FULLY COMPRESSIBLE SIMULATION OF LOW-SPEED PREMIXED REACTING FLOWS

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ABSTRACT

Low speed premixed combustion flows in industrial applications are generally simulated using the "incompressible" Navier-Stokes algorithms, which belong to the family of fractional step methods, or segregated methods. The approximations used for the combustion modelling in the framework of the segregated mathematical formulation, often represent important limitations for applying the combustion numerical simulation to a wider class of problems of engineering interest. Recent developments of preconditioning techniques allow to apply the same complete system of Navier-Stokes equations to a wide variety of fluid flow problems characterized by the whole range of Reynolds, Mach, Grashof, Prandtl and Damkoeler numbers. The present work describes the development of a fully "compressible" mathematical model for the simulation of low-speed turbulent premixed reactive flows. Issues on flow and fluid compressibility as well as on the two mathematical alternative formulations, are discussed. Also discussed are issues related to coupling the flamelet premixed combustion model (based on the solution of a transport equation for the progress variable) with one-equation turbulence models, instead of the classical two-equation $\kappa - \epsilon$ model. In this work the model by Spalart & Allmaras is used. The several advantages brought about by the use of the fully compressible formulation are discussed based on the results obtained on a test case taken from literature.

Intrroduction

Flows of engineering interest range from high speed aerodynamics to incompressible hydrodynamics, and include low speed reactive flows and heat exchange loops in natural and forced convection, just to make a few examples. On the other hand, fluid dynamics applications to different fluids bring into the mathematical formulation different equations of state, which in turn determine different levels of interaction between fluid dynamics and thermodynamics. The above range of thermo-fluid dynamics situations is described, in terms of non-dimensional parameters, by Reynolds, Mach, Grashof, Prandtl and Damkoeler numbers, just to mention the most important.

The desire of Computational Fluid Dynamics has long been the possibility to use a unique mathemathical formulation together with a unique numerical method to examine the variety of fluid dynamics problems, all of them governed by the Navier-Stokes system of equations. Going back to the infancy age of CFD (the '60s and '70s), numerical simulations for inviscid compressible aerodynamics and viscous incompressible flows represented two classes of methods which only shared the name of the governing equations. After the extraordinary pace of development of CFD methods, during the '80s and '90s, in more recent years, many efforts have been made to develop unified numerical approaches to the solution of a wider class of fluid flow problems. For this purpose, either typical "incompressible" methods are generalized for high speed compressible flows, or viceversa, the efficient use of "compressible" algorithms is extended to low-speed flows and to flows of incompressible fluids by means of suitable preconditioners. The two methods are now more often called coupled and segregated solution algorithms or, alternatively, density-based and pressure-based methods.

Combustion simulations have always used the segregated solution algorithm due to scientific and technical reasons (20 years ago) and to historical reasons in these days. When the coupled methods are used for incompressible or low-speed flow situations, the main problem is in fact to cope with the singularity of the Navier-Stokes equations when Mach number M approaches zero ($M \rightarrow 0$). The inviscid matrix of the coupled system of equations becomes in fact ill conditioned and though Mother Nature can cope with it, coupled numerical methods break down. As a result straightforward use of coupled methods gives severe convergence problems or even breakdown in the presence of regions with low Mach number. In order to cope with eigenvalue spreading, the efforts done by the scientific community led to the development of efficient preconditioning techniques. This is done by multiplying the system matrix by a preconditiong matrix which alters the speed of the acoustic waves making it of the same order of magnitude of the

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speed of the entropy and shear waves, i.e. the fluid local velocity. In this way a well conditioned system is recovered, and the coupled "fully compressible" algorithms regain their good convergence properties. This work is based on the works of Weiss and Merkle [1,2,3].

Compressible flow model

Reactive combustion flows, as all fluid flows, are governed by the coupled system of partial differential equations which represent the conservation of mass, momentum and energy, generally referred to as the system of the Navier-Stokes equations. One form of such a system is given by:

$$\begin{aligned}
\frac{D\rho}{Dt} &= -\rho\,\nabla\cdot\vec{V} \\
\rho\,\frac{D\vec{V}}{Dt} &= -\nabla p + \nabla\cdot\vec{\vec{\tau}} \\
\rho\,\frac{DE}{Dt} &= -p\nabla\cdot\vec{V} - \vec{V}\cdot\nabla p \\
&\quad +\nabla\cdot\left(\vec{V}\cdot\vec{\vec{\tau}}\right) - \nabla\cdot\vec{q}
\end{aligned} \tag{1}$$

where $E = e + V^2/2$ represents the total, or stagnation, energy, and $\vec{\vec{\tau}}$ and $\vec{q}$ represent the viscous stress tensor and the conductive heat flux respectively.

