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Numerical Simulation of Non-premixed Laminar and Turbulent Flames by means of Flamelet Modelling Approaches

DOCTORAL THESIS

Centre Tecnològic de Transferència de Calor
Departament de Màquines i Motors Tèrmics
Universitat Politècnica de Catalunya

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Doctoral Thesis

UPC – Febrer 2005

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TESI DOCTORAL

presentada al

Departament de Màquines i Motors Tèrmics
E.T.S.E.I.T.
Universitat Politècnica de Catalunya

per a l'obtenció del grau de

Doctor Enginyer Industrial

Terrassa, Febrer 2005

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Acknowledgements

En primer lloc vull remarcar el recolzament rebut pels directors d'aquesta tesi. A l'Assensi Oliva, ànima del CTTC, li agraeixo, per anomenar algunes coses, la passió i dedicació amb que viu la recerca i el fet d'haver-me-la transmesa. També per tot el suport que m'ha donat al llarg de la tesi. Al Carles David Pérez-Segarra pel rigor acadèmic i científic en el tractament dels problemes, fet en el que ha estat un mirall per a mi. També la seva autèntica passió pel coneixement. Al Ricard Cònsul pel moltíssim temps que m'ha dedicat al llarg de tots els anys de doctorat (de fet, això ja va començar abans), per haver compartit amb ell xerrades intenses i/o apassionades, infinitat de *brainstormings* (alguns ben acompanyats d'una o més cerveses...), pel rigor en els seus plantejaments i, a nivell més personal, per la seva amistat i franquesa. Sense tu, res hagués estat possible.

De la mateixa manera, agreixo al Jordi Cadafalch el seu suport en tota la part de CFD. El seu rigor en l'estructuració de codi i la capacitat alhora d'organitzar tasques sempre m'ha admirat. També la seva amistat.

Vull reconèixer al Ramiro i al Daniel l'ajuda i dedicació donada en tota la part informàtica al llarg del anys.

Com no podria ser d'altra manera, agraeixo l'oportunitat d'haver pogut conviure i compartir hores de feina, xerrades filosòfiques i termogresques amb tots els companys/es i/o amics i amigues del CTTC. Molt especialment al Carles, la Conxita, el Quim, el Miquel, el Cristian, el Dani i el Julian.

Dono les gràcies a la Generalitat de Catalunya per la concessió de la beca predoctoral l'any 1999 i al Col·legi d'Enginyers Industrials de Catalunya per la beca concedida per a la realització de Tesis Doctorals l'any 2002.

I am very grateful to Professor Jyh-Yuan Chen from the University of California at Berkeley and Professor Raymond Viskanta from the Purdue University for they help and kindness in my stays at their institutions.

Finalment, vull agrair amb un especial significat, com no, als meus pares(3) l'infinit amor, suport i mestratge en la vida que m'han donat sempre. Als meus avis i àvies per l'experiència que m'han transmès. En especial, a la meva iaia Elisa per la convivència durant aquests anys. A la meva germana, per haver-nos redescobert. Als meus amics i amigues el fet de ser-hi quan cal. A Martina pelo seu amor, ajuda e compreensão. A tots vosaltres, mai us ho podré agrair prou.

Contents

Chapter 1

Introduction

Combustion technology has played an important role in the development of our civilisation. Almost 80% of the worldwide energy support is provided by combustion equipment, a fact that is not expected to change in the near future. Therefore, deep knowledge, understanding and control of combustion phenomena is of great scientific and technological interest. Better design of combustion equipments can contribute both in the energy efficiency and in the reduction of pollutant formation.

Combustion is a complex phenomenon that involves several disciplines e.g. thermodynamics, heat and mass transfer, fluid dynamics and kinetic chemistry. Much advance has been achieved in the understanding of these disciplines and, furthermore, the coupling of all these fields in a problem such as combustion have also experienced a remarkable progress. Rigorous mathematical formulation of combustion phenomena is compiled in many text books, specially for laminar combustion. Turbulent combustion requires additional modelization such as statistical techniques to describe the flow and the inherent fluctuations involved. Accurate models for molecular transport phenomenon in multicomponent flows are also of deep interest, and much improvement has been acquired. Full chemical models for major fuels have received great attention from the scientific community, and very complete mechanisms for hydrocarbons, i.e. methane ($80 \div 90\%$ composition of natural gas), are now available. In addition, modelization of radiation heat transfer for participating media has also experienced a large development not only for combustion application but also for fields such as atmospheric knowledge.

Main phenomenological difficulties that arise from such complex phenomenon are summarised herewith: large chemical mechanism with a large number of chemical species and reactions with a wide range of time scales; sharp gradients of primitive variables (velocity vector, temperature and species mass fractions); usually turbulent regimes which imply three-dimensional and transient effects; radiation heat transfer in participating media since flames can absorb, emit and scatter radiation; phase-change problems when droplets combustion is considered; soot formation; etc. Each of these phenomena require a deep phenomenological understanding as well as an accurate mathematical description. Furthermore, the coupling among certain phenomenologies

must be considered and a suitable modelization is required.

