

Validation of a virtual chemistry combustion model in a fully technically premixed burner

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Abstract

In this paper a technically fully premixed burner fed with pure hydrogen is investigated through two different versions of the Thickened Flame Model. The main difference lies in the chemistry treatment: while the first is based on a detailed chemistry, the second embeds an in-house developed virtual chemistry mechanism. The models are validated against detailed flame imaging using the OH* radical to detect the flame front morphology and position. The results got through the virtual chemistry are in excellent agreement with the detailed mechanism allowing a strong reduction of the computational effort.

Introduction

Reactive CFD simulations represent nowadays a pillar in the design of modern GT combustors. Moreover, the most accurate combustion models like the Thickened Flame Model (TFM), based on the resolution of primitive variables (so-called species transport), have proven their reliability in capturing the most relevant aspects characterizing the performance of a combustion system, such as flame morphology, emissions and thermo-acoustic instabilities [1-2]. The main drawback of this approach is represented by the high computational cost driven by the need to properly discretize the flame front through extremely fine grids. This requirement is particularly severe when the system is operated at elevated pressure and aggressive fuels like hydrogen are burnt since the flame front can reach a thermal thickness of few micron. A significant computational time reduction can be reached adopting skeletal mechanisms avoiding the transport of those species that are not essential even if this doesn't fully resolve the issue when industrial geometries are simulated. Another option is the employment of global chemical schemes with a single or two steps, as per the original TFM formulation. Unfortunately, such approach lacks generality and even the use of optimized chemical mechanisms must be accurately verified. The virtual chemistry methodology [3] can combine the accuracy provided by a detailed/skeletal chemistry set with the extremely low wall-clock time of a global mechanism. This result can be achieved through customized algorithms able to extend their applicability to a wide range of operating conditions without compromising the accuracy of those parameters that are essential to make the TFM predictive. In this work, a virtual chemistry for pure hydrogen combustion is derived

and embedded within the TFM model. Its performance are measured against a skeletal mechanism and, more importantly, against the experimental measurements characterizing a technically fully premixed industrial burner.

Test Rig Description

The experiments are executed along an atmospheric rig with optical access for detailed imaging (Figure 1). The optical access is ensured by windows on the external casing and quartz windows on the flame tube allowing the visualisation of the primary zone. A Phantom VEO-640L camera is coupled with an IRO-x intensifier. A Nikon UV 85 mm lens with a bandpass filter set at 310 ± 2 nm is employed for the measure of OH* used as heat release rate marker. The sampling frequency is 400 Hz while the gate is equal to 0.4 ms. The time-averaged flame position is retrieved through 1000 samplings. Two independent air lines are installed: the first providing the combustion air and the cooling of the metallic pillars sustaining the quartz through internal passages, the second cooling the quartz and the metallic pillars by external convection.

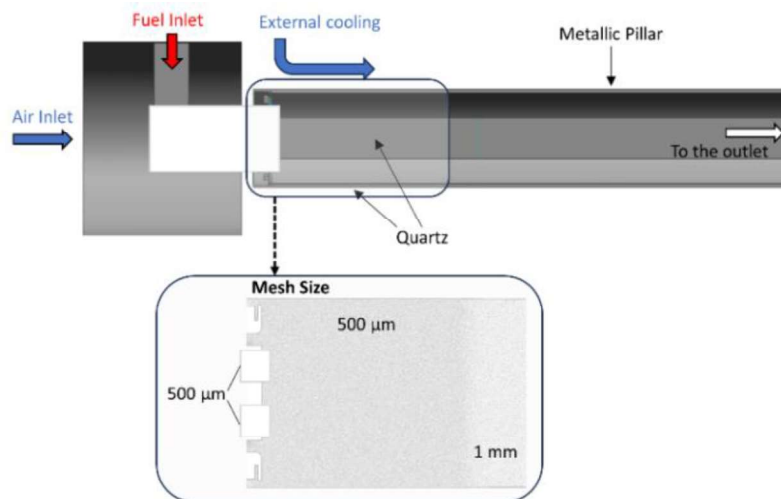


Figure 1. Combustion test rig (top) and computational mesh in the primary zone (bottom). Design details of the premixer are omitted as well as the external casing.

The investigated burner is technically fully premixed: the fuel is injected through several jets in cross flow inside the premixing channels ensuring an enhanced mixing with air. In the investigated test condition, pure hydrogen is used. Since the mass flow rates are controlled during the test, the corresponding values are used in the CFD model as boundary conditions. The flame temperature and the pressure drop at which the rig is operated correspond to the values of the NOVA LT16® at ISO base load conditions [4]. Regarding the thermal boundary condition at the combustor walls, an external heat transfer coefficient is coupled with the measured temperature.