Two equations of state of the form $\rho = \rho(p,T)$ and $h = h(p,T)$, and two fluid constitutive relations close the system. The constitutive relations relate the viscous stress tensor and the conductive heat flux to the velocity gradient tensor and to the temperature gradient respectively. Most fluids follow Newton's and Fourier's laws:

$$\tau_{i,j} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\delta_{i,j}\nabla\cdot\vec{V} \tag{2}$$

$$q_j = -\kappa\frac{\partial T}{\partial x_j} \tag{3}$$

System 1 is the most general and fully compressible formulation of the Navier-Stokes equations for it allows the reversible exchange between kinetic and internal energy (the term $p\nabla\cdot\vec{V}$), which can occur at the expense of density variations (through the continuity equation), thus including the fluid compressibility. The exchange term is responsible for the coupling between momentum and total energy equations.

An alternative way to identify the actual flow-fluid compressibility is by differentiating the equation of state $\rho = \rho(p,T)$:

$$\frac{D\rho}{Dt} = \left(\frac{\partial\rho}{\partial p}\right)_T\frac{Dp}{Dt} + \left(\frac{\partial\rho}{\partial T}\right)_p\frac{DT}{Dt} \tag{4}$$

which allows to relate the density changes associated to a fluid particle to pressure and temperature changes, rather than to a particular term in the partial differential equations. The two partial derivatives of density represent the fluid compressibility coefficients at constant temperature and at constant pressure respectively (often represented by $\rho\chi$ and $-\rho\beta$).

Incompressible fluids have $\beta = \chi = 0$, which implies that the density is constant throughout. This in turn inhibits the possibility of exchange between kinetic and internal energy, and the energy equation can be dropped out of the system. On the other hand, in typical compressible flows of gas dynamics, density changes occur in association with pressure changes, through the compressibility coefficient at constant temperature: $\left(\frac{\partial\rho}{\partial p}\right)_T = \rho\,\chi \propto \frac{1}{c^2}$ which implies that $\frac{D\rho}{\rho} \propto M^2$, where c is the speed of sound and M the Mach number (ratio of the local fluid velocity to the speed of sound). Therefore, density changes in flows of compressible fluids can only occur if the fluid speed is high enough compared to the local speed of sound.

Reactive processes in gas turbine combustors occur at approximately constant pressure and at low fluid speed, compared to the local speed of sound, with typical Mach number well below 0.3. Due to the volumetric heat addition the flow is however highly compressible and density changes are entirely due to the large temperature increase via the compressibility coefficient β, and not to the high fluid speed compared to the speed of sound.

Flows in gas turbine combustors

Premixed combustion flows are characterized by the complete and uniform mixing of fuel and oxidizer before their injection into the combustion chamber so that the mixture is ready to burn at any time and at any place. Once a steady flame has been ignited and stabilized, a fluid particle burns while travelling through the flame. The flame therefore separates the fresh mixture upstream from the burned mixture downstream. A suitable variable to describe the combustion process which takes place inside the flame is the so-called *progress variable* c which represents the degree of advancement of the combustion reaction, and assumes values in between $c = 0$ (100% of fresh mixture) and $c = 1$ (100% of burned mixture). A transport equation for the progress variable is given by:

$$\rho\,\frac{Dc}{Dt} = \nabla\cdot\left(\rho\mathcal{D}\nabla c\right) + W \tag{5}$$

Eq. 5 is equivalent to a one-step reaction, assuming equal mass diffusivities D for all species. CFD modelling of premixed combustion reduces to developing a suitable transport equation for c which is to be coupled to the main system of equations. From a thermodynamic point of view, reactive flows are processes in chemical non equilibrium (though thermal and mechanical equilibrium can still be assumed): with respect to the "cold" non reactive flows of ideal gases they need a more general equation of state of the form $\rho = \rho(p,T,c)$ and $h = h(p,T,c)$.

The two particular cases, upstream and downstream of the flame ($c = 0$ and $c = 1$), are described by the ideal gas behaviour (the fresh unburned mixture upstream) and by a complete thermochemical equilibrium state (the burned products downstream).

Pressure based model for reactive flows

The *pressure-based* algorithm is originally developed and used for incompressible and isothermal flows, and then extended to the simulation of flows with important compressibility effects. It represents the method historically used for combustion simulation, most often in conjunction with the $\kappa - \epsilon$ turbulence model. For premixed combustion applications the governing equations can be written for instance as:

$$\begin{aligned} \nabla \cdot (\rho \vec{V}) &= 0 \\ \rho \frac{D\vec{V}}{Dt} &= -\nabla p + \nabla \cdot \vec{\vec{\tau}} \\ \rho \frac{Dc}{Dt} &= \nabla \cdot (\rho \mathcal{D} \nabla c) + W \end{aligned} \tag{6}$$

where the progress variable replaces the energy equation. The algorithm is also called segregated or two-step, because the continuity equation is used as a constraint to derive an elliptic equation for the pressure p. The role of the pressure is to enforce a divergence free momentum and does not influence the density. The equation of state takes therefore the simplified form given by $\rho = \rho(c)$. The temperature T, as any other thermodynamic variable, depends only on the progress variable c.

Such a simplified model can only be applied to low-speed flows because the compressible energy exchange due to high fluid speed is missing. Furthermore, without a temperature equation, applications are limited to adiabatic flows with neither wall heat transfer (wall boundary conditions for c are of adiabatic type), nor internal heat diffusion (gas products at $c = 1$ must necessarily be at given and unique temperature, the adiabatic flame temperature).