Nowadays, one of the main limitations to predict and design combustion industrial equipment (furnaces, boilers, engines,...), or even predict simple flames such as jet flames or Bunsen flames, is in the resolution of the mathematical formulation. Analytical solutions of the governing equations are not feasible for most of the technological problems, and recently numerical techniques have received enormous interest. Given the ever-increasing computational capacity, numerical resolution of the formulation has become a powerful tool in the last decades and, therefore, numerical simulation of combustion phenomena is becoming a very useful ingredient in the design of industrial equipment.

Knowledge of local and instantaneous values of the primitive variables, i.e. velocity, pressure, temperature, mass fractions of the species involved in the combustion process, etc., constitute an essential component to completely understand the phenomena, to control the whole processes and, as a consequence, to get a better thermal and environmental design of the elements present in a combustion equipment. A virtual test bank can contribute to a dramatic reduction of the costs of the design decreasing the number of prototypes required and also the time-to-market of the products. Therefore, contributions to improve the mathematical and numerical tools are a challenge for the scientific community and a benefit for engineers, designers and, consequently, the whole society.

1.1 Background

This thesis pretends to contribute to the research that the international technical and scientific community is currently carrying out on the numerical simulation of laminar and turbulent flames. The state-of-the art in this topic is discussed in detail in Chapters 2, 3 and 4. In this section, a brief description of the antecedents of this topic in the Group where this thesis has been developed is given in order to locate the research carried out into this framework.

The present thesis has been developed at the Heat and Mass Transfer Technological Center (CTTC) of the Technical University of Catalonia (UPC), which has devoted human and economical resources to the basic understanding of fluid-dynamics and heat and mass transfer phenomena to acquire a powerful know-how and tools to improve the design of thermal systems and equipment. A deep understanding of the mathematical formulation that govern these phenomena, the detailed resolution by means of verified numerical simulations and experimental validation of the numerical results have been of great interest for the CTTC researchers.

Combustion phenomenon has received distinguished attention at CTTC, specially during the last decade. The main work developed on combustion modelling was the motivation of some contributions in different symposiums [1–11] and, to a large extent,

the PhD thesis of R. Cònsul [12] and two articles in prestigious journals [13, 14]. The main focus of the work was the rigorous formulation of chemically reacting flows and the detailed numerical simulation. Given the complexity of the detailed numerical simulation of combustion phenomena (finite rate kinetics, radiation in participating media, turbulence regimes, etc), the work was initially focused on the numerical simulation of laminar flames. Both premixed and non-premixed laminar flames were simulated. Numerical solutions were verified and the mathematical models validated with experimental data available in the literature.

Verification of numerical solutions has been considered a key issue in order to produce reliable results. Numerical results are successfully submitted to a verification procedure developed at CTTC [15] in order to assess their quality and establish criteria on the sensitivity of the simulation to the computational model parameters that account for the discretization. This tool estimates the order of accuracy of the numerical solutions, and the error band where the grid independent solution is expected to be contained, also giving criteria on the credibility of these estimations. Main contributions on verification techniques are compiled in the PhD thesis by J. Cadafalch [16].

In order to reduce the large computational resources required for the numerical simulation of laminar flames, a parallel multiblock algorithm using loosely coupled computers was proposed. Special emphasis was given to the parallel efficiency. The domain decomposition method itself has also received great attention at CTTC [17, 18]. These numerical techniques allow to increase the number of grid nodes in some phenomenologically complicated zones e.g. walls or flame fronts, and to reduce the number of grid nodes in other zones. As mentioned, this technique is specially attractive to be parallelised. Fast solvers for the resolution of large linear systems of equations are also essential tools to feasibly solve all these complex phenomena. Main contributions on these topics are compiled in the PhD thesis of M. Sòria [19] and J. Cadafalch [16], and publications such as [2, 3, 13, 20–22].

The flames studied were supposed to accomplish the hypothesis assumed with the Optically Thin Model (OTM). This means that the flame neither absorbs radiation coming from the hot gases nor scatters radiation. Nevertheless, researchers at the CTTC are working on a highest level of description considering the full RTE (Radiative Transfer Equation) solving it with DOM (Discrete Ordinates Method) [23–25]. In addition, a more accurate technique to evaluate the optical properties and to consider in a more detailed manner the spectral nature of these properties is also being developed. These models are likely to be applied to combustion simulations in the near future.

