Flamelet Generated Manifolds for Chemistry Representation in Partially-Premixed Flames

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Abstract—In this article it will be assessed how well partially-premixed one-dimensional flames are represented using premixed and non-premixed flamelet-based Flamelet Generated Manifold (FGM) databases. A procedure is introduced which enables combination of both types of FGM databases as a function of local conditions. This allows a more accurate description of detailed chemical kinetics while the considerable speedup of computations enabled by the FGM reduction method is retained.

I. INTRODUCTION

In LES and DNS simulations of turbulent reacting flows the high computational cost associated with the large system of stiff differential equations can become limiting or even prohibitive for moderate and high Reynolds numbers. To reduce the required efforts reduction methods are commonly used. The Flamelet Generated Manifold (FGM) [8], also known as Flamelet Prolongated ILDM (FPI) [6], tabulates thermochemical variables originating from one-dimensional laminar flame structures: flamelets. The FGM reduction method assumes that in (turbulent) three-dimensional flames locally flame structures can be identified which closely resemble flamelets in composition space; the FGM reduction method can therefore be considered to be a combination of classic flamelet- and manifold methods. Any thermochemical variable is now parameterized by a small number of control variables. FGM databases can be generated using either premixed or non-premixed flamelets. The question which is addressed in this work is how well partially-premixed flames are reproduced when premixed and non-premixed flamelet-based FGM databases are used to represent combustion chemistry. Bongers et al. [3] showed that a FGM database based on premixed flamelets can accurately describe the premixed part of partially-premixed counterflow flames. However, in this study the considered range in mixture fraction was limited since the fuel stream had the same composition as a premixed system at the upper flammability limit. Previous work from Fiorina et al. [5] showed that (premixed flamelet-based) FPI databases could not accurately predict combustion parameters in partially-premixed and non-premixed flamelets. A flame-index was introduced to distinguish between premixed and non-premixed combustion and in case of non-premixed combustion the chemical source term for the reaction progress variable was assumed to equal diffusive transport [1]. In other words, no detailed chemistry was used for the non-premixed combustion mode. From these two references it can be concluded that a premixed flamelet-based FGM database can be used to describe partially-premixed combustion provided that the gradient in mixture fraction is kept small.

The novelty of this article is the use of detailed chemistry for both the premixed and non-premixed combustion mode, including a switch-function to distinguish (locally) between the two different modes of combustion and thereby enabling the determination of the most appropriate type of FGM database. It will be discussed whether the switch should be based on mixture fraction and reaction progress variable gradients or using an additional control variable.

In the next section it will be explained how individual flamelets are computed and, subsequently, how FGM databases are generated from these individual flamelets. In the third section need to use an appropriate FGM database to describe chemical kinetics is outlined. In the last section a brief description of the work in progress is given.

II. FLAMELET GENERATED MANIFOLDS

FGM databases are composed of many individual flamelets, each flamelet having slightly different boundary conditions. Boundary conditions, above all, determine the type of flamelet: premixed or non-premixed. Schematic representations of these flamelets types are shown in figure 1. The main difference between these two types is the direction of diffusion in composition space. In premixed flamelets diffusion is only allowed along isomixture fraction contours while in non-premixed flamelets diffusion mainly takes place perpendicular to these iso-contours.

For this study, partially-premixed combustion parameters are mapped on two control variables describing mixing (mixture fraction $Z$) and reaction progress (reaction progress variable $Y$):

$$\psi = \psi(Z,Y)$$  (1)
in which $\psi$ can denote any thermo-chemical variable. The mixture fraction $Z$ is defined by Bilger [2] and the reaction progress variable, which has to be monotonous in both lean and rich mixtures in order to facilitate an unambiguous determination of dependent variables, is defined as:

$$\gamma = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{H_2O}}{M_{H_2O}} + \frac{Y_{H_2}}{M_{H_2}}$$  \hspace{1cm} (2)

in which $Y_i$ and $M_i$ denote a species mass fraction and a species its molar mass respectively.

