

APPLICATION OF THE LAMINAR FLAMELET CONCEPT IN THE NUMERICAL SIMULATION OF PARTIALLY PREMIXED FLAMES

R. Cònsul*, K. Claramunt[†], J. Cadafalch*, A. Oliva*, L.P.H. de Goey^{††}

*Centre Tecnològic de Transferència de Calor
Universitat Politècnica de Catalunya
Colom 11, 08222 Terrassa, Barcelona, Spain
e-mail: ricard@cttc.upc.edu

web page: <http://www.cttc.upc.edu>

[†]Department of Multi-Scale Physics

Delft University of Technology
Lorentzweg 1, 2628 CJ Delft, The Netherlands
e-mail: k.claramunt@ws.tn.tudelft.nl

^{††}Department of Mechanical Engineering, Combustion Technology
Eindhoven University of Technology
Den Dolech 2, 5600 MB Eindhoven, The Netherlands
e-mail: L.P.H.d.Goey@tue.nl

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Abstract. *The aim of this work is to analyse the application of flamelet models based on the mixture fraction variable and its dissipation rate to the numerical simulation of partially premixed flames. Although the main application of these models is the computation of turbulent flames, this work focuses on the performance of flamelet models in laminar flame simulations, removing in this way, turbulence closures influences. A co-flow methane/air laminar flame is selected. Five levels of premixing are taken into account from an equivalence ratio $\Phi=\infty$ (non-premixed) to $\Phi=2.464$. Results obtained using the flamelet approaches are compared to data obtained from the detailed solution of the complete transport equations using primitive variables. Numerical simulations with a counterflow flame are also presented to support the discussion of the results.*

1 INTRODUCTION

Flamelet models based on the mixture fraction variable using its dissipation rate for the mixing process are nowadays among the most extended models employed in the numerical simulation of non-premixed turbulent flames. Although the mathematical formulation of these flamelet models is derived from one-dimensional non-premixed flames, considering that the flame front can be viewed as an ensemble of thin locally one-dimensional elements [1], partially premixed turbulent flames are also often treated using flamelet approaches.

An example is the well-known SANDIA Flame D [2] defined by an equivalence ratio of 3.17 [3, 4, 5].

When modelling turbulent flames, the coupling between turbulence and chemistry makes the analysis of the appropriateness of the flamelet approach difficult. Thus, a more refined knowledge of the capabilities and limitations of the laminar flamelet approach can be revealed in the multidimensional numerical simulation of laminar flames.

The aim of this work is to analyse the appropriateness of the flamelet approach in partially premixed flames. To do so, a laminar co-flow methane/air flame is numerically simulated considering five levels of premixing between an equivalence ratio $\Phi=\infty$ (non-premixed) and $\Phi=2.464$. Results obtained using flamelet approaches are compared to data obtained from the resolution of the complete transport equations using primitive variables.

Steady state flamelet models (SFM) with species unity Lewis number are considered. When this hypothesis is used, as it is commonly employed when considering turbulent methane/air flames [3, 4], SFM models are able to predict accurately main flame structure (i.e. temperature and major species) in non-premixed laminar flames. See [6, 5], where a set of steady and unsteady flamelet approaches are compared in the simulation of the co-flow laminar non-premixed methane/air flame. This work focuses on the analysis of the validity of the steady state flamelet model when partially premixing is taken into account.

2 PROBLEM DESCRIPTION

The selected flame is the laminar partially premixed methane/air flame in a co-flow with the burner characteristics defined in [7]. Fuel mixed with primary air flows from an uncooled $r_i = 5.55$ mm inner radius tube. Air is injected from the annular region between this tube and a concentric $r_o = 47.6$ mm inner radius chimney.

Equivalence ratios and flow rates are listed in Table 2. Primary air is oxygen-enriched (25% O_2 by volume) and secondary air is “regular” (20.9% O_2). Secondary air flow rate is fixed to 44000 [cm^3/min]. See more details in [8, 9, 10].

Φ [—]	$\dot{m}_{CH_4}$ [cm^3/min]	$\dot{m}_{O_2}$ [cm^3/min]	Z_{st} [—]
∞	330	—	0.055
12.32	330	210	0.120
6.16	330	420	0.187
4.107	330	630	0.256
2.464	330	1050	0.397

Table 1: 2D co-flow methane/air flame. Inner jet reactant flow rates and stoichiometric mixture fraction for the different levels of partially premixing.

3 MATHEMATICAL MODELS

Full-calc model: Detailed model based on the full resolution of the transport equations [9, 10]. The fluid flow and heat and mass transfer phenomena of the reactive gas are assumed to be described by the governing equations for low-Mach number flows (continuity, species, momentum, energy and state equation).

Flamelet model: The fluid flow is calculated with the continuity and momentum equations. The mixture fraction equation is solved and the scalar dissipation rate evaluated. Species and temperature are obtained from the resolution of flamelet equations and stored in the flamelet libraries.

3.1 Mathematical sub-models

Transport coefficients of the molecular fluxes of momentum and heat are evaluated considering a mixture-averaged formulation. Pure-species transport properties are evaluated using CHEMKIN's database [11]. Mixture diffusion coefficients are calculated assuming unity Lewis numbers for all species. Chemical reactions are described by the skeletal mechanism presented in [12].