The TFC model for the progress variable

For premixed turbulent combustion, the classical model based on the progress variable c is the Bray-Moss-Libby (BML) model [4], where c is defined as the product concentration normalised by the equilibrium product concentration:

$$c = \frac{C_p}{C_p^{eq}} \tag{7}$$

The BML model belongs to the class of flamelet models which assume a probability density function $\mathcal{P}(c)$ for the progress variable given by two delta functions located at $c = 0$ (unburned gas mixture) and at $c = 1$ (equilibrium products). In flamelet models the flame is assumed infinitely thin and all intermediate conditions between unburned mixture and equilibrium products have zero probability to occur:

$$\mathcal{P}(c) = P_u \, \delta(c) + P_b \, \delta(1 - c) \tag{8}$$

where P_u and P_b represent the probabilities of finding fresh unburnt mixture or burnt equilibrium products at a certain location and time, and with $P_u = 1 - P_b$. As a result, the average of the progress variable represents the probability to find products at a given location and time:

$$\bar{c} = \int_0^1 c \, \mathcal{P}(c) \, dc = P_p \tag{9}$$

The relation of the Favre average $\tilde{\nu}$ with $\bar{\nu}$ can be obtained from the definition $\tilde{c} = \bar{\rho c}/\bar{\rho}$:

$$\tilde{c} = \frac{\rho_b \, P_b}{\rho_u + (\rho_b - \rho_u) P_b} \tag{10}$$

An unclosed equation for $\tilde{c}$ is given by:

$$\bar{\rho} \frac{D\tilde{c}}{Dt} = -\nabla \cdot \left(\widetilde{\bar{\rho} u" c"} \right) + \bar{W} \tag{11}$$

disregarding the molecular diffusion term. The TFC (Turbulent Flame Closure) model by Zimont and Lipatnikov [5] proposes a closed form for eq. 11 given by:

$$\bar{\rho} \frac{D\tilde{c}}{Dt} = \nabla \cdot (\rho \alpha_t \nabla \tilde{c}) + \rho_u U_t |\nabla \tilde{c}| \tag{12}$$

where α_t represents a turbulent thermal diffusivity (Lewis number unity) and U_t represents the turbulent burning velocity. In the TFC model, the correlation of the turbulent burning velocity with the Damkoeler number is given by:

$$U_t = 0.51 \, u' \, Da^{0.25} \, G \tag{13}$$

with: $u' = \sqrt{0.67 \, \kappa}$. The Damkoeler number is the ratio between a turbulent time ($\tau_t \approx \kappa/\epsilon$) and a laminar time scale (based on the laminar flame speed and a molecular diffusivity). Finally G respresents a stretch function which helps in describing the blow-off boundary (fully described in the appendix).

In the context of a pressure-based mathematical model, and from the above relations, once $\tilde{c}$ is available, then density and temperature can be obtained from (dropping bars and tildes):

$$\rho = \rho(c) = \left(\frac{1 - c}{\rho_u} + \frac{c}{\rho_b} \right)^{-1} \tag{14}$$

$$T = T(c) = T_u + (T_b - T_u) c \tag{15}$$

Density based model for reactive flows

Modern numerical techniques which allow to apply the fully coupled formulation, expressed for instance by eq. 1, for the numerical simulation of low-speed flows (no matter whether reactive or even truly incompressible) have been developed during the past years, and go under the name of preconditioning techniques. Multiplying the matrix of the system of the Navier-Stokes equations by a preconditioning matrix artificially changes the characteristic speeds (matrix eigenvalues) at which signals propagate in fluids: the use of the preconditioning technique alters the acoustic perturbation speed, making it of the same order of magnitude of the fluid velocity. In other words, the real stiff, low-speed world is transferred into a highly compressible one, in which the fully coupled formulation of the numerical algorithm does recover its original efficiency.

Within the coupled and preconditioned mathematical model, the progress variable equation is to be added to the full system of the Navier-Stokes equations together with two equations of state of the form:

$$\begin{aligned} \rho &= \rho(p,T,c) \\ h &= h(p,T,c) \end{aligned} \tag{16}$$

This would be the most general mathematical model governing reactive fluid flows with a one-step reaction and potentially allowing the simulation of all flow regimes in terms of the relevant non-dimensional numbers of Fluid Mechanics: Reynolds, Mach, Prandtl, Grashof and, eventually, Damkoeler.

