A STEADY PSEUDO-COMPRESSIBILITY APPROACH BASED ON UNSTRUCTURED HYBRIDFINITE VOLUME TECHNIQUES APPLIED TO TURBULENT PREMIXED FLAME PROPAGATION

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ABSTRACT
A pseudo-compressibility method for zero Mach number turbulent reactive flows with heat release is combined with an unstructured finite volume hybrid grid scheme. The spatial discretization is based on an overlapped cell vertex approach. An infinite freely planar flame propagating into a turbulent medium of premixed reactants is considered as a test case. The recourse to a flamelet combustion modeling for which the reaction rate is quenched in a continuous way ensures the uniqueness of the turbulent flame propagation velocity. To integrate the final form of discretized governing equations, a three-stage hybrid time-stepping scheme is used and artificial dissipation terms are added to stabilize the convergence path towards the final steady solution. The results obtained with such a numerical procedure prove to be in good agreement with those reported in the literature on the very same flow geometry. Indeed, the flame structure as well as its propagation velocity are accurately predicted thus confirming the validity of the approach followed and demonstrating that such a numerical procedure will be a valuable tool to deal with complex reactive flow geometries.

INTRODUCTION
Steady and unsteady zero Mach number reactive flows in the sense of Majda and Sethian (1985), are often encountered in many systems of practical interest such as furnaces or jet engines. In such cases, the pressure can be considered as being thermodynamically constant e.g. the density variations are uniquely related to the temperature changes due to the heat released by the combustion process. When compressible flow solvers are employed in such situations, their convergence rate is becoming so slow that specific procedures such as preconditioning techniques have to be employed to improve them, but in the limit $Ma \to 0$ even the recourse to such techniques is not sufficient to ensure a satisfactory convergence rate (Dourado and Azevedo, 1996 and 1999; Dourado et al., 2000). Accordingly, specific numerical strategies have to be employed such as the Simple, the PISO or the pseudo-compressibility technique (Chorin, 1967). The latter approach presents the immense advantage over the two others that its introduction in a compressible flow solver is easy and leaves the structure of the computer program largely unmodified while allowing the calculations of both inert and reacting flows (Corvellec, 1998; Corvellec et al.; 1999). On the other hand, during the last two decades, the finite volume unstructured grid technique has shown its ability to cope with a wide range of complex compressible flow geometries (Jameson et al., 1986, Barth and Jespersen, 1989) including the use of mesh refinement techniques (Batina, 1989, Trépanier et al., 1991, Nomura and Hughes, 1992) that are appealing for properly resolving the high spatial gradients that are potentially present in the flows under investigation. Thus, the temptation is strong to combine the advantages of both the pseudo-compressibility method and the finite volume unstructured grid technique to develop a computer code able to deal with low Mach number inert or reacting flows. Along these lines, the present work is devoted to the development and the test of such a combination that results in the development of a 2-D computer code that will be tested on the geometry of an 1-D freely propagating turbulent premixed flame whose velocity is known, thanks to the formulation retained for the combustion modeling.
PHYSICAL MODELING AND NUMERICAL STRATEGY

Combustion Model

Since the present study is mainly concerned with the numerical method of solution of the governing equations rather than the modeling of the combustion process itself, only a brief description of the modeling is given here. The formulation retained is similar to that of Corvellec et al. (1999). This choice is motivated by the fact that such a modeling yields a turbulent premixed flame that propagates at a velocity that can be directly derived from the so-called KPP analysis (Kolmogorov et al., 1937, Corvellec et al., 1999). Consequently, such a test case permits an unambiguous evaluation of the capability of the code to predict the correct turbulent flame speed which is intrinsic to the set of equations considered. So, the recourse to the comparison with experimental data is not required at this stage as long as it is not the physical modeling itself which is to be tested. A simplified Bray-Moss-Libby like formulation (Bray and Moss, 1977, Bray et al., 1984, Bray et al., 1988), thereafter referred to as BML is used with a quenched mean reaction rate. Accordingly, the isenthalpic combustion process takes place in infinitely thin-laminar like reactive interfaces (flamelets) whose thickness is less than the Kolmogorov scale and whose laminar flame velocity is negligible compared to the velocity fluctuations associated with turbulence. An observer recording the temperature signal at a given point within the flow would e.g. when \( \partial V \) vanishes. The pseudo-sound speed is given by:

\[
\alpha = \sqrt{\mu^2 + \beta}
\]

and the local corresponding pseudo-Mach number \( Ma^* \) defined by

\[
Ma^* = \frac{\mu}{\alpha}
\]

is thus always less than one as soon as \( \beta \) is larger than zero. For a 1-D turbulent flame and using an implicit structured finite differences approach, Bruel et al. (1996) have shown that i) the value of the pseudo-compressibility factor \( \beta \) influences strongly the convergence rate of the calculations and ii) a value \( \beta = 5u_{ref}^{-2} \) to 10\( u_{ref}^{-2} \) where \( u_{ref} \) is the largest convective velocity expected in the flow is found to be a good compromise in terms of convergence rate.

Mean Governing Equations

In spite of the fact that the test case considered here is one-dimensional, the governing equations are cast into a two-dimensional form since an unstructured approach for dealing with such equations cannot be formulated otherwise. For the simplified combustion model retained here, the main mean variables that describe the turbulent reactive flow are the density \( \rho \), the Cartesian velocity components \( \vec{u}_i \), the static pressure \( \vec{p} \) and the progress reaction variable \( \vec{c}_r \). The steady governing equations that include the pseudo-compressibility approach are given by:

\[
\frac{\partial \vec{c}_r}{\partial t} + \frac{\partial \vec{E}_{c_l}}{\partial x_j} - \frac{\partial \vec{E}_{c_l}}{\partial x_i} = S
\]
with \( x_1 = x \) and \( x_2 = y \), the various vectors can be expressed as:

\[
q = \begin{bmatrix}
\hat{p} \\
\hat{p}u \\
\hat{p}v \\
\hat{p}w
\end{bmatrix}
\quad \begin{bmatrix}
E_{x_1} = \begin{bmatrix}
\beta \hat{p}u \\
\hat{p}u^2 + \hat{p} & \hat{p}v \\
\hat{p}v & \hat{p}w
\end{bmatrix}
\quad \begin{bmatrix}
E_{x_2} = \begin{bmatrix}
\beta \hat{p}v \\
\hat{p}v^2 + \hat{p} & \hat{p}w
\end{bmatrix}
\quad E_{x_3} = \begin{bmatrix}
\beta \hat{p}w \\
\hat{p}w^2 + \hat{p}
\end{bmatrix}
\end{bmatrix}
\]

\[
E_{v_1} = \begin{bmatrix}
0 \\
\sigma_{x_1} - \rho u^{\prime} u^{\prime} \\
\sigma_{x_2} - \rho u^{\prime} v^{\prime} \\
\rho D_{x_1} u^{\prime} - \rho u^{\prime} c^{\prime}
\end{bmatrix}
\quad E_{v_2} = \begin{bmatrix}
0 \\
\sigma_{x_2} - \rho u^{\prime} v^{\prime} \\
\sigma_{y_2} - \rho v^{\prime} v^{\prime} \\
\rho D_{x_2} v^{\prime} - \rho v^{\prime} c^{\prime}
\end{bmatrix}
\quad E_{v_3} = \begin{bmatrix}
0 \\
\rho D_{x_3} u^{\prime} - \rho u^{\prime} c^{\prime}
\end{bmatrix}
\quad S = \begin{bmatrix}
0 \\
0 \\
0 \\
\hat{w}
\end{bmatrix}
\]