3.2 Flamelet equations

Steady state flamelet equations, assuming unity Lewis numbers and negligible Soret effect, and no radiation, can be written as follows [6]:

$$\frac{\rho\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} + \dot{w}_i = 0 \quad (1)$$

$$\frac{\rho\chi}{2} \frac{\partial^2 T}{\partial Z^2} + \frac{\rho\chi}{2c_p} \frac{\partial c_p}{\partial Z} \frac{\partial T}{\partial Z} - \frac{1}{c_p} \sum_{i=1}^N h_i \dot{w}_i = 0 \quad (2)$$

where T is temperature; Z mixture fraction; c_p specific heat; and Y_i , h_i , $\dot{w}_i$ are i^{th} species mass fraction, enthalpy and net rate of production, respectively.

The mixture fraction definition adopted for partially premixed methane/air flames reads:

$$Z = \frac{sY_{CH_4} - Y_{O_2} + Y_{O_2}^{ox}}{sY_{CH_4}^f - Y_{O_2}^f + Y_{O_2}^{ox}} \quad (3)$$

where the subscripts “ f ” and “ ox ” indicate fuel and oxidiser jets respectively, and s is the mass stoichiometric coefficient.

In flamelet equations, χ is the instantaneous scalar dissipation rate defined by:

$$\chi = 2D_z (\nabla Z \cdot \nabla Z) \quad (4)$$

where, D_z is the diffusion coefficient of the mixture fraction equation evaluated assuming also unity Lewis number.

In the integration of the flamelet equations the analytical approximation based on the counter-flow diffusion flame or the one-dimensional laminar mixing layer reported in [13, 1] is used:

$$\chi = \chi_{st} \frac{\Phi}{\Phi_{st}} \frac{f(Z)}{f(Z_{st})} \quad (5)$$

with,

$$\Phi = \frac{3}{4} \frac{\left(\sqrt{\rho_{\infty}/\rho} + 1\right)^2}{2\sqrt{\rho_{\infty}/\rho} + 1} \quad (6)$$

and where Z_{st} is the stoichiometric mixture fraction; Φ is a factor introduced in order to consider variable density effects [14]; the subscript ∞ means the oxidizer stream and $f(Z) = \exp\left[-2\left[\operatorname{erfc}^{-1}(2Z)\right]^2\right]$, where erfc^{-1} is the inverse of the complementary error function.

Using this expression in the flamelet equations, the flamelet library is built with two input parameters: Z and χ_{st} . The scalar dissipation rate at the stoichiometric conditions is evaluated where $Z = Z_{st}$. With this approach, the functional dependence of the scalar dissipation rate with the mixture fraction $\chi(Z)$ is parameterised by χ_{st} . This value acts as an external parameter that is imposed on the flamelet structure by the mixture fraction field [1].

4 NUMERICAL METHODOLOGY

The mathematical models are discretized using finite volume techniques over axisymmetric staggered grids. Central differences are employed for the evaluation of the diffusion terms, while third-order bounded schemes are used for the evaluation of the convective ones. A time-marching SIMPLE-like algorithm is employed to couple velocity-pressure fields [15]. Discretized equations are solved in a segregated manner using a multigrid solver. The convergence of the time-marching iterative procedure is truncated once normalised residuals are below 10^{-8} .

Domain decomposition method is used as a strategy to reduce the number of grid nodes far from the flame fronts and as a parallelisation technique. For further details see [9]. The computational domain is discretized considering several zones with different grid node distributions. The number of nodes is related to the grid parameter n . An h -refinement study is performed with five levels of refinement ($n = 1, 2, 4, 8$ and 16). For example, for the finest discretization level, $n = 16$, 141.856 control volumes are employed. See [10] for details about the grid node distribution.

Numerical results are submitted to a post-processing procedure based on the generalized Richardson extrapolation method for h -refinement studies and on the Grid Convergence Index (GCI). This tool estimates the order of accuracy of the numerical solution (observed order of accuracy p), and the error band where the grid independent solution is

expected to be contained (uncertainty due to discretization GCI), also providing criteria on the credibility of these estimations. See [9, 10, 16] for further details.

From these verifications studies the third level of refinement (i.e. $n = 4$) is selected to perform the numerical investigation hereafter presented. As an example of this uncertainty estimators, the GCI for the non-dimensional temperature ($T^* = T/298$) is estimated to be $\pm 0.16\%$.

Flamelet equations are converted into a discretized system using finite volume techniques. An operator-splitting procedure and/or a Damped-Newton method is used to reach steady state solutions [9]. Mixture fraction coordinate is discretized with 160 nodes concentrating the mesh around $Z=Z_{st}$. Numerical results are stored in *flamelet libraries*.

When solving the flamelet model, temperature and species mass fractions are obtained from flamelet libraries (i.e. $T = T(Z, \chi_{st})$, $Y_i = Y_i(Z, \chi_{st})$). At each axial position, χ_{st} is evaluated using Eq. (4) at $Z = Z_{st}$.