Even though turbulence regimes have been applied to reactive flows recently, a large experience is acquired at CTTC for incompressible non-reactive flows. This experience comes from the PhD by C.D. Pérez-Segarra [26] where the boundary layer

case was characterised. Next steps were the implementation of turbulence RANS models (Reynolds-Averaged Navier-Stokes Simulations) and the resolution of different natural convection flows [27–30] and forced convection flows [16, 31–34]. DNS (Direct Numerical Simulation) of incompressible flows have also been investigated [22, 35–37] more recently.

1.2 Outline

In the remainder of this chapter, the basic mathematical formulation for chemically reactive gas flows is presented, focusing the attention on combustion. Transport equations for mass, momentum, species and energy are taken into account as well as the state equation. Furthermore, modelization of molecular transport terms, thermal radiation and the chemistry involved are also exposed. Continuing in this chapter, the main simulation methodology employed in this thesis is presented. A parallel multiblock algorithm using loosely coupled computers is commented and the verification tool employed in the subsequent chapters is presented. Numerical tools are basically compiled in [13].

The results presented in the second chapter are compiled from the PhD thesis by R. Cònsul [12] and the article [14] published in the journal *Combustion and Flame*, where the author of the present thesis made a significant contribution. The chapter shows a deep analysis of the multidimensional mathematical modelling and a numerical investigation of a co-flow partially premixed methane/air laminar flame. Detailed simulations based on the full resolution of the transport governing equations are performed. The capabilities and limitations of the numerical simulations of laminar combustion are given showing the highest resolution level of this powerful tool. A verification and validation of the numerical solutions in a wide range of partially premixed levels are presented. Different chemical approaches (from reduced mechanism to full mechanism of GRI-Mech 3.0 of 325 reactions and 53 species), radiation effects, mass transport models, and inlet boundary conditions are carefully studied. Special emphasis is paid to the description of the pollutant formation, i.e. CO and NO_x formation.

The third chapter is dedicated to the formulation of flamelet equations for non-premixed combustion and the modelling considerations for an accurate application in the numerical simulation of multidimensional non-premixed laminar flames. Steady and unsteady flamelets are compared showing the limitations and capabilities of each approach. Special attention is paid to the assumptions of the flamelet equations, the scalar dissipation rate modelling, and the evaluation of the Lagrangian type flamelet lifetime when unsteady flamelets are considered. The validation of the flamelet mathematical formulation is performed with verified numerical solutions based on the full resolution of the transport equations (discussed in Chapter 2). Four phenomenologi-

cal situations related to the mass transfer process and the inclusion of the radiation heat transfer are identified: i) Unity-Lewis numbers and radiation not included; ii) Unity-Lewis numbers and radiation included; iii) Fixed-Lewis numbers and radiation not included; iv) Fixed-Lewis numbers and radiation included. Special emphasis is given again to the proper characterisation of the pollutant formation.

As a complement of the discussion presented in Chapter 3 about the laminar flamelet concept, an appendix is contributed. In this appendix, the flamelet libraries used for the flamelet modelling simulations of the confined co-flow axisymmetric non-premixed methane/air laminar flame performed in Chapter 3 are studied. Part of the contents of this appendix are published in *Proceedings of the 42nd AIAA Aerospace Sciences Meeting and Exhibit*, 2004 [9].

Once the flamelet model has been applied and deeply analysed for the numerical simulation of multidimensional laminar flames, its application is investigated in a well-known piloted non-premixed methane/air turbulent flame. The fourth chapter is dedicated to expose the mathematical formulation for turbulent combustion based on mass-weighted time-averages (Favre-averaging) techniques and using RANS EVM two-equation models and the laminar flamelet concept with a presumed PDF. Verification of the numerical solutions and validation of the mathematical formulation using available experimental data have been carefully performed. Steady and unsteady flamelet modelling simulations are compared giving idea of the limitations and improvements of each approach. An extended version of the Eddy Dissipation Concept (EDC) model is also employed to compare its results with the flamelet simulations.

Finally, a general conclusion chapter is written to summarise the achievements, the capabilities, and also the main difficulties and limitations of the methodology employed for the numerical simulation of combustion phenomena both for laminar and turbulent regimes. Future actions are also suggested.

1.3 Basic Mathematical formulation for a reactive gas.

Next sections present the basic mathematical formulation employed in this thesis. The governing transport equations for reactive gas mixtures are expressed in a differential form. Models for the molecular transport fluxes are provided for gas mixtures taking into account main effects and the commonly used simplifications.