RANS equations

The complete coupled system of the Reynolds averaged Navier-Stokes equations that has to be solved includes an equation for the progress variable c and a turbulence model closure. In this work the Spalart & Allmaras model [6] has been chosen for its robustness, convergence properties and accuracy. The full system in conservative formulation is given by:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &+ \frac{\partial}{\partial x_j}(\rho u_j) &= 0 \\ \frac{\partial \rho u_i}{\partial t} &+ \frac{\partial}{\partial x_j}(\rho u_i u_j + \delta_{ij} p - \tau_{ij}^T) &= 0 \\ \frac{\partial \rho E}{\partial t} &+ \frac{\partial}{\partial x_j}(\rho H u_j - u_i \tau_{ij}^T + q_j^T) &= 0 \end{aligned} \tag{17}$$

$$\begin{aligned} \frac{\partial \rho c}{\partial t} &+ \frac{\partial \rho c u_j}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho \alpha^T \frac{\partial c}{\partial x_j}\right) &= S_c \\ \frac{\partial \rho \tilde{\nu}}{\partial t} &+ \frac{\partial \rho \tilde{\nu} u_j}{\partial x_j} - \frac{\rho C_{b2}}{\sigma}\frac{\partial \tilde{\nu}}{\partial x_k}\frac{\partial \tilde{\nu}}{\partial x_k} &- \\ & \frac{1}{\sigma}\frac{\partial}{\partial x_j}\left[\rho(\nu+\tilde{\nu})\frac{\partial c}{\partial x_j}\right] &= S_{\tilde{\nu}} \end{aligned}$$

where the two non-zero source terms are given by:

$$\begin{aligned} S_c &= \rho_u U_t |\nabla \tilde{c}| \\ S_{\tilde{\nu}} &= C_{b1}\rho\tilde{\Omega}\tilde{\nu} - C_{w1} f_w \left[\tfrac{\tilde{\nu}}{d}\right]^2 \end{aligned} \tag{18}$$

and where superscript ^{T} indicates the sum of viscous and turbulent counterparts for the both the diffusivities and the diffusion terms:

$$\tau_{i,j}^T = (\mu+\mu_t)\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{i,j}\frac{\partial u_k}{\partial x_k}\right] \tag{19}$$

$$q_j^T = -\left(\kappa + \frac{\mu_t\, c_p}{Pr_t}\right)\frac{\partial T}{\partial x_j} \tag{20}$$

where c_p is the specific heat at constant pressure and $Pr_t = 0.92$ represents the turbulent Prandtl number. The expression of the eddy (turbulent) viscosity of the Spalart & Allmaras model is $\mu_t = \rho\ \tilde{\nu}\ f_{v1}$. All model constants are summarised in the appendix.

System preconditioning

Preconditiong the system (17) is achieved multiplying the unsteady terms by a suitable matrix $\mathbf{P}^{-1}$ or, in equivalent way, the fluxes and the source terms by its inverse $\mathbf{P}$:

$$\frac{\partial Q}{\partial t} + \mathbf{P}\frac{\partial F_j}{\partial x_j} = \mathbf{P}S \tag{21}$$

where Q represents the vector of conservative variables $(\rho, \rho u, \rho v, \rho w, \rho E, \rho c, \rho\tilde{\nu})^T$, F_j the corresponding fluxes and $S = (0,0,0,0,0,S_c,S_{\tilde{\nu}})^T$ the source term vector. The preconditioning matrix is given by $\mathbf{P} = \mathbf{M}\mathbf{M}_m^{-1}$. $\mathbf{M}$ represents the Jacobian matrix of the vector Q with respect to the vector of the so-called viscous-primitive variables $Q_v = (p,u,v,w,T,c,\tilde{\nu})^T$. $\mathbf{M}_m$ represents a modified version of $\mathbf{M}$. No modification brings back the original not preconditioned system ($\mathbf{P} = \mathbf{I}$). All matrices are given in reference [7].

Due to the form of the equations of state 16, the matrix $\mathbf{M}$ contains arbitrary thermodynamics in terms of derivatives of density and enthalpy with respect to pressure, temperature and progress variable. However, due to the flamelet nature of the turbulent combustion model (only two constant states can exist: either $c = 0$ or $c = 1$), only derivatives with respect p and T are needed: $\rho_p,\ \rho_T,\ h_p,\ h_T$. The matrix $\mathbf{M}_m$ contains "modified" thermodynamics in terms of ρ_p^m. To keep the condition number of system 21 of $\mathcal{O}(1)$, rescaling of the characteristic speeds is obtained with the following choice of ρ_p^m:

$$\rho_p^m = \frac{1}{V_p^2} - \frac{\rho_T}{\rho h_T} \tag{22}$$

where V_p, a local preconditioning velocity, plays a crucial role for it should be as low as possible, but not smaller than any local transport velocity for stability considerations:

$$V_p = min\left[max\left(u, \frac{\nu}{\Delta_x}, \frac{\alpha}{\Delta_x}, \sqrt{\frac{\Delta p}{\rho}}\right), c\right] \tag{23}$$

Where α represents the thermal diffusivity. The criterium based on the local fluid speed u is dominant in turbulent flows, at high Reynolds numbers. The velocity based on the local pressure gradient prevents vanishing V_p at stagnation regions. The two criteria based on diffusion velocities depend strongly on the grid stretching inside the boundary layers, where the flow is viscous or heat conduction dominated. Where the velocity V_p based on the maximum characteristic speed grows higher than the local speed of sound, then $V_p = c$ and the preconditioning is locally and automatically switched off where the flow is supersonic ($\rho_p^m = \gamma/c^2 = \rho_p$ and $\mathbf{M}_m = \mathbf{M}$). This is particularly useful in all test cases where subsonic and supersonic regions are both present.