5 RESULTS

In Fig. 1-3 illustrative results obtained with the full resolution of the governing equations (*full-calc model*) and with the flamelet model are presented for the five levels of premixing. Temperature and two major species mass fractions (i.e. Y_{O_2} and Y_{H_2O}) centreline profiles are plotted. As can be observed, the agreement between detailed and flamelet model solutions is excellent for the non-premixed situation (i.e. $\Phi=\infty$), but as the equivalence ratio decreases, the disagreements between both computations increase. However, at the post-flame region, good agreement is obtained between detailed and flamelet simulations for all equivalence ratios.

As a main important feature, it is shown that flamelet model simulations tend to over-predict the inner flame temperature as the equivalence ratio is decreased. This fact is specially relevant for the highest level of partially premixing considered (i.e. $\Phi=2.464$) where a double flame is formed. Here, the inner flame height is clearly under-predicted (see Fig. 4).

6 DISCUSSION

Authors argue that two main reasons can cause differences. On one hand the scalar dissipation profile obtained in the CFD computations disagrees with the profile employed during the solution of flamelet equations. Remember that the flamelet equations are solved using the analytical approximation based on the one-dimensional laminar mixing layer (Eq. (5)). See for instance Fig.5, where the χ radial profile for $\Phi = 2.464$ is plotted at different flame heights.

On the other hand, as the level of partial premixing increases, the dependence of the flamelet equation solutions on χ_{st} also increases (i.e. $T(Z, \chi_{st})$, $Y_i(Z, \chi_{st})$). For instance, while for the non-premixed case the temperature profiles maintain almost the same shape for the whole range of χ_{st} solved, for the $\Phi = 2.464$ case, temperature profile differs

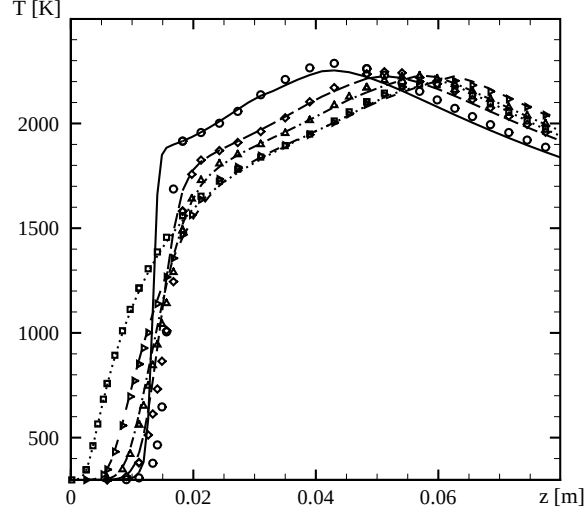


Figure 1: 2D co-flow flame. Full-calc vs Flamelet simulations. Temperature centreline profiles. Symbols: Full-calc simulations. Lines: Flamelet simulations. Dotted line and square: $\Phi=\infty$. Dashed line and right triangle: $\Phi=12.32$. Dashed-dot line and delta: $\Phi=6.16$. Dashed-dot line and diamond: $\Phi=4.107$. Solid line and circle: $\Phi=2.464$.

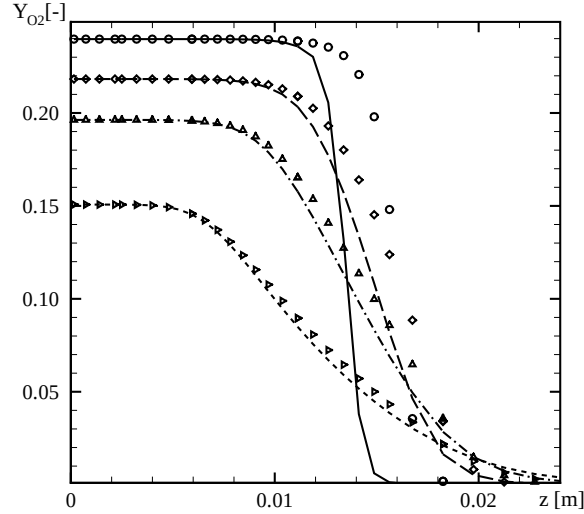


Figure 2: 2D co-flow flame. Full-calc vs Flamelet simulations. Y_{O_2} centreline profiles. Symbols: Full-calc simulations. Lines: Flamelet simulations. Dashed line and right triangle: $\Phi=12.32$. Dashed-dot line and delta: $\Phi=6.16$. Dashed-dot line and diamond: $\Phi=4.107$. Solid line and circle: $\Phi=2.464$. Non-premixed results are not included as the mass fraction is almost negligible in this range.

notably depending on the χ_{st} considered. See Fig. 7.

Furthermore, for low equivalence ratios, the range of values of χ_{st} for which one is able to solve flamelet libraries is reduced (see Fig. 7). The lowest value of χ_{st} reached during the solution of flamelet equations increases as the equivalence ratio also decreases (i.e.