1.3.1 Basic transport equations for multicomponent reactive flows

The governing equations for a low-Mach number reactive gas (continuity, species, momentum, energy and state equation) can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{1.1}$$

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) = -\nabla \cdot \vec{j_i} + \dot{w}_i \tag{1.2}$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{g} \tag{1.3}$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \vec{v} h) = -\nabla \cdot \vec{q} - \nabla \cdot \vec{q}^{\,R} + \vec{\tau} : \nabla \vec{v} + \frac{\partial p}{\partial t} + \vec{v} \cdot \nabla p \tag{1.4}$$

$$\rho = \frac{pM}{RT} \tag{1.5}$$

where t is time; ρ mass density; $\vec{v}$ average velocity of the mixture; $\vec{\tau}$ shear stress tensor; p pressure; $\vec{g}$ gravity; h specific enthalpy of the mixture; $\dot{w}_i$ net rate of production of *ith* species; M molecular weight of the mixture; $\vec{q}$ diffusion heat flux; $\vec{q}^{\,R}$ radiant heat flux; Y_i mass fraction of *ith* species; $\vec{j_i}$ diffusion mass flux of *ith* species; T temperature, and R the gas universal constant.

The energy equation 1.4 can be simplified neglecting some effects. The third term on the r.h.s. describes the frictional heating and is negligible for low speed flows. Next term, the time derivate of the pressure, should be retained in applications for reciprocating engines but can be neglected in open flames where the pressure is approximately constant and equal to the static pressure. In the small Mach number limit, the term $\vec{v} \cdot \nabla p$ can also be neglected [38]. Taking into account these considerations, the energy equation reads:

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \vec{v} h) = -\nabla \cdot \vec{q} - \nabla \cdot \vec{q}^{\,R} \tag{1.6}$$

Enthalpy and temperature are related as,

$$h = \sum_{i=1}^{N} h_i Y_i = \sum_{i=1}^{N} \left(h_i^o + \int_{T^o}^{T} c_{p_i} dT \right) Y_i \tag{1.7}$$

where h_i is the specific enthalpy of *ith* species; h_i^o is the standard heat of formation of *ith* species; N is the total number of chemical species; c_{p_i} is the specific heat of *ith* species and T^o is the standard state temperature. Thermodynamic properties have been evaluated using the NASA thermodynamic data [39].

1.3.2 Modelization of the molecular transport terms

In a multicomponent dilute gas, species mass diffusion fluxes $\vec{j}_i$, from a rigorous kinetic theory formulation, are associated to three mechanical forces and to one thermal force. Molecular mass diffusion fluxes are caused by: i) concentration gradients $\vec{j}_{X,i}$; ii) pressure forces $\vec{j}_{p,i}$, for example in a rotating gas formed by heavy and light species; iii) body force $\vec{j}_{b,i}$, for instance, in a mixture submitted to an electrical field and where the mixture contains some species with magnetic properties; iv) temperature gradients $\vec{j}_{T,i}$. These contributions are usually called *ordinary*, *pressure*, *forced* and *thermal* diffusion respectively. The last one is also known as *Soret effect*. Here, only the *ordinary* (equivalent Fickian diffusion) and the *thermal* diffusion effects are taken into account. Contributions due to both pressure gradients and body forces are neglected since they are small compared to ordinary and thermal diffusion [40]:

$$\vec{j_i} = -\rho \mathcal{D}_{im} \nabla Y_i - D_i^T \nabla \ln T \tag{1.8}$$

where, $\mathcal{D}_{im}$ and D_i^T are the multicomponent ordinary and thermal diffusion coefficients respectively.

The shear stress tensor is evaluated taking into account Stokes' law for Newtonian fluids:

$$\vec{\tau} = 2\mu\vec{\gamma} - \frac{2}{3}\left(\mu \nabla \cdot \vec{v}\right)\vec{\delta} \tag{1.9}$$

where μ is the mixture viscosity; $\vec{\delta}$ is the Kronecker Delta; $\vec{\gamma}$ is the rate of strain tensor which can be expressed as:

$$\vec{\gamma} = \frac{1}{2}\left(\nabla\vec{v} + \nabla\vec{v}^T\right) \tag{1.10}$$

Diffusion heat flux considers Fourier's conduction and the energy transport by inter-diffusion is given by:

$$\vec{q} = -\lambda \nabla T + \sum_{i=1}^{N} h_i \vec{j_i} \tag{1.11}$$

where λ is the thermal conductivity of the mixture. Molecular fluxes of momentum $\vec{\tau}$, heat $\vec{q}$ and mass $\vec{j_i}$, have to be modelled requiring the introduction of transport coefficients. These coefficients are evaluated considering a mixture-averaged formulation. Pure-species transport properties are evaluated using CHEMKIN's database [41]. The Duffour effect (flux of energy produced by concentration gradients) has been neglected.