Equations of state

In the above described mathematical model, the choice of the working fluid is totally arbitrary. Any chosen fluid can be defined by two equations of state of the form of eq. 16 and via the matrix **M** which requires the derivatives of density and enthalpy with respect to pressure, temperature and, eventually, with respect to the progress variable as well. In particular, when treating gas mixtures in thermochemical equilibrium, look-up tables can be provided instead of closed analytical form of equations 16. The tables can be obtained from typical chemical equilibium codes (often open source codes) such as NASA CEA code or Stanford University Stanjan code. In this way, chemical energy (the heat of combustion and the energy of dissociation and ionization) are hidden inside the enthalpy and the specific heat and they are fully accounted for via the equation of state.

The form of the equations of state 16 for such a flamelet combustion mechanism is suggested by their original "incompressible" counterpart given by equations 14 and 15:

$$\begin{aligned} \rho &= \rho(p^*, T^*, c^*) = \left[\frac{1-c^*}{\rho_u} + \frac{c^*}{\rho_b}\right]^{-1} \\ h &= h(p^*, T^*, c^*) = h_u + (h_b - h_u)\, c^* \end{aligned} \tag{24}$$

where subscripts $_u$ and $_b$ refer to the unburned and burned conditions respectively and are functions of the local pressure and temperature p^* and T^*.

Coupling the TFC model with the S&A model

The core of the TFC turbulent premixed combustion model is represented by the formulation of the turbulent burning velocity U_t, given in eq. 13, which is proportional to the turbulent velocity fluctuations u' and depends, weakly, on the Damkoeler number as well:

$$U_t \propto \sqrt{\kappa}\left(\frac{\kappa/\epsilon}{\tau_l}\right)^{0.25} \propto C\, \kappa^{3/4}\, \epsilon^{-1/4} \tag{25}$$

where τ_l is a laminar time scale based on the thermal diffusivity and the laminar flame speed.

When using a Spalart & Allmaras turbulence model, only a single turbulence quantity is solved. A second turbulence quantity must be available in order assemble a turbulent kinetic energy and its dissipation rate, say κ_{SA} and ϵ_{SA}. A natural choice would be using the absolute value of the vorticity $|\Omega|$, a quantity related to turbulent production and dissipation rates in most of two-equation models. However the sought quantity, and the available eddy diffusivity $\tilde{\nu}$, combined together should produce the two new turbulent quantities κ_{SA} and ϵ_{SA} which must fulfill a number of requirements:

[1] should assume given and arbitrary constant values at inflow boundaries: the flame form, position and stability strongly depend on the turbulence level of the incoming flow;

[2] should have the same wall behaviour as the true turbulent kinetic energy and the true turbulent dissipation.

The choice of using $\tilde{\nu}$ and $|\Omega|$ would lead to: $\kappa_{SA} \propto \tilde{\nu}\,|\Omega|$ and to a dissipation rate proportional to $\tilde{\nu}\,\Omega^2$. Such a choice however would not satisfy the first requirement: a uniform stream at inlet have zero vorticity. A better choice may be given by:

$$\begin{aligned} \kappa_{SA} &= \left(\frac{\tilde{\nu}}{l_t}\right)^2 \\ \epsilon_{SA} &= C_\mu\, \frac{\kappa_{SA}}{\tau_t} = C_\mu\, \frac{\kappa_{SA}}{d^2/\tilde{\nu}} \equiv C_\mu\, \frac{\tilde{\nu}^3}{l_t^2\, d^2} \end{aligned} \tag{26}$$

where $C_\mu = 0.09$ and l_t is a turbulent integral scale and $\tau_t = d^2/\tilde{\nu}$ represents the "true" dissipation time scale of the eddy viscosity in the S&A one-equation model, with d representing the distance from the nearest solid boundary. Relations 26 do satisfy the second requirement: the turbulent viscosity has wall behaviour similar to the turbulent kinetic energy and ϵ_{SA} is constructed in order to mimic a true turbulent dissipation. The turbulent kinetic energy from eq. 26 does satisfy also the first requirement. Furthermore, since the turbulent dissipation occurs at very short distances d from solid boundaries, if the length scale d is replaced by $d = min(d, l_t)$, then the first requirement is also satisfied by ϵ_{SA} almost everywhere apart from a very thin layer close to solid walls.