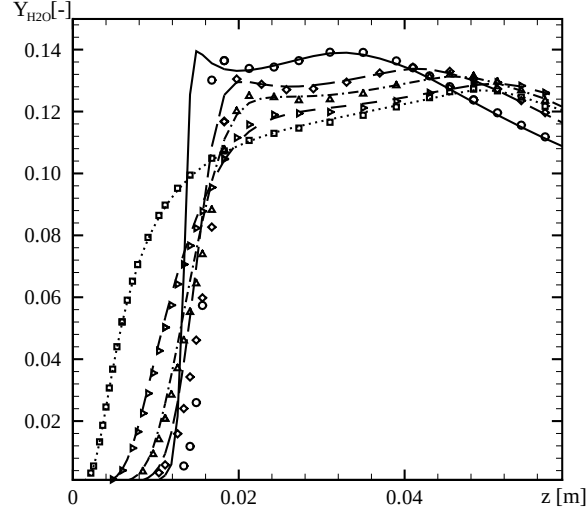


Figure 3: 2D co-flow flame. Full-calc vs Flamelet simulations. Y_{H_2O} centreline profiles. Symbols: Full-calc simulations. Lines: Flamelet simulations. Dotted line and square: $\Phi = \infty$. Dashed line and right triangle: $\Phi = 12.32$. Dashed-dot line and delta: $\Phi = 6.16$. Dashed-dot line and diamond: $\Phi = 4.107$. Solid line and circle: $\Phi = 2.464$.

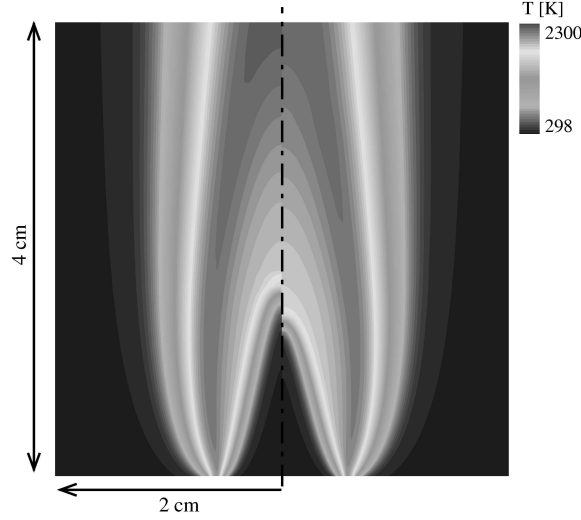


Figure 4: 2D Co-flow flame. $\Phi = 2.464$. Temperature contours. Full-calc (left) vs Flamelet simulations (right).

$\chi_{st,min} = 10^{-3} \text{ s}^{-1}$ for $\Phi = \infty$ and 12.32, $\chi_{st,min} = 10^{-1} \text{ s}^{-1}$ for $\Phi = 6.16$, and $\chi_{st,min} = 1 \text{ s}^{-1}$ for $\Phi = 4.107$ and 2.464). Moreover, it can be observed also that a sudden increase of the temperature in the rich fuel zones (i.e. $Z=1$) for low equivalence ratios arises. For all Φ , the same temperature boundary condition has been considered (i.e. $T=298 \text{ K}$).

In Fig. 6, the stoichiometric scalar dissipation rate (χ_{st}) and mixture fraction (Z)

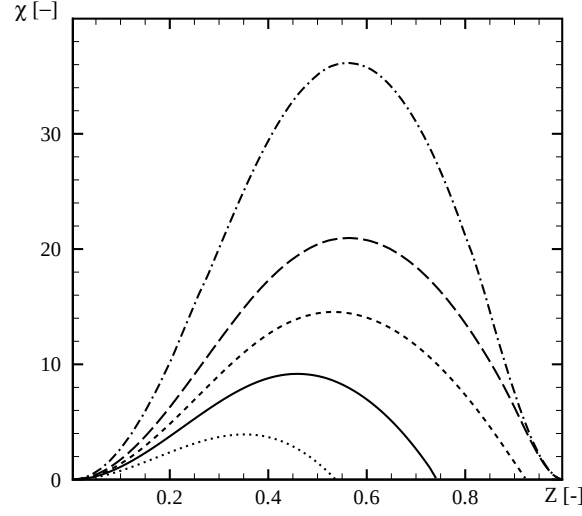


Figure 5: 2D co-flow flame. $\Phi=2.464$. Scalar dissipation rate profiles obtained from the co-flow flame computation using flamelet model at different heights. Dashed-dot line: $z = 0.5$ cm. Long-dashed line: $z = 1$ cm. Dashed line: $z = 1.5$ cm. Solid line: $z = 2$ cm. Dotted line: $z = 3$ cm.

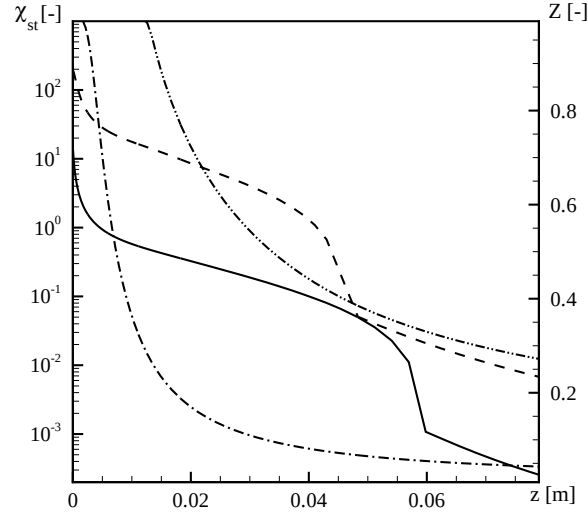


Figure 6: 2D co-flow flame. Flamelet simulations. Centreline profiles for the stoichiometric scalar dissipation rate (χ_{st}) and for the mixture fraction (Z) for the extreme levels of premixing. $\Phi=\infty$: solid line χ_{st} , dashed-dot-dot line Z . $\Phi=2.464$: dashed line χ_{st} , dashed-dot line Z .

