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Citation for published version (APA):

Abtahizadeh, E., Bastiaans, R., de Goey, P., & van Oijen, J. (2015). Extension of the FGM technique for autoignition and preferential diffusion effects. In *5th International Workshop on Model Reduction in Reaction Flows (IWMRRF)*, 28 June - 1 July 2015, Spreewald, Germany

Document status and date:

Published: 28/06/2015

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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Extension of the FGM technique for autoignition and preferential diffusion effects

Ebrahim Abtahizadeh, Rob Bastiaans, Philip de Goey and Jeroen van Oijen
Eindhoven University of Technology, Eindhoven, the Netherlands

Abstract—Flamelet Generated Manifolds (FGM) has been extended to account for preferential diffusion effects and autoignition. Such development is made in order to study stabilization mechanism of turbulent lifted CH₄/H₂ flames of the Delft JHC burner. In this burner, methane based fuel has been enriched from 0 to 25% of H₂. The main stabilization mechanism of these turbulent flames is autoignition based on the formation of ignition kernels which is very challenging to model. Addition of hydrogen makes the modeling even more challenging due to preferential diffusion effects. The proposed FGM model is implemented in DNS of unsteady mixing layer and LES of lifted jet flames. It is revealed that the proposed model has the capability to accurately predict main features of CH₄/H₂ turbulent flames.

INTRODUCTION

Combustion devices are often optimized in order to increase thermal efficiency and reduce pollutant emissions such as carbon monoxide (CO) and nitrogen oxides (NO_x). For these purposes, strategies have been developed which deploy autoignition of a fuel jet emerging in a preheated and diluted oxidizer stream. This is often called Mild combustion which usually yields flameless oxidation [1]. In the laboratory scale Mild burners (JHC burners), stabilization of reaction zone is very often occurred by autoignition. This requires sophisticated models which are able to predict complex autoignition events. Since these autoignition events are typically initiated at very small mixture fractions due to an intense dilution of oxidizer stream, turbulent structures in the fuel stream can hardly intrude these ignition events. This induces that influence of molecular diffusion on autoignition is comparable to that of turbulence transport (eddy viscosity). In this condition, addition of H₂ to fuel makes molecular diffusion and preferential diffusion effects increasingly important.

In this study, a novel flamelet model so-called “Igniting Mixing Layer (IML) flamelet is proposed in order to predict preferential diffusion effects in autoigniting flames. IML flamelets are basically similar to the commonly used one-dimensional Igniting Counter-Flow diffusion flamelets (ICF flamelets) with a notable distinction in the initial condition. In ICF flamelets, a steady-state molecular mixing field is assumed between the fuel and oxidizer stream with frozen chemistry ($\dot{\omega} = 0$). This situation implies that a steady-state mixing field is reached before any chemical reaction takes place. This assumption is mainly valid if the time scale of mixing is much shorter than the chemical time scales. However, such an assumption might lead to unrealistic

predictions if molecular diffusion terms are comparable in size to the chemical source terms (for example in CH₄/H₂ mixtures). In this case, molecular diffusion has a large influence on autoignition time scales.

In IML flamelets, in contrast to ICF flamelets, fuel and oxidizer streams are initially unmixed. This unmixed profile permits us to include preferential diffusion effects in the pre-ignition stage. In this situation, the initial thermo-chemical properties have a step-function profile in physical space. Their values are equal to the fuel boundary on one side of the domain and equal to the oxidizer boundary at the other side. Due to the steep gradient of mixture fraction at the interface, the scalar dissipation rate $\chi = 2D (\partial Z/\partial x)^2$ is very large at this point. During the molecular mixing process, the scalar dissipation rate decreases and chemical reactions may start at any time during the mixing process. In IML flamelets, the gradient of mixture fraction is not enforced by an inflow momentum (i.e. an applied strain). However, it is governed purely by molecular diffusion. In the absence of an applied strain, the species mass fractions and temperature approach chemical equilibrium for infinite time. More detailed information on IML flamelets can be found in [2-4].

RESULTS

A quantitative comparison of the autoignition time scales between the ICF flamelets and IML flamelets is shown in Fig. 1. ΔT represents the maximum temperature rise in mixture fraction ζ space:

$$\Delta T(t) = \max(T(\zeta, t) - T(\zeta, 0)) \quad (1)$$

The evolution of ΔT is shown in Fig. 1a for IML flamelets which are computed by using transport models $Le_i = 1$ and $Le_i = c_i$. It is observed that the autoignition time scale of the IML flamelets decreases significantly by inclusion of preferential diffusion effects for the Case D25H2. In ICF flamelets, it is possible to use different transport models for the initial profile ($t = 0$ s) and its time evolution ($t > 0$ s). This means that $Le_i = c_i$ transport can be used to generate the initial condition (IC: $Le_i = c_i$) while $Le_i = 1$ is used to compute the evolution from such an initial condition and vice versa. Assuming unity Lewis numbers for the computation of the initial condition leads to linear profiles of Y_i in mixture fraction space, which were used in some previous studies. Fig. 1b shows that the autoignition delay time of the ICF flamelets depends solely on the assumed transport model for initial conditions regardless of the transport model used to compute the flamelets. When $Le_i = c_i$ transport is used to generate the initial condition for the ICF flamelets, using both transport models in the actual

simulation results in the same autoignition time scale. The same trend can be observed when unity Lewis numbers are used to compute the initial condition ($IC:Le_i = 1$).