(10)

where \( \hat{w} \) is the mean reaction rate given by Eq. (6) and \( \sigma_{ij} \) is the laminar stress tensor expressed for a Newtonian fluid by:

\[
\sigma_{ij} = \mu_j \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)
\]

(11)

In Eq. (10), \( D = \frac{V_{y_i}}{S_{c_i}} \) is the laminar diffusion coefficient, \( V_{y_i} \) the kinematic laminar viscosity and \( S_{c_i} \) the laminar Schmidt number. The Reynolds stress, present in Eq. (10) are closed with a Boussinesq-like expression, namely (Frisch, 1995):

\[
\rho \hat{u}_i u_j^{\prime} = -\mu_j \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)
\]

(12)

Where \( \hat{k} = \frac{1}{2} \frac{\rho u_i u_j^{\prime}}{\rho} \) is the turbulence kinetic energy. The turbulent viscosity coefficient can be expressed as a function of \( \hat{k} \) and of its dissipation rate \( \hat{e} \) by (Launder and Spalding, 1974):

\[
\mu_t = \hat{C}_\mu \frac{k^3}{\hat{e}}
\]

(13)

with \( C_\mu \), being equal to 0.09.

In the present work, the turbulence field is supposed to be frozen at the level that prevails in the fresh reactants so that \( \hat{k} = \hat{k}_r \) and \( \hat{e} = \hat{e}_r \), with:

\[
\hat{k}_r = \frac{1}{2} u_r^2 \quad \hat{e}_r = C_{\mu}^{0.75} \frac{k_{y_r}^{1/2}}{l_i}
\]

(14)

where \( u_r = \sqrt{\rho u_r^2} \) and \( l_i \), to be prescribed, stand for the rms velocity fluctuations and the turbulence integral length that prevail in the fresh reactants, respectively.

The turbulent mass flux present in Eq. (10) is also expressed through a gradient approximation, namely (Bray et al., 1984):

\[
\hat{p} u_i u_j^{\prime} = -\hat{p} D_{ij} \frac{\partial c^i}{\partial x_j}
\]

(15)

where \( D_{ij} = \frac{V_{y_i}}{S_{c_i}} \) is the turbulent diffusion coefficient, \( \nu_t \) the turbulent kinematic viscosity and \( \hat{n} \) the turbulent Schmidt number. The closed form of Eqs. (9) is now written in an integral form using the Green’s theorem:

\[
V_{y_i} \frac{\partial}{\partial x_j} q dV + \int_{S_y} \mathbf{E}_i \cdot \hat{n} \mathbf{d} \mathbf{S} + \int_{S_y} S dV
\]

(16)

where \( \hat{n} \) represents the outgoing normal unitary vector to surface \( S \) of volume \( V \) and \( \mathbf{E}_i \) and \( \mathbf{S} \) are the convective and diffusion flux vectors whose components are given in Eq. (10). In two dimensional Cartesian notation, the product \( \hat{n} \mathbf{d} \mathbf{S} \) is equal to \( \Delta y \hat{1} - \Delta x \hat{j} \) where \( \hat{1} \) and \( \hat{j} \) are the basis vectors.

Spatial Discretization

As the control volume can be constructed \( a \ priori \) with different type of elements (triangles and/or quadrangles) on hybrid grid topologies, the elementary cell of the grid considered here is simply called an element. Thus, the control volume \( V \) is defined by the external boundary surface of all elements sharing a common node, as sketched in Fig. (1). The spatial discretization adopted here is based on a cell center finite volume method adapted for cell vertex hybrid elements (Jameson et al., 1986). This scheme proved to be efficient for dealing with steady and unsteady inert flows as reported by Mavriplis et al. (1989), Mavriplis and Venkataraman (1995), Dourado and Azevedo (1996), Mavriplis (1998), Dourado and Azevedo (1999) and Dourado et al. (2000). The discretized form of Eq. (16) is written as:

\[
\int_{V} \frac{\partial}{\partial x_j} (\mathbf{E}_i) dV + \sum_{e_{xy}} (\mathbf{E}_{e_{xy}} dV - \mathbf{E}_{e_{xy}} dV) + V S
\]

