A transported thickening factor strategy for multi-regime combustion

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Abstract
This paper investigates the necessity for a spatial and temporal relaxation of the thickened flame model (TFM) in multi-regime combustion applications. Two definitions of flame index are employed as combustion regime sensor for both the standard model and in a dynamic relaxation strategy. The effectiveness of all modeling approaches is assessed on a Large Eddy Simulation (LES) of a two-dimensional triple flame, which is developed within a shear layer comprising fuel and oxidizer.

Introduction
Numerical modeling of multi-regime flames is inherently complex, as they may simultaneously exhibit different combustion regimes locally. While offering lower relative computational cost, tabulated chemistry approaches are difficult to apply in multi-regime scenarios, due to the complexity of generating a representative tabulation. In contrast, species transport approaches such as the thickened flame model, although computationally expensive, require fewer *a priori* assumptions, and therefore are still one of the main strategies for multi-regime combustion modeling. TFM [1] is based on the artificial thickening of the flame front to enable its resolution on a numerical LES grid, while retaining the original flame speed. This concept is applicable to premixed flames, which exhibit a well-defined flame front and speed. However, this approach cannot be applied to high Damkhöler non-premixed flames [2], as the chemical source term is not the limiting factor for the consumption speed. The current state of the art for multi-regime modeling with TFM involves the application of the dynamically thickened flame model (DTFM) [3] on the premixed zones of the flame, thanks to a regime identifier [4,5]. A subsequent switch to a finite-rate closure no-modelling strategy on the non-premixed areas is then applied. Diffusive flames, in fact, are already thickened on a LES grid, due to the non-resolved stretch. This strategy may result in a spatially discontinuous definition of the thickening factor F when neighbouring cells have different combustion regimes [6]. Furthermore, an abrupt change of the thickening factor between subsequent time steps may lead to localised numerical quenching. The reaction rates are instantaneously divided by F, while time is needed by the flame to recover its thickness. In industrial applications with low-Mach solvers these issues may be significant, as coarser grids and high values of F with larger time step, are often used.

This work aims to study a relaxation in time and space of the thickening strategy via a transport equation of F, coupled with a flame index based on the gradients of mixture fraction and progress variable.

Methodology

Flame index definition

In the standard DTFM the switch between the premixed and non-premixed treatment of the flame is done thanks to a flame regime sensor, usually a scalar. In this paper, two possible definitions of the so-called flame index concept are investigated. The first is the normalized Takeno Flame Index (FI) [7], which is based on the dot product of the fuel and the oxidizer. Since this definition doesn't explicitly account for the mixing process, expressions which include the mixture fraction Z have been introduced in the literature. For this work, the intermediate expression of the Premixedness Index (PMI) proposed by Illana et al. [8] has been used. This flame index is based on the alignment of the direction cosines of the gradients of Z and a reaction progress variable c. If the flame is locally premixed, the gradients will be perpendicular ($PMI = 1$), while in a non-premixed or weakly stratified region, the dot product will be close to 1 ($PMI = 0$).

$$PMI = 1 - \left| \frac{\nabla c}{\|\nabla c\|} \cdot \frac{\nabla Z}{\|\nabla Z\|} \right| \tag{1}$$

Since PMI has a continuous definition, a threshold value is selected to allow a certain degree of mixture stratification.

Thickening relaxation strategy

The relaxation strategy of the TFM takes its cues by the transport equation for the DTFM flame sensor Ω, introduced by Jaravel [9]. The author aim is to regularize and extend the application of F toward the preheat zone of the flame, avoiding numerical issues that arise from the sharp gradients at the flame base. Otherwise, in this work the objective is to smooth the sharp transition between premixed and non-premixed cells, through convective transport of the thickening factor. The application of F in the premixed zones is achieved directly thanks to a source production term, while a sink term is responsible for the gradual switch to the no-model approach, where $F = 1$. Furthermore, since the molecular diffusivity is alone not sufficient to correctly widen the thickened area toward the preheat zone, the actual transported scalar is multiplied by a factor n. Subsequently, the local value obtained is clipped to the minimum between F and F_{max}, given by the desired points needed to resolve the flame front. The following set of equations therefore depicts this dynamic relaxation strategy just outlined.