Numerical method

Equations are integrated with a cell-centered Finite-Volume method on block-structured meshes. Convective inviscid fluxes are computed by second order Roe's scheme [8,9] based on the decomposition of the Euler equations in waves so that proper upwinding can be applied to each wave depending on the sign of the corresponding wave speed. This implies an eigenvector decomposition of the matrix of the Euler system. The first order Roe's scheme numerical flux vector is given by:

$$\begin{aligned} F^*_{i+1/2} &= \frac{F_i + F_{i+1}}{2} - \\ &\frac{1}{2}\left[\mathbf{P}^{-1}\,\mathbf{R}_p\,|\Lambda_p|\,\mathbf{L}_p\right]_{i+1/2} \quad (Q_{i+1} - Q_i) \end{aligned} \tag{27}$$

made of a central part and a matrix dissipation part computed at the cell interface, denoted by $(i + 1/2)$. $\mathbf{R}_p$ and $\mathbf{L}_p$ represent the matrices of right and left eigenvectors of $\mathbf{D}_p = \mathbf{PD}$, where:

$$\mathbf{D} = \frac{\partial F_x}{\partial Q}\, n_x + \frac{\partial F_y}{\partial Q}\, n_y + \frac{\partial F_z}{\partial Q}\, n_z \tag{28}$$

and $|\Lambda_p|$ represents the diagonal matrix whose elements α_p are the absolute values $|\lambda_p|$ of the eigenvalues of the system matrix $\mathbf{D}_p$. Second order accuracy is achieved (see reference [9] for a thourough review) computing the elements α_p as:

$$\alpha_p = |\lambda_p| + \Psi(R^+) - \Psi(R^-) \tag{29}$$

with:

$$\begin{aligned} R^+ &= \frac{\lambda^+\,(Q_i - Q_{i-1})}{\lambda^+\,(Q_{i+1} - Q_i)} \\ R^- &= \frac{\lambda^-\,(Q_{i+2} - Q_{i+1})}{\lambda^-\,(Q_{i+1} - Q_i)} \end{aligned} \tag{30}$$

where the function Ψ represents an appropriate limiter which assures monotonicity of the solution. Preconditioned eigenvectors are given in [7] for a general equation of state. Viscous fluxes and source terms are calculated with standard cell-centered Finite-Volume techniques and they are both second order accurate.

In Finite-Volume and semidiscrete form, system 21 becomes:

$$\Omega \frac{\partial Q}{\partial t} = -\mathbf{P}\, RES \equiv -\mathbf{M}\mathbf{M}_m^{-1}\, RES \qquad (31)$$

where RES represents the vector of residuals for the conservative variables and Ω the cell volume. Updating is done in terms of the viscous primitive variables Q_v, previously defined. This is done by multiplying the above system by $\mathbf{M}^{-1}$ to the left:

$$\Omega \frac{\partial Q_v}{\partial t} = -\mathbf{M}_m^{-1}\, RES \qquad (32)$$

Systems 31 and 32 are equivalent. If an implicit numerical scheme is used to discretize the time derivative then:

$$\Omega \frac{Q_v^{new} - Q_v^{old}}{\Delta t} = -\mathbf{M}_m^{-1}\, RES^{new} \qquad (33)$$

After linearization about the old time level:

$$\Omega \frac{\Delta Q_v}{\Delta t} = -\mathbf{M}_m^{-1}\, \left[RES^{old} + \mathbf{J}\, \Delta Q_v\right] \qquad (34)$$

where the Jacobian matrix $\mathbf{J}$ is given by:

$$\mathbf{J} = \left(\frac{\partial RES}{\partial Q_v}\right)^{old} \qquad (35)$$

Re-arranging, multiplying by $\mathbf{M}_m$ to the left, and dropping superscripts:

$$\left(\mathbf{M}_m \frac{\Omega}{\Delta t} + \mathbf{J}\right)\, \Delta Q_v = -RES \qquad (36)$$

At each time-step the linearization leads to a linear system which is to be solved by an iterative method. When unconditional stability is achievable, eq. 36 may become in principle a Newton method able to deliver quadratic convergence if the linear system solution is pushed till full convergence at each linearization step. In the real implementation the Jacobian matrix of the residual vector is done using a shorter stencil (equivalent to first order scheme) leading to a quasi-Newton method in case the numerical scheme can stand infinite CFL number. The choice of the red-black relaxation scheme is due to the fact that allows a straightforward implementation on multi-block domains and multi-processor machines without loss of convergence and computational efficiency.

Together with the CFL number, the global convergence properties of the method are determined by the convergence level chosen for the solution of the linear system (namely, the number of sweeps of relaxation) as well as by the underrelaxation parameter.

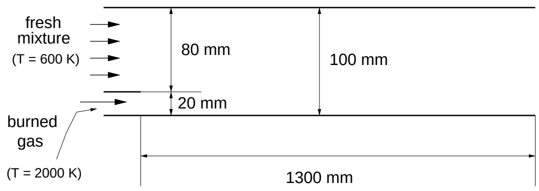

Figure 1: Skematic description of the experimental combustor

Results

Figure 1 shows a skematic description of an experimental combustor for premixed flows [10].

Two streams feed the combustor: one of fresh lean mixture ($\Phi = 0.87$) of methane and air flowing at 65 m/s and at 600 K, and the other made of gas product flowing at 108 m/s and at 2000 K. The second stream stabilises the flame. Tables 1 and 2 describe the gas mixture:

pressure	1 bar
temperature	600 K
specific heat	1120 J/kg K
gas constant	299.5 J/kg K
viscosity	2.5×10^{-5} Ns/m^2
Prandtl number	0.71
equivalence ratio	0.87

Table 1: Properties of inflow gas mixture.

species	mole fraction	mass fraction
CH_4	0.0837	0.04832
O_2	0.1925	0.22174
N_2	0.7238	0.72994

Table 2: Definition of gas mixture in terms of mole fraction and mass fraction for $\Phi = 0.87$.