For the mixture-averaged viscosity μ and thermal conductivity λ, the semi-empirical formulae by Wilke (1950) and modified by Bird (1960), is used [40]. Mixture diffusion coefficients $\mathcal{D}_{im}$ that appear in Eq. 1.8 are calculated considering three possibilities, from higher to lower level of detail:

- From *Stefan-Maxwell* equation and considering the *trace-species* approximation [40]. Assuming that a given species sees the rest moving with the same averaged velocity, and when the mixture is composed by one majority species, the equivalent Fickian diffusion coefficient of one species into the mixture can be formulated as [40]:

$$\mathcal{D}_{im} = \frac{1 - Y_i}{\sum_{\substack{j=1 \\ j \neq i}}^{N} X_j / \mathcal{D}_{ij}} \tag{1.12}$$

  Here, $\mathcal{D}_{ij}$ are the binary diffusion coefficients and X_j the molar fraction of *jth* species.

- Consideration of a fixed Lewis number for each species, e.g. $Le_{CH_4} = 0.97$, $Le_{O_2} = 1.11$, $Le_{H_2} = 0.3$. Species $\mathcal{D}_{im}$ coefficients, are evaluated from their Lewis number value:

$$\mathcal{D}_{im} = \frac{\lambda}{\rho Le_i c_p} \tag{1.13}$$

  For major species, these fixed Lewis numbers are provided in the literature (see, for example [42]). In this work and when Lewis numbers are not known, they have been evaluated by averaging the local Lewis values obtained from the numerical results performed with the previous approximation. See [12] for further details.

- Consideration of a unity Lewis number for all the species involved in the chemical model ($Le_i = 1.0$, $i = 1, 2, ...N$). This approximation is commonly used, for example, for the flamelet approach [43, 44].

$$\mathcal{D}_{im} = \frac{\lambda}{\rho c_p} \tag{1.14}$$

Thermal diffusion coefficients are obtained using calculated $\mathcal{D}_{im}$ values. This coefficients are related to the thermal diffusion ratios by:

$$D_i^T = \frac{\rho_i \mathcal{D}_{im}}{X_i} \Theta_i \tag{1.15}$$

where Θ_i is the thermal diffusion ratio of *ith* species and is given by:

$$\Theta_i = \sum_{j=1}^{N} \theta_{ij} X_i X_j \tag{1.16}$$

Here, θ_{ij} are the pairs of thermal diffusion ratios for light species into all other components of the mixture. These ratios are only given for chemical species with mass weights lower than 5 g/mol.

1.3.3 Energy equation in terms of temperature

The energy equation is expressed in terms of temperature. We define the mixture enthalpy as follows:

$$h = \sum_{i=1}^{N} h_i Y_i \tag{1.17}$$

Differentiating this expression, the following equation can be posed:

$$dh = \frac{\partial h}{\partial T} dT + \sum_{i=1}^{N} \frac{\partial h}{\partial Y_i} dY_i = c_p dT + \sum_{i=1}^{N} h_i dY_i \tag{1.18}$$

In order to write the energy equation in terms of temperature, the expression 1.18 is introduced into the energy equation (Eq. 1.6) obtaining:

$$c_p \frac{\partial (\rho T)}{\partial t} + c_p \nabla \cdot (\rho \vec{v} T) = -\sum_{i=1}^{N} h_i \left[\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{v} Y_i) \right] - \nabla \cdot \vec{q} - \nabla \cdot \vec{q}^{\,R} \tag{1.19}$$

Substituting the energy transport flux defined in Eq. 1.11 and introducing the species equation 1.2 into the term in brackets the following expression can be written:

$$\begin{aligned} c_p \frac{\partial (\rho T)}{\partial t} + c_p \nabla \cdot (\rho \vec{v} T) = &-\sum_{i=1}^{N} h_i \left[-\nabla \cdot \vec{j_i} + \dot{w}_i \right] + \nabla \cdot (\lambda \nabla T) \\ &- \sum_{i=1}^{N} \nabla \cdot h_i \vec{j_i} - \nabla \cdot \vec{q}^{\,R} \end{aligned} \tag{1.20}$$

Rearranging, grouping the enthalpy inter-diffusion terms and taking into account that $dh_i = c_{p_i} dT$ the following energy equation in terms of temperature is written:

$$c_p \frac{\partial (\rho T)}{\partial t} + c_p \nabla \cdot (\rho \vec{v} T) = \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^{N} h_i \dot{w}_i - \sum_{i=1}^{N} \left(c_{p_i} \vec{j_i} \cdot \nabla T \right) - \nabla \cdot \vec{q}^{\,R} \tag{1.21}$$

1.3.4 Thermal radiation

In the formulation of the energy conservation equation one of the physical contributions involved is the radiant heat flux $\vec{q}^{\,R}$, actually the net input rate of heat transfer by radiation expressed in terms of the divergence of radiant heat flux, $-\nabla \cdot \vec{q}^{\,R}$.