centreline profiles are plotted for the extreme levels of equivalence ratios. For the non-premixed simulations flamelet libraries can provide the full range of χ_{st} appearing in CFD simulations. However, this is not the case for the lowest equivalence ratio (i.e. $\Phi=2.464$), where for $\chi_{st} < 1$, scalar values (temperature and species mass fractions) are set from the lowest χ_{st} available in the flamelet libraries (i.e. $\chi_{st}=1$). This is specially important to

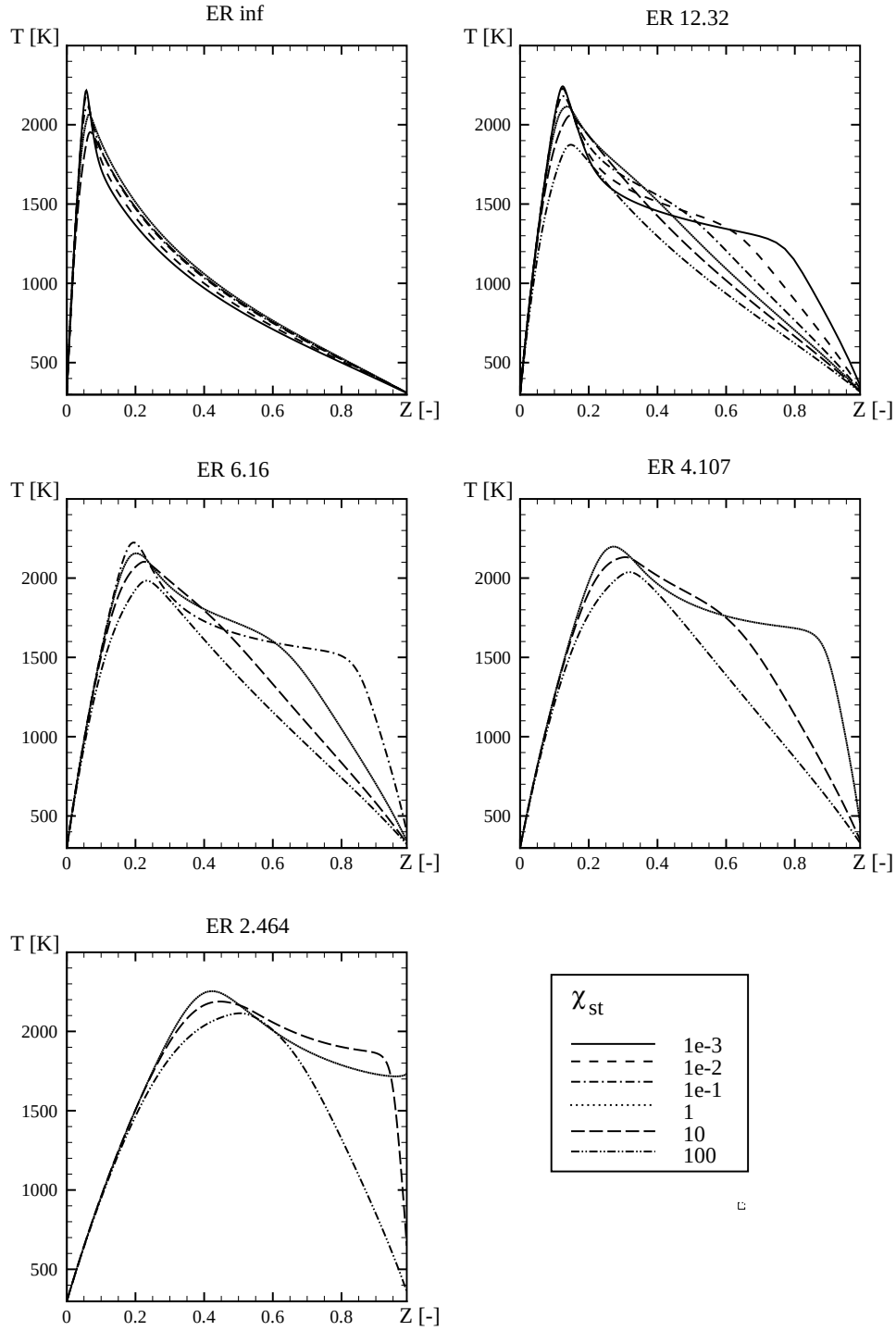


Figure 7: Temperature profiles obtained from the solution of the flamelet equations for the five equivalence ratios considered.

be taken into account. Please notice that the value χ_{st} in the flame front ($Z_{st}=0.397$), is lower than unity. This latter feature, could justify the under-prediction of the flame front height observed in flamelet model CFD simulations.