The following table shows the turbulent characteristics of the two streams at the combustor inlet, and the values assigned to the S&A eddy viscosity (the integral scale needed in eq. 26 was taken equal to $l_t = 3.06 \times 10^{-3}$):

quantity	fresh mixture	burned mixture
V [m/s]	65	108
T [K]	600	2000
κ [m^2/s^2]	91	770
ϵ [m^2/s^3]	25000	2×10^6
$\tilde{\nu}$ [m^2/s]	2.92×10^{-2}	8.50×10^{-2}

Table 3: Inlet conditions for the two streams. The integral scale was taken equal to $l_t = 3.06 \times 10^{-3}$ in the relations 26.

Fig. 2 shows the computed field of the turbulent burning velocity, key feature of the TFC model, based on the Spalart & Allmaras turbulence model, showing a reasonable about constant field:

The simulation was carried out with CFL=100, an underrelaxation factor $\omega = 0.70$ and 15 red-black relaxation sweeps per time step (linearization step). Figure

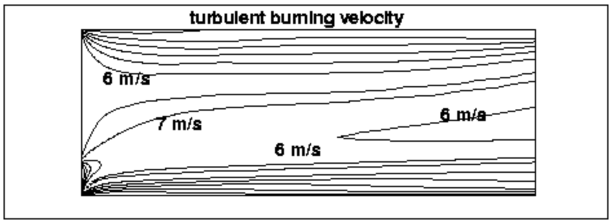

Figure 2: The calculated field of the turbulent burning velocity U_t of the TFC premixed combustion model. Dimensions not to scale.

3 shows the convergence history for the axial momentum, the progress variable and the S&A eddy viscosity equations:

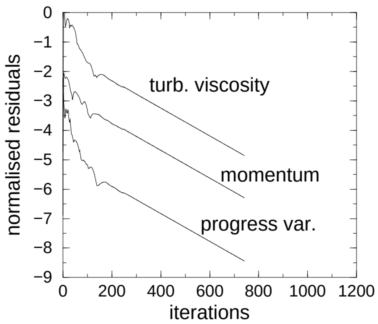

Figure 3: Convergence history: residuals of axial momentum, progress variable and S&A eddy viscosity. Simulation used CFL=100, an underrelaxation factor $\omega = 0.70$ and 15 red-black sweeps per linearization step.

A qualitative description of the computed solution is given in fig. 4 where the isolines of the progress variable, the axial velocity and the temperature are shown.

Finally, fig. 5 shows velocity and concentration profiles at three combustor sections. A small difference in the inlet value of methane concentration can be noticed. The results are however satisfactory. More investigations on physical aspects of the combustion flows are scheduled as future activities.

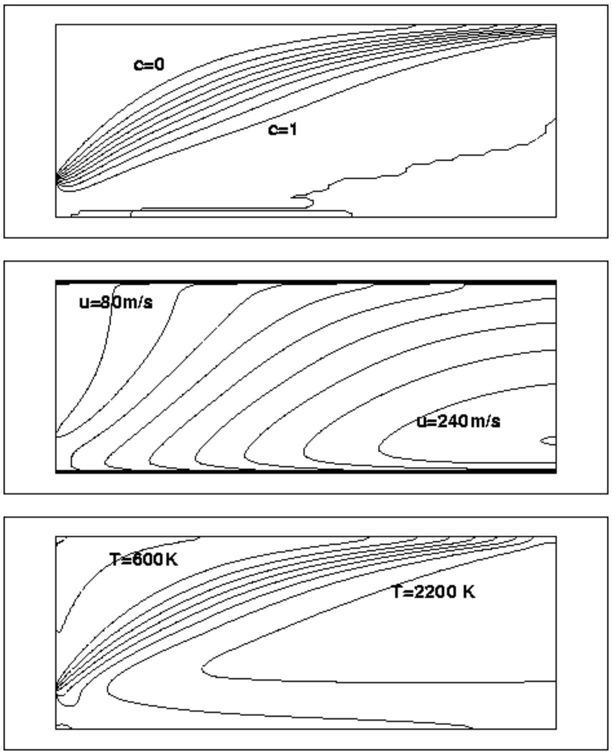

Figure 4: Isolines of the prograss variable (top), the axial velocity (middle) and the temperature (bottom). Dimensions not to scale.

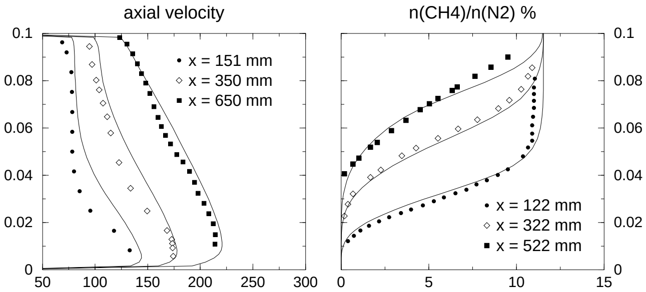

Figure 5: Velocity and methane concentration profiles at three sections of the combustor.