(17)

where \( q = \frac{1}{V} \int_{V} q dV \)

(18)

is the average main variables vector, and
Figure 1 - Domain of influence of nodes 1, 2 and 3 and its local stretching for hybrid unstructured grid.

$$\bar{S} = \frac{1}{V} \int_V \bar{s} dV$$

(19)

is the average source term vector. $\bar{E}$ is the average flux vector at face $f$ calculated as the arithmetic average of the two fluxes located on nodes which delimit this face. Further details on triangular and hybrid elements in unstructured grids are presented in the studies that have been referred to above.

**Artificial Dissipation**

For high Reynolds number flows, it is frequently required to stabilize the calculations by adding explicitly some artificial dissipation to damp out numerical oscillations. These additional dissipative terms must be kept at a level that does not endanger the accuracy of the numerical solution. Accordingly, and as suggested by Dourado et al. (2000), the dissipation terms introduced in the systems of equations are written as:

$$D_i(q_i) = \sum_{k=1}^{nm} [\Delta_k - \Delta_i] \left[ \frac{\Delta_x + \Delta_y}{2} \right]$$

(20)

where

$$\Delta(q) = -k^{(4)} \nabla^2 q$$

(21)

and $nm$ is the number of nodes located on the boundary of the control volume $i$, as it is sketched in Fig. (1).

The constant $k^{(4)}$ which defines the level of the fourth order dissipation term is taken equal to 1/256 for all the calculations presented in this work and the coefficient $A$ is adjusted according to the grid stretching by:

$$A_k = \alpha_1 \cos^2 \theta_k + \alpha_2 \sin^2 \theta_k$$

(22)

Subscripts $i$ and $k$ refer to the variable evaluation at nodes $i$ and $k$, respectively. At each mesh point, the coefficients $\alpha_1$ and $\alpha_2$ of Eq. (22) are calculated with the maximum eigenvalue $\lambda$ associated with the convective terms by:

$$\alpha_1 = \phi(s) \frac{\lambda}{s+1} \lambda \quad \alpha_2 = \phi(s^{-1}) \frac{s}{s+1} \lambda$$

(23)

where $s$ represents the magnitude of the stretching vector $\bar{S}$ (see Fig. (1)) and $\phi(r) = 1 + r^{2/3}$. For an unstructured mesh, the maximum eigenvalue $\lambda$ at each mesh point is evaluated by the following discrete approximation:

$$\lambda = \sum_{j=1}^{nf} \left[ \bar{u}_j \Delta y_j - \bar{v}_j \Delta x_j \right] + \bar{a} \sqrt{\Delta x^2 + \Delta y^2}$$

(24)

where $\bar{u}$, $\bar{v}$ and $\bar{a}$ are the average values of the velocity components and of the sound speed calculated from the two nodes which delimit the face $f$ and cumulated over all the boundary faces of the control volume considered. Finally, since the code is edge based database organized, the artificial dissipation term formulation was enhanced in order to be usable in the context of hybrid grids where triangular and quadrilateral elements coexist. One should observe that, although quadrilateral meshes were used in the present simulations, the code treats all grids in a fully
unstructured way. The reader should be aware that the definition of an unstructured grid is not necessary related to the shape of the control volumes but to the form in which these control volumes are addressed in the code.

Pseudo-time marching

As exposed before, when one has recourse to the pseudo-compressibility method to solve the flow governing equations, the solution is physically meaningful only when a steady state in pseudo-time is reached, so, even to seek steady state solutions, a time-stepping procedure has to be used. Thus, the discretized equations system (17) is first written as:

$$V_i \frac{dq_i}{dt} + [C(q_i) - Dv(q_i) - D_a(q_i)] = S(q_i) \quad i = 1 \ldots n$$

(25)

where the residuals of the convective, diffusive and stabilizing terms are denoted by $C(q)$, $Dv(q)$ and $D_a$, respectively, and the source term is represented by $S(q)$.