6.1 Scalar dissipation rate profile dependence

In order to analyse the dependence of the flamelet model simulations to the scalar dissipation rate profile used during the integration of flamelet equations, a 1D counterflow partially premixed flame is numerically simulated in physical space instead of Z-space. The five levels of partially premixing are also considered in this problem. The jets separation is 1.27 cm, and the jet exit velocities are chosen so as to consider different values of the scalar dissipation rate evaluated at the stoichiometric position (i.e. $\chi_{st}=8, 15, 25, 50$ and 100 s^{-1}). The main purpose pursued here is to avoid the approximations considered in a multidimensional simulation when the flamelet approach is taken into account.

When solving the flames using the flamelet libraries built with the pre-assumed χ_Z distribution, an excellent agreement between detailed and flamelet results is obtained for non-premixed flames, while expected disagreements are observed when the level of partially premixing is increased. However, these disagreements are only important for low values of χ_{st} . In Fig. 8, temperature profiles for the equivalence ratio of $\Phi=2.464$ are shown. Relevant disagreements are only observable for $\chi_{st} \leq 15 \text{ s}^{-1}$.

Considering that in this problem, the flamelet model formulation is just the solution of the same problem in mixture fraction space (Z) in spite of the physical space (z), the differences between *full-calc* and flamelet results can only be caused by the pre-assumed scalar dissipation rate profile $\chi(Z)$ used in the flamelet equations integration. As can be observed in Fig. 9 for low values of χ_{st} , important differences appear between the scalar dissipation rate profile obtained from the *full-calc* simulation and the pre-assumed analytical approximation used to built the flamelet libraries.

An alternative possibility to be considered in the construction of the flamelet libraries is the evaluation of the real scalar dissipation rate profiles obtained in the flame simulations and the consequent update of the flamelet libraries [6]. This procedure needs an interactive procedure between flame and flamelet library computations (*interactive flamelet*).

In Fig. 10 numerical solutions obtained with the *interactive flamelet model* are compared with *full-calc* results. Three flame-flamelet interactions have been performed. As can be seen an excellent agreement is obtained.

6.2 Application of the interactive flamelet in the co-flow flame

The interactive flamelet model has been also applied in the numerical simulation of the 2D axisymmetric co-flow flame. The most difficult case (i.e. $\Phi=2.464$) has been taken into account. Considering this interactive procedure, the scalar dissipation rate distribution is evaluated at each axial position using the radial scalar dissipation rate distribution to integrate the flamelet equations. Fig. 5 shows the scalar dissipation rates profiles evaluated

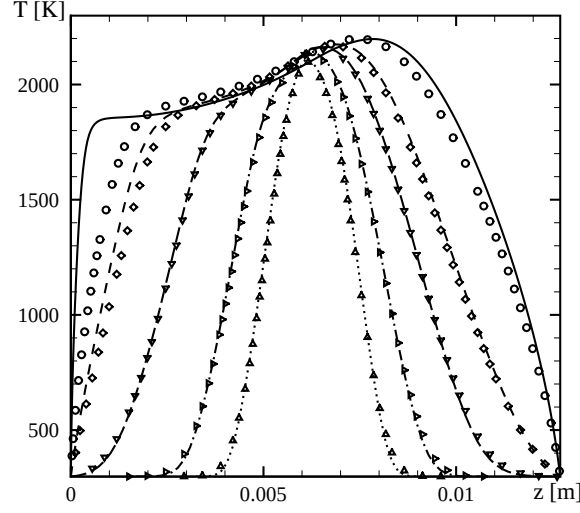


Figure 8: 1D counterflow flame in physical space. Full-calc vs Flamelet simulations. $\Phi=2.464$. Temperature distribution for different strain rates defined by χ_{st} . Symbols: full-calc simulations. Lines: Flamelet simulations. Solid line and circle: $\chi_{st}=8 \text{ s}^{-1}$. Dashed line and diamond: $\chi_{st}=15 \text{ s}^{-1}$. Long-dashed line and gradient: $\chi_{st}=25 \text{ s}^{-1}$. Dashed-dot line and right triangle: $\chi_{st}=50 \text{ s}^{-1}$. Dotted line and triangle: $\chi_{st}=100 \text{ s}^{-1}$.

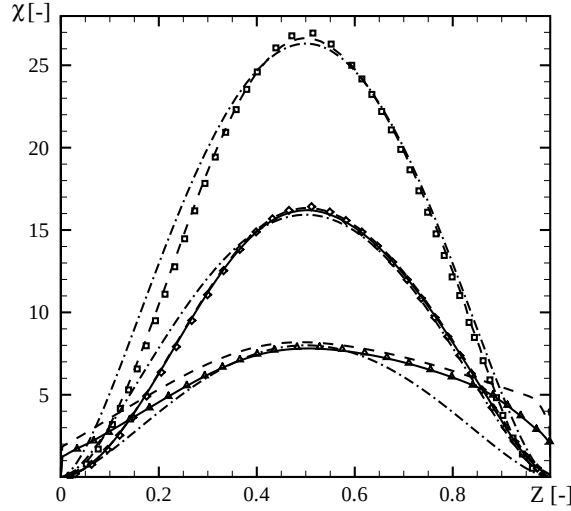


Figure 9: 1D counterflow flame in mixture fraction space. Full-calc vs Flamelet simulations. $\Phi=2.464$. Scalar dissipation rate distributions $\chi(Z)=2 D_z (\nabla Z \cdot \nabla Z)$ for different strain rates defined by χ_{st} ($\chi_{st}=8, 15, 25 \text{ s}^{-1}$). Symbols: full-calc simulation. Solid line: flamelet simulation with the pre-assumed analytical approximation. Dashed line: interactive flamelet simulation. Dashed-dot line: analytical approximation (Eq. 5).