Conclusions

A coupled and fully compressible mathematical model for the simulation of low-speed turbulent premixed combustion flows has been deveoped. The combustion model is based on flamelet mechanism and on a transport equation for the progress variable. The turbulence model used was the one-equation model by Spalart & Allmaras. The coupling between the two models has been discussed.

The mathematical model is made of 7 PDEs in 7 unknowns and it is closed by two general equations of state of the form $\rho = \rho(p, T, c)$ and $h = h(p.T, c)$. The fully general model for fluid dynamics simulation is here summarised:

- the progress variable equation is added to the fully coupled compressible system of the Reynolds averaged Navier-Stokes equations with the Spalart & Allmaras one-equation turbulence model;
- updating, at the end of each iteration (time-step), is done in terms of the pressure, the temperature, the three components of the velocity, the Spalart & Allmaras turbulence variable and the progress variable;
- total freedom is given in defining the thermodynamic properties of the working fluid, either in analytical closed form or by means of look-up tables obtained by chemical equilibrium codes;
- the density is then obtained as

$$\rho = \rho(p^*, T^*, c^*) = \left[\frac{1 - c^*}{\rho_u} + \frac{c^*}{\rho_b}\right]^{-1} \quad (37)$$

where: $\rho_u = \rho_u(p^*, T^*, c = 0)$ is calculated via the ideal gas equation of state, for the unburned gas mixture, and $\rho_b = \rho_b(p^*, T^*, c = 1)$ is obtained via look-up tables for the equilibrium gas products;

- multiple and different inflow boundaries can be provided in terms of independent values of temperature and progress variable;
- pressure is an independent variable whose variations may contribute to the definition of the thermodynamic state.

Such a complete model can in principle be ready for studying the influence of pressure instabilities on the flame stability, once equipped with time accuracy capabilities, and can also be used for high speed combustion where compressibility effects become important.

Appendix

Spalart & Allmaras turbulence model

$$\mu_t = \rho\,\tilde{\nu}\,f_{v1}$$

$$\begin{aligned}\frac{D\tilde{\nu}}{Dt} &= C_{b1}\,\tilde{\Omega}\,\tilde{\nu} + \frac{1}{\sigma}\frac{\partial}{\partial x_i}\left[(\nu+\tilde{\nu})\frac{\partial\tilde{\nu}}{\partial x_i}\right] \\ &+ \frac{C_{b2}}{\sigma}\frac{\partial\tilde{\nu}}{\partial x_k}\frac{\partial\tilde{\nu}}{\partial x_k} - C_{w1}\,f_w\left[\frac{\tilde{\nu}}{d}\right]^2\end{aligned}$$

$$f_{v1} = \frac{\chi^3}{\chi^3 + c_{v1}^3}$$

$$\chi = \frac{\tilde{\nu}}{\nu}$$

$$\tilde{\Omega} = \Omega + \frac{\tilde{\nu}}{\kappa^2\,d^2}\,f_{v2}$$

$$f_{v2} = 1 - \frac{\chi}{1+\chi\,f_{v1}}$$

$$f_w = g\,\left(\frac{1+c_{w3}^6}{g^6+c_{w3}^6}\right)^{1/6}$$

$$g = r + c_{w2}(r^6 - r)$$

$$r = \frac{\tilde{\nu}}{\tilde{\Omega}\,\kappa^2\,d^2}$$

$$c_{w1} = \frac{C_{b1}}{\kappa} + \frac{1+C_{b2}}{\sigma}$$

C_{b1}	C_{b2}	σ	κ	C_{w3}	C_{w2}	C_{v1}
0.135	0.622	2/3	0.41	2	0.3	7.1

where Ω represents the absolute value of vorticity, and d the distance from the closest solid boundary.

TFC premixed combution model

$$\frac{\partial\rho c}{\partial t} + \frac{\partial\rho c u_j}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\rho\alpha^T\frac{\partial c}{\partial x_j}\right) = \rho_u U_t|\nabla\tilde{c}|$$

$$U_t = A\,G\,u'\,Da^{0.25} \equiv A\,G\,\frac{u'^{3/4}\,U_l^{1/2}\,L^{1/4}}{\chi_u^{1/4}}$$

with $A = 0.51$, where χ_u represents the thermal diffusivity of the gas mixture and U_l the laminar flame speed. The integral length scale is $L = 0.37\;u'^3/\epsilon$, and the stretch function G is expressed by:

$$G = 0.5\,erfc\{-(1/2\sigma)^{0.5}\;[\ln(\epsilon_{cr}/\tilde{\epsilon}) + \sigma/2]$$

where $erfc$ represents the complementary error function, $\sigma \simeq \mu\ln(L/\eta)$ is standard deviation from the log-normal distribution, with $\eta = L\;Re_t^{-3/4}$ and $\mu = 0.26$. The critical value of the dissipation ϵ is $\epsilon_{cr} = 15\;\nu\;g_{cr}^2$, with g_{cr} a critical velocity gradient.

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