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# Evaluation of the approximated diffusion flamelet concept using fuels with different chemical complexity

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ABSTRACT

The ability of flamelet models to reproduce turbulent combustion in devices such as diesel engines or gas turbines has enhanced the usage of these approaches in Computational Fluid Dynamics (CFD) simulations. The models based on turbulent look-up tables generated from counterflow laminar diffusion flames (DF model) permit drastic reduction of the computational cost of the CFD calculation. Nevertheless, for complex molecular fuels, such as n-heptane, the oxidation process involves hundreds of species and the calculation of the transport equations together with the ODE system that models the chemical kinetics for the DF solution becomes unaffordable for industrial devices where hundreds of flamelets are required. In this context, new hypotheses have to be introduced in order to reduce the computational cost maintaining the coherence of the combustion process. Recently, a new model known as Approximated Diffusion Flamelet (ADF) has been proposed with the aim of solving the turbulent combustion for complex fuels in a reduced time. However, the validity of this model is still an open question and has to be verified in order to justify subsequent CFD calculations. This work assesses the ADF model and its ability to reproduce accurately the combustion process and its main parameters for three fuels with different chemical complexity and boundary conditions by its comparison with the DF model. Results show that although some discrepancies arise, the ADF model has the ability to correctly describe the ignition delay and the combustion structure in the auto-ignition zone that is the most relevant one for industrial processes.



## 1. Introduction

During recent decades, the development of industrial combustion systems in terms of efficiency and pollutant emissions has encouraged the analysis of these systems by means of numerical simulations. In this context, the Computational Fluid Dynamics (CFD) is a powerful technique that allows the researcher to obtain very valuable knowledge of the turbulent combustion. Nevertheless, the models used for turbulent combustion are based on a set of hypotheses whose suitability depends on the combustion regime [1,2]. Together with the model hypotheses, the computational cost is another important factor that determines the model capabilities for practical applications.

Among the different models that can be found in the literature, the flamelet model is reported to be one of the most powerful models for solving the turbulent combustion [3,4]. For non-premixed turbulent combustion, the key underlying assumption of this model consists of describing the local structure of the turbulent flame by an ensemble of igniting and

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extinguishing laminar diffusion flames called flamelets. Thus, this assumption requires the chemistry to be much faster than physical processes such as the mixing process, corresponding to large Damköhler numbers. However, despite seeming very restrictive, this is usually a suitable description for non-premixed turbulent combustion in industrial devices and means that combustion takes place in a very thin layer in which the flamelets are embedded [2].

For non-premixed combustion systems, these flamelets usually follow a counterflow diffusion flame (DF) configuration. With the proper mathematical operations and simplifications, the flamelet can be described by a simplified 1D structure in the mixture fraction space [5]. The transport equations for temperature and species describing the flamelet evolution retain the transient, mixing and source terms. Mixing terms include the scalar dissipation rate ($\chi$), which controls the diffusion rate of species in the mixture fraction space and depends on the strain rate ($a$) imposed by the flow [2]. Source terms for species transport equations are particularly critical since they are calculated by solving the stiff non-linear ODE system that models the chemical kinetics for each mixture fraction at each time step. As the fuel increases in molecular complexity, its oxidation involves hundreds or even thousands of species and reactions. Therefore, the number of transport equations to be solved and the number of equations of the ODE system that models the chemical kinetics accordingly increase.

In recent decades, the flamelet model has been implemented following different approaches and it has been extensively applied especially in the field of the design and analysis of internal combustion engines.

In the representative interactive flamelet (RIF) model approach and its variants, the flamelet or set of flamelets required to reproduce the characteristics of the turbulent combustion is solved during the CFD computation [6,7]. However, despite the interesting results reported using this model, for instance in the field of diesel engines [8], this interactive coupling presents some important drawbacks related to the computational cost, i.e. the on-the-fly resolution of the set of flamelets, especially for fuels with high molecular complexity. In those cases, only a few flamelets are considered and the modeling of the turbulence-chemistry interaction (TCI) is partially lost [9].

In the approaches known as Flame Prolongation of Intrinsic Low-Dimensional Manifold (FPI), Flamelet Generated Manifold (FGM) and their respective variants, the set of flamelets required to reproduce the characteristics of the turbulent combustion is pre-calculated and, consequently, decoupled from the CFD computation. Results are stored in a look-up database in terms of thermochemical parameters [10,11,12]. These models are gaining attention since once the database is generated, the time required by the CFD computation for solving a given turbulent combustion problem is very limited. However, for fuels with high molecular complexity, the generation of the flamelet database is still too expensive in terms of computational cost and sometimes becomes unaffordable when the boundary conditions span over wide ranges of values and, consequently, a great number of flamelets have to be computed.

Recently, the Approximated Diffusion Flamelet (ADF) concept was developed with the aim of decreasing the computational effort required to generate the flamelet database while keeping complex chemistry [13]. The ADF concept is based on solving only the 1D flamelet transport equation for the progress variable, which is a linear combination of selected species that accounts for the transient evolution of the flamelet, in the mixture fraction space. Additionally, it decouples the mixing and the source terms of this transport equation. The chemical source term of the progress variable is pre-calculated by solving the corresponding ODE system related to the chemical kinetics. For this purpose, the temporal evolution of a set of homogeneous reactors (HRs) for different mixture fractions is solved storing the results in a look-up table used when solving the progress variable transport equation [14]. It is important to note that since chemistry is decoupled from the diffusion processes the ADF model permits the modeling of complex chemistry in completely acceptable amounts of time.

The considerable reduction of calculation time gained with these simplifications allow the application of this flamelet model when the boundary conditions encompass a great variety of values, with flamelets belonging to the whole range of strain rates, while managing complex chemistry. These capabilities are particularly important in complex problems such as diesel engines where so many processes interact and the proper modeling of the phenomena is critical for describing the turbulent structure of the flame as well as predicting pollutant emissions.

Finally, these required modeling capabilities argue for the use of comprehensive mechanisms instead of reduced mechanisms that, certainly, would permit the application of the DF model but with losses that are not admissible for the previous modeling objectives.

In this context, the analysis of the flamelet steady-state conditions and their transient temporal evolution for both DF and ADF models are evaluated in the present investigation.

In a previous published study, the validity of the ADF assumptions was preliminarily investigated by directly comparing with the DF model keeping the same boundary conditions [13]. This analysis focused on evaluating the differences between DF and ADF related to the ignition delay, the initial ignition propagation across the flamelet and the steady-state reacting equilibrium conditions. In this research, despite the fact that noticeable discrepancies were clearly identified in all of the three characteristic flamelets investigated, the observed differences were considered acceptable. Nevertheless, the information reported was not sufficient to understand the extent of the differences between ADF and DF and/or how to decrease them since only very few flamelets (few strain rates) were considered [13]. The ADF concept was integrated into two similar flamelet combustion models, known as ADF-PCM (ADF Presumed Conditional Moment) and ADF-PCM$\chi$ (ADF-PCM with probability density function in $\chi_{st}$), and for both models the flamelet database was generated using this simplification.

These models have been applied during the last years to different problems such as lifted methane flames in a vitiated coflow [14], diesel-like sprays [15,16], diesel engines [17] and furnaces [18] and, in all cases, results were very promising. However, the validity of the ADF concept is still an open question nowadays under evaluation and more research effort is required.