The radiation transfer equation (RTE) describes the transfer of radiant energy in a participating medium. RTE can be derived from a simplification of the Maxwell equations in which, for example, polarisation effects are not considered. RTE accounts

for the rate of change of radiation intensity along a path in terms of the physical processes of absorption, emission and scattering [45, 46]. From the resolution of RTE, radiative fluxes involved in the thermal energy equation can be evaluated.

Simplified radiation model: optically thin approximation

Flame radiation is typically modelled using the assumption of optically thin transfer between the hot combustion gases and the cold surroundings [47, 48]. This assumption implies that each radiation point has an unimpeded isotropic view of the cold surroundings, considered as a black body. The radiative heat loss term per unit of volume is expressed as:

$$\nabla \cdot \vec{q}^{R} = 4\sigma T^4 \sum_{i=1}^{N} (p_i \kappa_{P_i}) - 4\sigma T_s^4 \sum_{i=1}^{N} (p_i \kappa_{I_i}) \tag{1.22}$$

where σ is Stefan-Boltzmann constant; p_i is the partial pressure of species i; κ_{P_i} is the Planck-mean absorption coefficient for species i; T_s background temperature; κ_{I_i} is the incident-mean absorption coefficient for *ith* species.

The summation terms on the r.h.s of Eq. 1.22 account for the different radiating species present in hydrocarbon flames. The radiating species considered in order of importance are CO_2, H_2O, CH_4 and CO.

The approximation of an optically thin gas establish that self-absorption is negligible compared to emission. The first term on the r.h.s accounts for the radiation emission and the second term accounts for the absorption of radiation coming from the surrounding background. When T_s is low, this term can be neglected.

Spectral absorption coefficients for each species are predicted using a narrow-band model, together with a combination of tabulated properties and theoretical approximations. From running RADCAL [49], both Planck-mean and incident-mean absorption coefficients are obtained at different temperatures, which are fitted to polynomial expressions [47].

1.3.5 Chemical models

All chemical reactions proceed at a defined rate that depends on different parameters such as the concentration of the different species, the temperature and the pressure. For a given reaction, the rate of reaction is the quantitative measure of its evolution, namely, the number of moles of products produced (or reactants consumed) per unit of time and volume. The *rate law* describes an empirical formulation of these reaction rates.

The reaction rate of the *jth* reaction can be evaluated by the following expression:

$$q_j = k_j^f \prod_{i=1}^{N} [X_i]^{\nu_{i,j}^{'}} - k_j^b \prod_{i=1}^{N} [X_i]^{\nu_{i,j}^{''}} \tag{1.23}$$

Here, $[X_i]$ are the molar concentrations, $\nu_{i,j}^{'}$, $\nu_{i,j}^{''}$ the stoichiometric coefficients appearing as reactants and as products respectively for the *ith* species in the *jth* reaction, and k_j^f, k_j^b the forward and backward kinetic rate constants.

The forward rate constants k_j^f are evaluated with the modified Arrhenius law:

$$k_j^f = AT^{\beta} exp\left(-\frac{E}{RT}\right) \tag{1.24}$$

where A is the pre-exponential factor; β is the temperature exponential; E is the activation energy; R is the gas universal constant.

On the other hand, and since usually only forward rate parameters A, β and E are given in the literature, the backward rate constants k_j^b are evaluated taking into account the equilibrium constant of reaction K_c which is calculated with thermodynamic properties [50]. The relation of the rate constants and the equilibrium constant is:

$$K_c = \frac{k_j^f}{k_j^b} \tag{1.25}$$

The evaluation of the net rate of production/destruction of each species, due to the N_r reactions, is obtained by summing up the individual contribution of each reaction:

$$\dot{w}_i = M_i \sum_{j=1}^{N_r} \left(\nu_{i,j}^{''} - \nu_{i,j}^{'}\right) q_j \tag{1.26}$$

where M_i are the molecular weights of the species.

Different levels of chemical modelization can be considered. For methane combustion, for example, mechanisms from full chemistry (e.g. GRI mechanisms releases 1.2, 2.11 or 3.0 [39, 51]), reduced mechanism (e.g. mechanism from Jones [52]) or irreversible single-step models [53], can be taken into account.

1.4 Simulation Methodology

A brief explanation of the most relevant aspects of the numerical methodology employed in this thesis (for details see the paper by R. Còsul et al. [13]) is exposed below.

1.4.1 Numerical Method

Finite volume technique over orthogonal staggered grids is applied with a fully implicit temporal differentiation. Central differences are employed for the evaluation of the diffusion terms, while upwind scheme [54] or third order bounded schemes [55] are used for the evaluation of convective terms. A segregated SIMPLE-like algorithm is considered in order to couple the velocity and pressure fields [54]. A multigrid solver is used to solve the algebraic linear systems of equations [56].