TFM: Reference vs Virtual Chemistry Formulation

The two combustion models are indeed different in their mathematical formulation, even if both are based on the TFM. The reference model employs a Flame Index (FI ,

Eq. 1), to switch from the TFM for the premixed regime to a finite-rate closure for the diffusive one, as explain in [1].

$$FI = \frac{\nabla Y_{H_2} \cdot \nabla Y_{O_2}}{|\nabla Y_{H_2} \cdot \nabla Y_{O_2}|} \quad (1)$$

Eq. 2, representing the transport equation of the generic scalar ϕ , is modified as follows: when the FI is negative, the efficiency function E and the thickening factor F are imposed equal to 1, leading to the finite-rate closure. Conversely, for positive FI , they are calculated according to the original TFM formulation [5].

$$\frac{\partial \bar{\rho} \tilde{\phi}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{\rho} (EFD + (1 - \Omega)D_t) \frac{\partial \tilde{\phi}}{\partial x_j} \right) + \frac{E}{F} \dot{\omega}(\tilde{\phi}) \quad (2)$$

The thickening factor F leverages the flame sensor Ω to apply the artificial thickening only inside the flame front:

$$F = \Omega(F_{max} - 1) + 1 \quad (3)$$

with $F_{max} = \Delta x N / LFT(\Phi)$. The adopted mesh resolution inside the primary zone, Δx , (Figure 1) can limit F_{max} to values close to around 6, having chosen a number of points $N = 8$ inside the flame front thickness ($LFT(\Phi)$). The reference reaction for the calculation of the flame sensor Ω selected within the skeletal mechanism of Boivin et al. [6] is $H_2 + OH \rightarrow H_2O + H$. Despite the differentiation between the premixed and the diffusive regime proposed by the reference combustion model, the low fuel unmixedness at the flame front makes the latter practically negligible: Figure 2, shows that the FI is always positive inside the flame front location identified by the contour plot of Ω . Basing on this finding, the VC model is developed without any combustion regime differentiation.

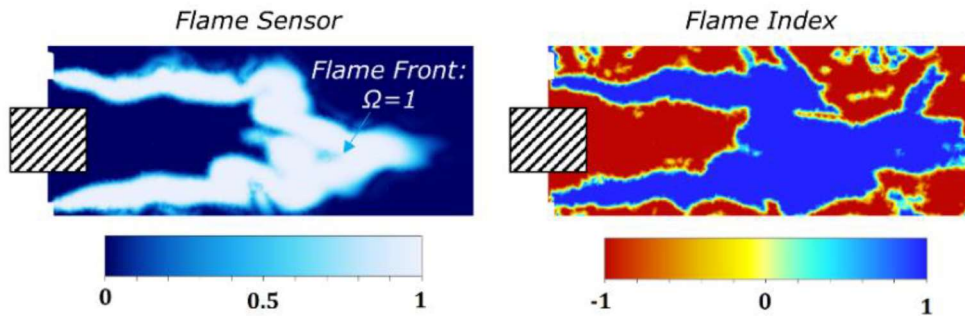
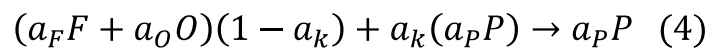


Figure 2. Flame Sensor (left) and Flame Index (right) proving that the combustion regime is dominantly premixed.

The virtual chemistry, originally introduced by Callier et al. [3], is based in this study on a single-step irreversible reaction:



where O is the oxidiser, F the fuel, P the generic product and a is the stoichiometric mass coefficient. a_k controls the amount of products included in the reactants. The introduction of the products into the reactants prevents the autoignition enabling the correct laminar flame thickness prediction. Every species in the reaction is a virtual

entity and must be based according to the specific conditions that the mechanism aims to reproduce. The information needed for the virtual species definition are the Schmidt number, the *NASA7* polynomial coefficients, and the molecular weight W . Finally, the Prandtl number and the laminar viscosity μ have to be determined as overall mixture properties, not depending on the mixture composition. Indeed, the Pr is constant, while the laminar viscosity is defined as a polynomial function of the temperature. The forward reaction rate is subjected to optimisation: all the parameters that define the Arrhenius expression as well as all the other mentioned quantities are subjected to an optimization process. These control variables are the parameters calibrated to reproduce the performance of a detailed reaction mechanism in the specific thermodynamic conditions of interest. The algorithm maximises a fitness function that is evaluated by means of Cantera as difference between a reference solution based on the detailed mechanism and the virtual mechanism prediction. This calibration is achieved through a genetic algorithm that is schematically reported in Figure 3.

