master degree in Nuclear Engineering at the University of Rome “La Sapienza”.

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