1.4.2 Resolution of species equations

An operator-splitting procedure has been employed. This technique is based on the split of each species equations into two steps: the convective-diffusion step, and the chemical step. Several possibilities can be found in the literature considering different kinds of operator-splitting strategies [2, 57–62]. Depending on how the convection-diffusion equation for species mass conservations is split, and how the chemical source terms are integrated, the method represents a numerical approximation to the original non-split discretized equations. The operator-splitting method used in this work is based on a pseudo-time splitting procedure. Referring to the standard treatment, some new peculiarities have been introduced to increase its efficiency. A brief explanation of the method is given below.

The two-dimensional discretized species mass transport equations, with a fully implicit formulation and after introducing the mass conservation equation, take the form, according to standard notation (see e.g. [54]):

$$\begin{aligned}\rho_P^o \frac{Y_{i,P} - Y_{i,P}^o}{\Delta t} V_P + (J_e - F_e Y_{i,P}) - (J_w - F_w Y_{i,P}) \\ + (J_n - F_n Y_{i,P}) - (J_s - F_s Y_{i,P}) = \dot{w}_{i,P} V_P\end{aligned} \tag{1.27}$$

where F and J represent the mass fluxes and the convection-diffusion terms at the faces of the control volume. E.g. for the east face and without considering Soret effect:

$$J_e = \left(\rho u Y_i - \rho D_{im} \frac{\partial Y_i}{\partial x} \right)_e S_e \tag{1.28}$$

Defining an intermediate species mass fractions (Y_i^*), the discretized equation (1.27) is split forcing an implicit resolution of the second-step (key aspect in these kinds of stiff system of equations). The consistency of each species equation is maintained when the evaluation of the intermediate species (i.e. first step) is treated explicitly. Therefore:

- First step, convection-diffusion terms:

$$\rho_P^o \frac{(Y_{i,P}^* - Y_{i,P}^o)}{\Delta t} V_P + (J_e - F_e Y_{i,P}) - (J_w - F_w Y_{i,P}) + (J_n - F_n Y_{i,P}) - (J_s - F_s Y_{i,P}) = 0 \tag{1.29}$$

- Second step, chemistry term:

$$\rho_P^o \frac{Y_{i,P} - Y_{i,P}^*}{\Delta t} V_P = \dot{w}_{i,P} V_P \tag{1.30}$$

To increase the robustness of the method, the implicit resolution of the first step has been enforced via a deferred correction [63]:

$$\rho_P^o \frac{(Y_{i,P}^* - Y_{i,P}^o)}{\Delta t} V_P + (J_e^* - F_e Y_{i,P}^*) - (J_w^* - F_w Y_{i,P}^*) + (J_n^* - F_n Y_{i,P}^*) - (J_s^* - F_s Y_{i,P}^*) = b_{spl} \tag{1.31}$$

where the deferred term (b_{spl}), is evaluated subtracting both the actual mass fluxes and the convection-diffusion terms as:

$$\begin{aligned} b_{spl} \quad &= (J_e^* - J_e) - (J_w^* - J_w) + (J_n^* - J_n) - (J_s^* - J_s) \\ &+ (F_e - F_w + F_n - F_s)(Y_{i,P} - Y_{i,P}^*) \end{aligned} \tag{1.32}$$

For each outer iteration, the split convection-diffusion equations (1.31) are solved in a segregated manner, while the chemical step (1.30) is solved in a coupled manner for all species and for each control volume using the Modified Damped Newton's method for stiff ordinary differential equations [42].

It is interesting to point out that the intermediate species mass fractions (Y_i^*) loses its physical concept in this approach. The intermediate values are those that the discretized species diffusion equations (1.27) are fully satisfied at each time-step. In fact, and depending on the considered species, Y_i^* can even take negative values. Thus, source terms linearizations, usually recommended in finite volume discretizations for always-positive variables [54], are not used.

1.4.3 Treatment of the energy equation

As can be observed in equation 1.6, the transient and convective terms in the energy equation are written in terms of enthalpy, while the heat fluxes are evaluated considering Fourier's law in terms of temperature gradients. On the formulation of a discretized energy equation, two main approaches are usually followed: i) the energy equation is solved in terms of temperature after introducing some numerical

approaches for the convective fluxes; ii) the energy equation is solved in terms of enthalpy after rewriting the heat transfer diffusion term.

When the second approach is considered, temperature is usually evaluated from the enthalpy-temperature relationship specified by Eq. 1.7, using for example Newton's method [62].