from flamelet model solution. Flamelet library temperature profile computed with the above mentioned profiles is shown in Fig. 11. In these computations, temperature and

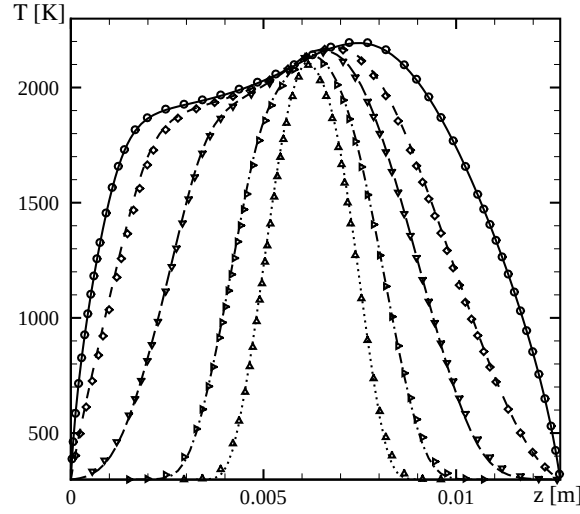


Figure 10: 1D counterflow flame in physical space. Full-calc vs Interactive Flamelet simulations. $\Phi=2.464$. Temperature distribution for different strain rates defined by χ_{st} . Symbols: full-calc simulations. Lines: Flamelet simulations. Solid line and circle: $\chi_{st}=8 \text{ s}^{-1}$. Dashed line and diamond: $\chi_{st}=15 \text{ s}^{-1}$. Long-dashed line and gradient: $\chi_{st}=25 \text{ s}^{-1}$. Dashed-dot line and right triangle: $\chi_{st}=50 \text{ s}^{-1}$. Dotted line and triangle: $\chi_{st}=100 \text{ s}^{-1}$.

species mass fractions are limited to the mixture fraction range where $\chi(Z)$ is available.

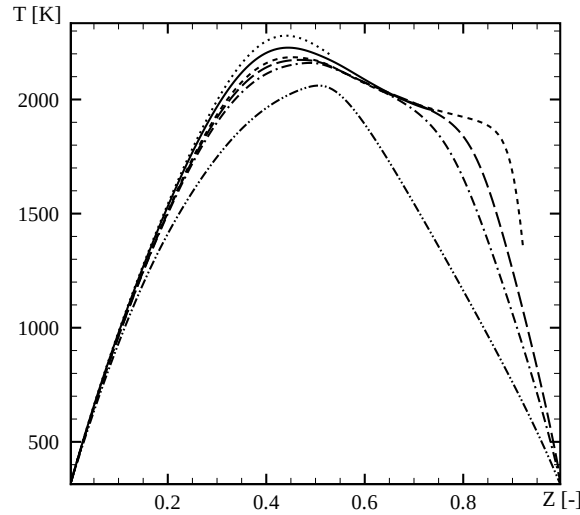


Figure 11: 2D co-flow flame. Temperature profiles obtained from the solution of flamelet equations using χ profiles. Dashed-dot-dot line: $z = 0 \text{ cm}$. Dashed-dot line: $z = 0.5 \text{ cm}$. Long-dashed line: $z = 1 \text{ cm}$. Dashed line: $z = 1.5 \text{ cm}$. Solid line: $z = 2 \text{ cm}$. Dotted line: $z = 3 \text{ cm}$.

In Fig. 12, *Full-cal* vs *interactive flamelet model* solutions are plotted for this equivalence ratio. Five interactions are performed to reach a converged solution. As can be

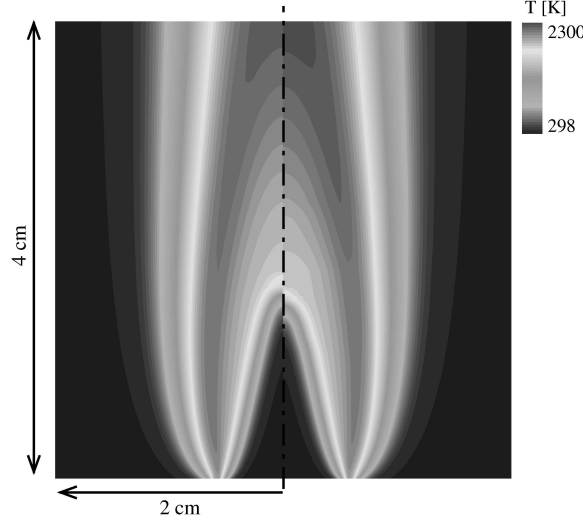


Figure 12: 2D co-flow flame. $\Phi=2.464$. Temperature contours. Full-calc (left) vs Interactive flamelet simulations (right).

seen, with this interactive strategy the under-prediction of the inner flame front is reduced considerably, and the agreement is improved.