Then, a Runge-Kutta explicit three-stage hybrid time-stepping scheme is adopted due to its satisfactory performance, simplicity and low computational cost. The scheme proposed by Manzari et al. (1998), to advance the solution in pseudo-time is implemented here under the following form:

$$q_i^{(0)} = q_i^{(n)}$$

$$q_i^{(0)} = q_i^{(0)} - \alpha_1 \frac{\Delta t}{V_i} \left[ C(q_i^{(\kappa-1)}) - Dv(q_i^{(\kappa-1)}) + S(q_i^{(\kappa-1)}) \right]$$

$$q_i^{(\kappa)} = q_i^{(\kappa-1)} + \alpha_2 \frac{\Delta t}{V_i} \left[ C(q_i^{(\kappa-1)}) - Dv(q_i^{(\kappa-1)}) + S(q_i^{(\kappa-1)}) \right]$$

$$q_i^{(\kappa+1)} = q_i^{(\kappa)} \quad \kappa = 1, 2, 3$$

(26)

The operators $C$, $Dv$ and $S$ are expressed by using the vector properties $q_i^{(\kappa-1)}$ from stage $\kappa-1$, while the added artificial dissipation term is calculated only in the first stage and held constant throughout the next stages. The coefficients appearing in Eq. (26) are given the values $\alpha_1 = 0.6$, $\alpha_2 = 0.6$ and $\alpha_3 = 1.0$.

**RESULTS**

The 1-D turbulent premixed flame referenced by Corvellec (1998) as Case I is considered here to test the present numerical approach. The parameters defining such a slow propagating flame are given in Table (1).

<table>
<thead>
<tr>
<th>$X$</th>
<th>$X_c^*$</th>
<th>$S_i$ (m/s)</th>
<th>$\bar{u}_r$ (m/s)</th>
<th>$l_i$ (m)</th>
<th>$Sc_i$</th>
<th>$C_w$ kg/m$^3$/s</th>
<th>$\rho_r$ kg/m$^3$/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.03958</td>
<td>0.5</td>
<td>1.0</td>
<td>10$^{12}$</td>
<td>0.75</td>
<td>200</td>
<td>1.1886</td>
</tr>
</tbody>
</table>

Table 1 – Parameters defining the 1-D turbulent premixed flame considered as test case.

The boundary condition imposed at the reactants side e.g. $\bar{u}_r = S_i$ and $\bar{c} = \bar{c} = 0$ has been chosen so that the turbulent flame brush will be steady in the computational domain which consists of a strip of $0.5 \text{ m}$ long and $0.1 \text{ m}$ in height with only one division in the latter direction. An example of grid, called *mesh I* with 355 nodes in the longitudinal direction and 354 quadrilateral elements is presented in Fig. (2). In order to properly resolve the strong gradients that are to be expected in the turbulent brush near the quenching point, the mesh is highly refined in the region located between $0.17 \text{ m} \leq x \leq 0.33 \text{ m}$ with a minimum mesh spacing $\Delta x_{\text{min}}$ equal to $5.33 \times 10^{-4} \text{ m}$.

Due to the high Reynolds number flow hypothesis, the laminar diffusive transports will be neglected in front of their turbulent counterparts. To ensure 1-D like conditions on such a 2-D mesh, a symmetry condition is imposed at the lower and upper boundary lines parallel to the flow and are applied to the corresponding nodes and faces. Such a condition corresponds to the imposition of zero transverse velocity and gradients. At the burned products side, the pressure is imposed and all other variables are extrapolated. The initial condition for the progress variable $\bar{c}$ is given by a ramp form function that goes from $\bar{c} = 0$ at $x = 0.27 \text{ m}$ to $\bar{c} = 1$ at $x = 0.32 \text{ m}$. The Courant-Frederich-Lewis (CFL) number used in these calculations is equal to 0.94 and is kept constant throughout the computational domain. Accordingly, the pseudo time step $\Delta \tau$ is variable in the computational domain with a minimum value used in the region of greatest refinement. Such a CFL number is given by:

$$CFL = \lambda_\tau \frac{\Delta \tau}{\Delta x_{\text{min}}}$$

(27)
where $\lambda = u + a_s$ is the largest convective eigenvalue based on the pseudo-sound speed given by Eq. (8). As a consequence, the minimum pseudo-time step for mesh 1 is equal to $2 \times 10^{-5}$ s. The convergence criterion set to $10^{-4}$ was met after 27500 iterations through a convergence history presented in Fig. (3). The corresponding profiles of pressure gradient, mean progress variable and mass flux obtained on mesh 1 are presented in Fig. (4).

The curvature at the foot of the flame brush is extremely strong and this illustrates why such a highly stretched mesh has to be used to capture properly the progress variable and pressure gradients in that zone. The profile of pressure gradient plotted against the progress reaction variable $c$ is displayed in Fig. (5).

Consequently, the criterion convergence chosen here appears to be correctly adapted to get accurate converged results. To investigate the sensitivity of our results to the mesh refinement, three other meshes have been considered that differ from mesh 1 by their refinement: i) mesh 2 possesses 50% more divisions in the $x$-direction in the interval $[x_{\min}, x_{\max}] = [33, 017, 0]$ with $\Delta x_{\min} = 3.5610^{-4} m$; ii) mesh 3 has 100% more divisions in the $x$-direction on the same interval, which gives $\Delta x_{\min} = 2.6710^{-4} m$ and iii) mesh 4 has the same number of nodes as mesh 3 but the interval of refinement is reduced to $[0.22 m, 0.30 m]$, which gives a minimum mesh discretization of $\Delta x_{\min} = 1.3310^{-4} m$.

A good agreement is obtained between the present results and those of Corvellec (1998) with a difference in the maximum value of the pressure gradient of less than 6%.
minimum spacing $\Delta x_{\min}$ equal to $7.1 \times 10^{-5} \, m$. The results obtained with the different grids are presented in Fig. (6) where the profiles of the pressure gradient are plotted versus the mean reaction progress variable.

The dependence on the value of $\hat{\beta}$ of the number of iterations required to meet the convergence criterion $LRHS_{nu} \leq 10^{-4}$ is presented in Fig. (8). The optimum value of $\hat{\beta}$, around 10, obtained here confirmed the results reported by Bruehl et al. (1996), and shows that such an optimum is poorly dependent on the numerical approach retained and thus can be considered as specific of the pseudo-compressibility approach itself.

**CONCLUDING REMARKS**

The proposed combination of the pseudo-compressibility method with an unstructured formulation to solve the governing equations of a turbulent premixed flame proves to work properly and to produce results that compare well with those obtained in the literature on the very same flow geometry. Due to the centered type of spatial discretization used here, a fourth-order artificial numerical dissipation has been added to stabilize the calculations but the results show that the accuracy of the final solution has been preserved. The use of an explicit three-stage hybrid time stepping scheme shows that it is powerful enough to calculate the steady solution in the pseudo-time of the system of discretized governing equations. Nevertheless, the use of such an explicit time stepping scheme has the drawback of limiting the maximum possible CFL-number value resulting in an increased total number of pseudo-time steps required to achieve convergence. If needed, an implicit formulation could be considered to speed-up the convergence process. Finally, an auto-adaptive Lagrangian-Eulerian approach on unstructured grid (Téranier et al., 1991; Nomura and Hughes, 1992) could greatly help in reducing the total number of grid elements required to resolve properly the high gradients present in the flow while preserving the overall accuracy of the calculations. Future work will focus on these directions.

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