$$F_{max} = \frac{N}{\delta_T} \Delta x \;\rightarrow\; F_{corr} = nF_{max} \tag{2}$$

$$\frac{\partial F}{\partial t} + \frac{\partial \rho U F}{\partial x_i} = \nabla \cdot (\rho D_F \nabla F) + S_F \tag{3}$$

$$S_F = \begin{cases} \frac{F_{corr} - F}{\tau_0} \dot{R}_k + \frac{1 - F}{\tau_1} & if\ flame\ index = premixed \\ \frac{1 - F}{\tau_1} & if\ flame\ index = non\ premixed \end{cases} \tag{4}$$

Where N is the number of points desired in the flame front, δ_T the flame thermal thickness, Δx a one-dimensional mesh size. S_F is the global source term of the transport equation and $\dot{R_k}$ the kinetic rate of a reaction o k of choice. In addition, τ_0,τ_1 are constants that control the magnitude of the production and destruction of F. Finally, to ensure that the turbulent diffusivity contribution in the flame front is correctly switched off, as in the original DTFM formulation, a hyperbolic tangent sensor Ω is introduced.

$$\Omega = \tanh\left(\frac{F}{F_{trsh}}\right) \tag{5}$$

Where F_{trsh} is a threshold value.

Computational domain and numerical setup

Both the relaxation strategy and the standard DTFM model are investigated with LES of a 2D triple flame, developed in a shear layer of H2 and air at 3 bar. The computational domain is a 100mm x 20mm rectangle with fuel and oxidizer inlets separated by the major axis of symmetry. The boundary conditions for hydrogen and air are 12 m/s at 293 K and 3 m/s at 450 K, respectively. To validate the model, a flame-resolved reference case is discretized on a numerical grid of 40 million uniform quadrilateral elements. The Navier-Stokes equations are solved using the density-based explicit solver AVBP [10] with third-order accurate in time and space schemes. In addition, as the thickened flame model comparisons are performed on the pressure-based implicit solver ANSYS FLUENT 2022R2, a sampling of the inlet velocity profiles of the reference run has been performed, to be used as boundary conditions in the subsequent calculations. A coarser mesh of 3e-4m size is used for all LES simulations of TFM, resulting in a maximum value of $F \approx 22$ in the triple point, for a desired target of 7 points. This high value of the thickening factor is desired to exacerbate the numerical problems arising from an impulsive application of F and to represent coarser grids employed in industrial applications. Nevertheless, a separate run of the DTFM on a finer grid ($F \approx 7$) has been performed, to ensure that results are not overly dependent on the thickening factor value. Table 1 summarizes the numerical grid details.

Table 1. Grid size and relative flame thickness in the triple point.

	Reference	Coarse grid	Fine grid
$\Delta x\ [m]$	$7e-6$	$3e-4$	$1e-4$
$\delta_{T,trp}\ [m]$	$9.4e-5$	$9.4e-5$	$9.4e-5$
N_{trp}	≈ 134	≈ 0.32	≈ 0.96

Second order accurate schemes are chosen for both space and time, with a time step of 5e-6s. Mass diffusivity is accounted for through the mixture average approach, with the inclusion of Soret effects. Due to recent discussions on the direct use of the Bilger mixture fraction to evaluate the local δ_T [11], it has been decided to also investigate the F transport strategy and PMI, with the addition of a passive scalar. Furthermore, all TFM simulations are performed with the efficiency function set to 1. The authors acknowledge that this may not be correct and that it's also necessary to recover the real stretch effects on turbulent flames [12]. Nevertheless, this approach has been chosen to isolate the effects of the discontinuous application of F. The TFM simulations are initially run for 3.6e-2 s, with the source terms deactivated up to a height of 30 mm from the inlet. The aim is first to achieve a stable flame configuration and then subsequently investigate the ability of the flame to propagate upstream. A scheme of the domain and flame shape is depicted in Fig. 1. For the flame chemistry, the reaction scheme of Boivin [13] is chosen, comprising of 9 species and 12 reactions. The third body reaction $H + O_2 + M \rightleftarrows HO_2 + M$ is selected for the source term of equation 4, due to its role on the heat release of the $H2$-air triple flame and its maximum towards the preheat zone [14]. For these same reasons, the definition of the progress variable is $c = Y_{H2O} + Y_{HO2}$.