Nevertheless, it has been observed that flamelet equation solutions are very sensitive to the scalar dissipation rates profiles used during its integration, and the limitation imposed in the mixture fraction range due to the limited $\chi(Z)$ profile. For instance, no significant improvements are obtained when considering an equivalence ratio of $\Phi=4.107$.

7 CONCLUSIONS

The appropriateness of steady flamelet models in partially premixed flames has been analysed in a laminar co-flow partially premixed methane/air flame considering five equivalence ratios.

An excellent agreement in temperature and major species mass fractions has been obtained for the non-premixed situation (i.e. $\Phi=\infty$), but as the equivalence ratio decreases, the disagreements between detailed and flamelet results increase, specially at the inner flame zone. At the post-flame region, good agreement has been observed.

The disagreements obtained between detailed and flamelet models for low equivalence ratios have been estimated to be caused by: the scalar dissipation rate profile used to compute the flamelet libraries, the strong dependence of the solution of the flamelet equations to the χ_{st} , and the sharp gradients observed in low χ_{st} in rich-fuel zones.

The influence of the scalar dissipation rate profile has been assessed in a counterflow flame. Excellent agreement is obtained when considering an interactive strategy between flame simulation and flamelet equations integration using in-situ χ profiles.

The interactive strategy also tends to improve the flamelet model results in the 2D

axisymmetric co-flow flame, but they remain very sensitive to the evaluated χ field, and to the integration of the flamelet equations for the whole mixture fraction range when no information about the scalar dissipation rate profile is available.

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REFERENCES

- [1] N. Peters. *Turbulent combustion*. Cambridge University Press, 2000.
- [2] R.S. Barlow and J.H. Frank. Effects on Turbulence on Species Mass Fractions in Methane/Air Jet Flames. In *Proceedings of the Twenty-Seventh Symposium (International) on Combustion*, pages 1087–1095, 1998.
- [3] P.J. Coelho, O.J. Teerling, and D. Roekaerts. Spectral radiative effects and turbulence/radiation interaction in a non-luminous turbulent jet diffusion flame. *Combustion and Flame*, 133:75–91, 2003.
- [4] M. Sheikhi, T. Drozda, P. Givi, F. Jaber, and S. Pope. In *Proceedings of the Twenty-Third Symposium (International) on Combustion*, pages 549–556, 2005.
- [5] K. Claramunt. *Numerical Simulation of Non-premixed Laminar and Turbulent Flames by means of Flamelet Modelling Approaches*. PhD thesis, Universitat Politècnica de Catalunya, 2005.
- [6] K. Claramunt, R. Cònsul, D. Carbonell, and C.D. Pérez-Segarra. Analysis of the laminar flamelet concept for non-premixed laminar flames. Application to the numerical simulation of a confined co-flow methane/air flame, *In Press. Combustion and Flame*, 2005.
- [7] C.S. McEnally and L.D. Pfefferle. Experimental study of nonfuel hydrocarbon concentrations in coflowing partially premixed methane/air flames. *Combustion and Flame*, 118:619–632, 1999.
- [8] B.A. Bennett, C.S. McEnally, L.D. Pfefferle, and M.D. Smooke. Computational and experimental study of axisymmetric coflow partially premixed methane/air flames. *Combustion and Flame*, 123:522–546, 2000.
- [9] R. Cònsul, C.D. Pérez-Segarra, K. Claramunt, J. Cadafalch, and A. Oliva. Detailed numerical simulation of laminar flames by a parallel multiblock algorithm using loosely coupled computers. *Combustion Theory and Modelling*, 7(3):525–544, 2003.

- [10] K. Claramunt, R. Cònsul, C.D. Pérez-Segarra, and A. Oliva. Multidimensional mathematical modeling and numerical investigation of co-flow partially premixed methane/air laminar flames. *Combustion and Flame*, 137:444–457, 2004.
- [11] R.J. Kee, F.M. Rupley, and J.A. Miller. The Chemkin Thermodynamic Database. Technical report, Sandia National Laboratories, 1987.
- [12] M.D. Smooke, C.S. McEnally, and L.D. Pfefferle. Computational and experimental study of soot formation in a coflow, laminar diffusion flame. *Combustion and Flame*, 117:117–139, 1999.
- [13] N. Peters. Laminar diffusion flamelet models in non-premixed turbulent combustion. *Progress in Energy and Combustion Science*, 10:319–339, 1984.
- [14] J.S. Kim and F.A. Williams. Structures of flow and mixture-fraction fields for counterflow diffusion flames with small stoichiometric mixture fractions. *Journal of Computational Physics*, 53:1551–1566, 1993.
- [15] S. V. Patankar. *Numerical heat transfer and fluid flow*. Hemisphere Publishing Corporation, 1980.
- [16] J. Cadafalch, C.D. Pérez-Segarra, R. Cònsul, and A. Oliva. Verification of finite volume computations on steady state fluid flow and heat transfer. *Journal of Fluids Engineering*, 124:11–21, 2002.