In this thesis, a different methodology has been followed. The energy equation has been considered in its original form (Eq. 1.6). An energy convection-diffusion equation with temperature as dependent variable has been formulated, introducing the enthalpy convective fluxes in the source term by means of a deferred correction (terms in brackets in Eq. 1.33).

$$\begin{aligned} c_p\frac{\partial(\rho T)}{\partial t} + c_p\nabla\cdot(\rho\vec{v}T) = \nabla\cdot(\lambda\nabla T) - \nabla\cdot\vec{q}^{\,R} \\ -\left[\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\rho\vec{v}h) + \sum_{i=1}^{N}\nabla\cdot\left(h_i\vec{j_i}\right) - c_p\frac{\partial(\rho T)}{\partial t} - c_p\nabla\cdot(\rho\vec{v}T)\right] \end{aligned} \tag{1.33}$$

Then, Eq. 1.33 is directly solved as a standard convection-diffusion equation in terms of temperature without any further mathematical approach. However, enthalpy terms are rigorously evaluated from Eq. 1.7 and introduced in the source terms.

1.4.4 Domain Decomposition Method - Parallel algorithm

The domain decomposition method has been used as a strategy to reduce the number of grid nodes far from the flame fronts and as a parallelisation technique. The whole domain is divided into several overlapping blocks or *subdomains* joined by the interpolation boundaries. The overlapping zones are generated by stretching the length of the subdomains. Four control volumes to define these zones have been selected in order to maintain the accuracy of the numerical solutions (remember that third-order schemes are employed to evaluate convective terms).

The discretized governing equations are solved in each block (subdomain) with the appropriate boundary conditions and the required grid (inner iteration). Once all blocks have been calculated, information of the interpolation boundaries is transferred among the different blocks in an explicit manner (outer iteration). This strategy allows to solve several blocks simultaneously by different CPUs. The processors communicate only once per outer iteration. Thus, the communication work is notably lower than the calculation work. This property benefits the use of the proposed algorithm in *Beowulf clusters*.

Boundary conditions at the interpolation boundaries, which are responsible for the information transfer among subdomains, are calculated using appropriate *interpolation schemes*. In this work, for the Navier-Stokes equations the normal boundary

velocity is calculated via local mass balances, and the tangential velocity using local balances of the tangential-momentum fluxes [17]. For the scalar fields (Y_i and T) an asymptotically conservative scheme based on bi-quadratic Lagrangian interpolations has been employed [2, 21]. When operator-splitting techniques are used for the species equations, the interpolated boundary conditions are only needed for the intermediate species mass fractions (Y_i^*), while species mass fractions (Y_i) are directly evaluated decoupled at each CV from the chemistry step (equation 1.30).

The parallel implementation of the code has two main goals: allow maximum portability between different computing platforms, and keep the code as similar as possible to the sequential version. To achieve the first, the MPI library has been used as message passing protocol (LAM 6.1). To achieve the second, all the calls to low-level message passing functions have been grouped on a program module, and a set of input-output functions has been implemented. The code for the solution of a single-domain problem remains virtually identical to the previous sequential code. In fact, it can still be compiled without the MPI library and invoked as a sequential code [3].

All the numerical simulations have been performed on a *Beowulf cluster* composed by the following standard PCs with a conventional network: 48 AMD (K7) Athlon 900 MHz and 512 Mbytes (256 Kb cache); 40 AMD (K7) AthlonXP 2600+ (1938 Mhz) and 1 Gbyte (512 Kb cache); 26 Intel Pentium4 2800 Mhz and 1 Gbyte and (512 Kb cache); 2 AMD (K7) AthlonMP 1900+ (1600 Mhz), double CPU and 2 Gbytes (256 Kb cache),

1.4.5 Verification of the numerical solutions

All numerical solutions here presented have been submitted to a verification process by means of a post-processing procedure [15] based on the Generalised Richardson extrapolation for h-refinement studies and on the Grid Convergence Index (GCI) proposed by Roache [64]. With this procedure, global and local estimates are calculated giving criteria about the sensitivity of the numerical solutions to the computational model parameters that account for the discretization (the mesh spacing and the order of accuracy), and for the credibility of the estimates themselves.

The procedure processes three consecutive numerical solutions of the h-refinement study. These solutions are interpolated at the post-processing grid. In this thesis, the post-processing grid is assigned to the coarsest grid of the three consecutive solutions. The most relevant parameters arisen from the verification process are the GCI, the observed order of accuracy of the numerical solution, p, and the percentage of nodes of the post-processing grid where the application of the post-processing procedure has been possible (these nodes are here referred as Richardson nodes). These estimates are obtained for the finest mesh and for each of the dependent variables of the problem.

Both global and local estimators of the GCI and p for each dependent variable

are calculated. Global GCI are obtained by means of a volume weighted average. These estimations are credible when the global observed order of accuracy p for each variable, approaches the theoretical value (e.g. 2 in second differencing schemes), and when the number of Richardson nodes is high enough. These global estimates permit a uniform reporting of the results of the verification procedure in a compact manner. On the other hand, local estimates help to locate local sources of error, such as zones with inadequate mesh concentration or problems with an inadequate formulation of the boundary conditions. For more details see [15].

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