The most accurate FGM model in which preferential diffusion effects are included both in flamelets and transport equations for controlling variables (FGM C model) is assessed in an unsteady mixing layer where there is interaction of flow field with chemistry. For this purpose, Direct Numerical Simulation (DNS) has been carried out in an unsteady mixing layer configuration. These mixing layers resemble conditions of JHC burners downstream of the fuel injection point where the fuel stream mixes and ignites in the hot coflow stream.

Comparison of the temperature rise ΔT obtained from detailed chemistry and the FGM C model is shown in Fig. 2. In the simulations with the FGM C model, three different manifolds are created and used which are either based on IML flamelets (IML manifold) or ICF flamelets (ICF manifold) with $a = 100 \text{ s}^{-1}$ and 500 s^{-1} . These three manifolds are implemented in the FGM C model to compare predictions of the IML manifold with those of the widely-used ICF manifold. It is observed that the IML methodology can predict autoignition time scales more accurate compared to the ICF method.

Fig. 3 shows instantaneous snapshots of the filtered Y_{OH} which is obtained from the LES of Case D00H2 with FGM.C model. It is observed that at $t = 96 \text{ ms}$, a kernel is formed at approximately $Z = 200 \text{ mm}$. Subsequently, this kernel grows and convects downstream at $t = 100 \text{ ms}$ and $t = 104 \text{ ms}$. This mechanism, which is repeated in subsequent

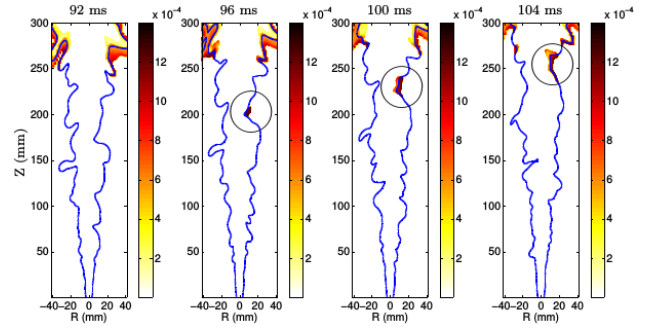


Fig. 3. Computed instantaneous snapshots of Y_{OH} using FGM C model for Case D00H2. Blue lines indicate stoichiometric mixture fraction ζ_{st} .

times, governs stabilization of the flame. At far downstream location, these kernels further grow and ignite the surrounding mixture. It is apparent that this flame is stabilized by autoignition in which ignition kernels are formed, grow and convect downstream corresponding to experimental observations by Artega et al. [5].

CONCLUSIONS

The IML methodology has been introduced to account for preferential diffusion effects and autoignition. First, this method has been assessed and validated in the DNS of unsteady mixing layer. Afterwards, it has been implemented within LES of lifted jet flames. It is revealed that the proposed model has the capability to accurately predict autoignition and stabilization mechanism of CH_4/H_2 turbulent flames.

ACKNOWLEDGMENT

The authors gratefully acknowledge the financial support of the Dutch Technology Foundation (STW) under project No. 10414.

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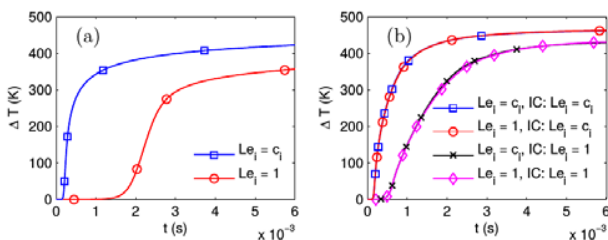


Fig. 1. Temperature rise ΔT computed using detailed chemistry and different transport models for (a) IML flamelets and (b) ICF flamelets. In fig. (b), different transport models have been used to compute the initial condition (IC) for the ICF flamelets. Case D25H2.

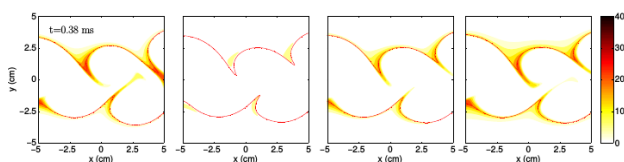


Fig. 2. Comparison of the temperature rise ΔT obtained by DNS of unsteady mixing layers using (from left to right) detailed chemistry, the ICF manifolds ($a = 100 \text{ s}^{-1}$), the ICF manifolds ($a = 500 \text{ s}^{-1}$) and IML manifold. Red lines correspond stoichiometric mixture fraction.