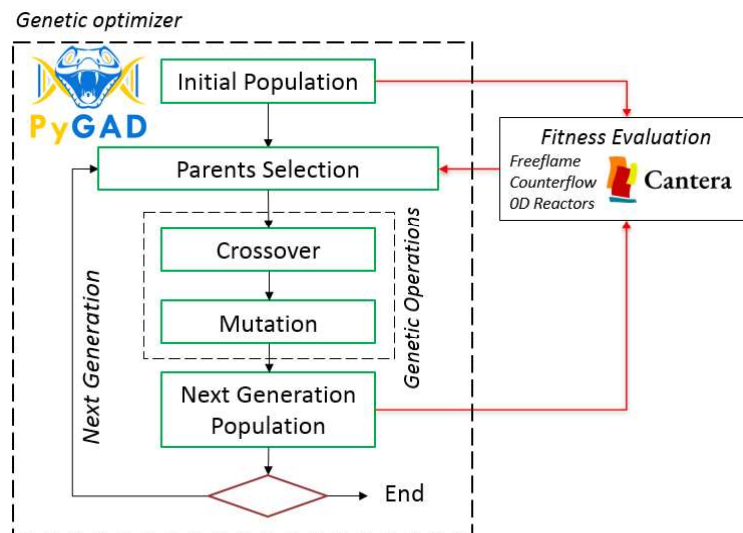


Figure 3. Genetic optimizer workflow for the calculation of the virtual chemistry.

Results and Discussion

Flame morphology

The numerical *HRR* is used to retrieve the predicted flame shape and position and Figure 4 reports the comparison with the experimental OH^* map: the numerical fields are integrated in orthogonal direction to calculate the Line of Sight (LoS) and make them comparable with the chemiluminescence. The dashed horizontal line helps to identify the experimental flame length and highlight the differences with the numerical results. It can be seen that the reference TFM, based on the skeletal mechanism, is affected by a limited difference in terms of flame length. The small difference that can be detected is the rate of decay between the OH^* and the *HRR* intensity: moving from the flame front, the intensity of OH^* drops in few millimetres while a smoother decay is present for the *HRR* in the reference numerical case. The same drawback is present in an even more significant way for the VC simulation:

here a more intense signal is present downstream the main heat release region. Such defect is due to a small overprediction of the heat release on the product side using the virtual single step mechanism. Despite that, the flame morphology seems to be reproduced quite accurately also with this approach.

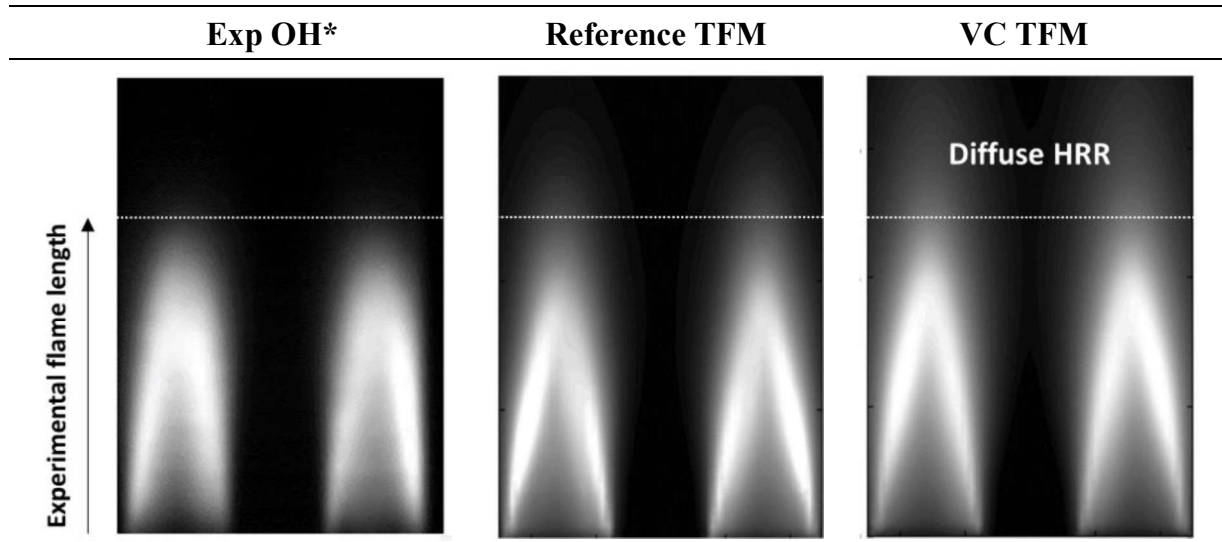


Figure 4. Experimental time-averaged OH^* LoS (left), time-averaged HRR LoS for reference *TFM* (centre) and the *VC* model (right). Colorbar: 0-black, maximum-white.