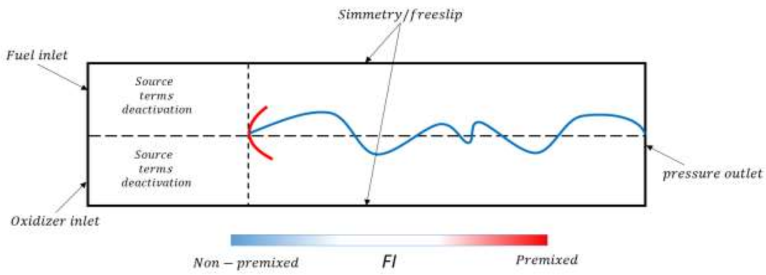

Figure 1. Schematic visualization of the computational domain and boundary conditions, with an added sketch of the expected flame shape.

Results

A 3 mm wide moving window was created based on the stoichiometric mixture fraction and maximum release location, to identify the triple point shift during the simulations. Fig. 2 clearly shows how the standard model experiences detachment for both flame indices, and for the finer grid. The impulsive discontinuous application of F does not allow the flame to anchor at the edge of the zone where the reactions are deactivated, resulting in advection from the domain.

Moving to the F transport simulations, identified as T-TFM, both flame indices capture the ability of the flame to propagate upstream. PMI is helpful in recovering the flame propagation, which is slightly improved using the passive scalar (T-TFM-

PMI-PS). Selecting the right flame index definition is more critical than in the standard DTFM, since the thickening production source is activated whenever the premixed regime is identified. Overestimation of these zones will result in unwanted thickening, as F is advected downstream. On the other hand, underestimation may lead to under-resolution of the flame front, especially in the lean branch of the triple flame.

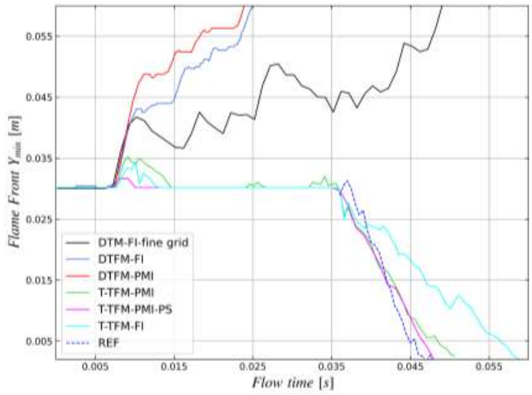

Figure 2. Minimum position of the triple flame front Y_{min} during the flame stabilization and propagation phases.

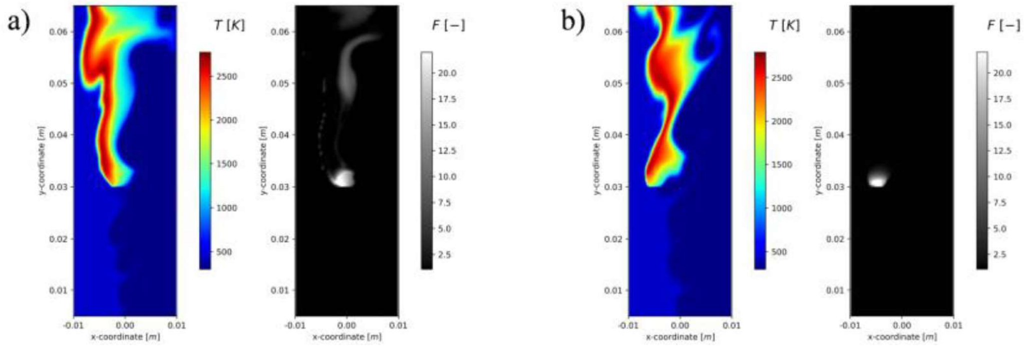

Figure 3. Contours of temperature and thickening factor for the T-TFM during the stabilization phase for FI (a) and PMI (b), respectively.

Figs. 3a and 3b show the effect of the different flame indices on the T-TFM. The PMI (see Fig 3b) results in a much smaller thickened area, localized in the triple flame leading edge. In Fig. 3a FI, on the other hand, produces thickening trails downstream of the front.

Conclusions

The purpose of this study is to demonstrate the need for spatial and temporal relaxation in the application of the thickened flame model in multi-regime flames, and to develop a strategy based on the transport of the thickening factor. In addition, two definitions of the flame index have been studied as a sensor for switching between the thickened model and the no-model approach. The results show that relaxing the thickening factor application helps in recovering the correct behavior of the reference flame.

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