Another interesting comparison between the reference *TFM* and the *VC* approach can be done in terms of fuel mixing: the mixture fraction is calculated according to Bilger's formulation in the former while it is transported through a user defined scalar in the latter. In the reference case, the laminar flame properties, tabulated as a function of the mixture fraction, are influenced by H_2 preferential diffusion. This is not totally correct since the tabulated laminar properties shouldn't be influenced by the strain rate. Conversely, when the mixture fraction is transported, the influence of the H_2 preferential diffusion on the laminar properties is neglected making the approach more consistent. The corresponding differences can be observed in Figure 5 reporting the mixture fraction fields on a longitudinal plane for one of the several burner-tubers with overlapped the iso-line of the *HRR* at 90%. It can be seen that the reference *TFM* is characterized by a slightly lower mixture fraction within the flame front while minor differences are observed elsewhere. This is demonstrated also by the contour plots of the mixture fraction at the tuber exit and by the corresponding mixture fraction radial profiles: the maximum difference among them falls at about 70% of the radial span and is less than 0.5%.

Regarding the computational cost, the *VC* allows a drastic reduction of the delivery time that can be quantified in about -63% compared to the reference *TFM*. This saving can be significantly higher when such approach is applied to even more complicated chemistry sets, like for example natural gas or blends between different fuels.

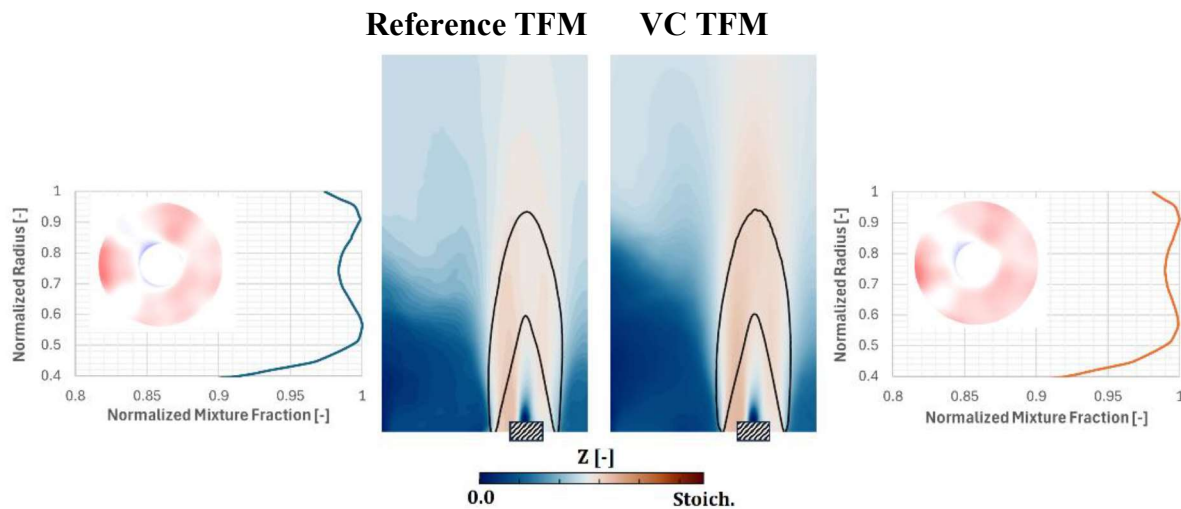


Figure 5. Mean mixture fraction from the Reference TFM (left) and the VC case (right). The graphs report the profile at the burner exit.

Conclusion

In this paper, a virtual mechanism for pure hydrogen combustion has been derived and validated against detailed experimental flame imaging and a skeletal mechanism. The comparison with the test data shows a good prediction of the flame morphology while a not relevant difference can be appreciated against the results obtained with the skeletal mechanism. The discrepancy in terms of fuel mixing between the two models can be related only to different numerical strategies. As next step, the virtual chemistry approach will be validated against data for hydrogen-natural gas blends.

Nomenclature

CFD	Computational Fluid Dynamics	HRR	Heat Release Rate
CPU	Central Processing Unit	LoS	Line of Sight
FI	Flame Index	TFM	Thickened Flame Model
GT	Gas Turbine	VC	Virtual Chemistry

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