**A. Flamelet equations**

The flamelet equations [8] form a set of specific transport equations for one-dimensional reacting flows describing conservation of mass, species and enthalpy. When unit Lewis numbers are assumed for all species the set of equations reduces to:

$$\frac{\partial (\rho)}{\partial t} + \frac{\partial (\rho u)}{\partial x} = -\rho K$$  \hspace{1cm} (3)

$$\frac{\partial (\rho Y_i)}{\partial t} + \frac{\partial (\rho u Y_i)}{\partial x} - \rho K Y_i + \dot{\omega}_i = -\rho K Y_i$$  \hspace{1cm} (4)

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u h)}{\partial x} + \frac{\partial}{\partial x} \left( \rho u c_p (h - \frac{\lambda}{c_p} \frac{\partial h}{\partial x}) \right) = -\rho K h$$  \hspace{1cm} (5)

in which $x$, $\rho$, $u$, $K$ denote the physical coordinate perpendicular to the flame, the mixture density, the velocity and the adiabatic flame propagation velocity and is an eigenvalue of the system. Subscripts 1 and 2 refer to the fuel- and oxidizer stream, respectively. The parameter of this system is the stoichiometry of the fresh mixture denoted by the mixture fraction $Z_{st}$. Beyond flammability limits thermo-chemical variables are linearly interpolated between the leanest flamelet and pure oxidizer and the richest flamelet and pure fuel, respectively. Chemical equilibrium has been explicitly added to all flamelets.

When FGM databases are constructed from strained counterflow diffusion flamelets, equations 3, 4, 5 and 6 are solved. The equation of state again closes the system of equations. Boundary conditions for strained counterflow diffusion are:

$$Y_i (x \to -\infty) = Y_{i,1} \hspace{1cm} h (x \to -\infty) = h_1 \hspace{1cm} Y_i (x \to +\infty) = Y_{i,2} \hspace{1cm} h (x \to +\infty) = h_2 \hspace{1cm} K (x \to +\infty) = a(t)$$

in which subscripts 1 and 2 again refer to the fuel- and oxidizer stream, respectively. The parameter of this system is the applied strain rate $a$, which can be a function of time in case of unsteady computations, and is defined at the oxidizer side ($x = \infty$). Solving the unsteady equations for conservation of mass, species mass fractions and enthalpy results in a natural continuation of the profiles in $Z$-$\gamma$ space beyond the extinction strain rate. The time-dependent solution of the unsteady equations, which is treated as a family of solutions, is tracked until the solution equals the mixing limit starting from a steady solution with a strain rate equal to unity.

**III. FGM VERSUS DETAILED CHEMISTRY**

Laminar, one-dimensional $CH_4$/air (21% $O_2$ and 79% $N_2$ by volume) flames are simulated in a counterflow setup. The boundary conditions will be varied from premixed to fully non-premixed resulting in realizations ranging from a premixed double flame, via a triple-flame structure to a (single) diffusion flame structure. All setups are simulated at ambient conditions ($p = 1.01325 \times 10^5$ Pa and $T = 300$ K) and Lewis numbers are set to unity for all species. The GRI 3.0 reaction mechanism [10] is used to represent combustion chemistry.

For the FGM database based on unstrained, steady premixed flamelets, 400 flamelets with $Z \in [0.25Z_{st}, 2.0Z_{st}]$ have been used. For a given inlet composition, determined by $Z$, $\gamma$ is tracked. Equation 6 is removed from the system of equations since $K$ equals zero everywhere. Beyond the flammability limits linear extrapolation between the leanest flamelets and pure oxidizer, and the richest flamelet and pure fuel respectively, has been applied. The resulting database has been interpolated onto an equidistant grid with 375 points in both $Z$ and $\gamma$ direction. For the FGM database based on non-premixed flamelets, 600 flamelets with increasing strain rate have been used. The unsteady...
flamelet equations, equation 3, 4, 5 and 6 are solved while the strain rate at the oxidizer side is increased by 1 s$^{-1}$ on average using a Wiebe function, starting with a strain rate equal to unity. For each solution, dependent on time, $\mathcal{Y}$ is recalculated at each point according to equation 2 while for $Z$ the transport equation is solved. The steady, slow increase in strain rate implies that the flamelet will extinguish at a given moment: the (extinguishing) flamelet is tracked until it equals the mixing limit. By this means the entire composition space between (near) chemical equilibrium and the mixing limit can be spanned. The resulting database has again been interpolated onto an equidistant grid with 375 points in both $Z$ and $\mathcal{Y}$ direction. In figure 2 the OH mass fraction, which is a function of the two control variables $Z$ and $\mathcal{Y}$, is shown as an example.

When the FGM databases are used in flamelet computations equations 4 and 5 are replaced by transport equations for the two control variables only:

$$\frac{\partial (\rho Z)}{\partial t} + \frac{\partial}{\partial x} \left( \rho u Z - \frac{\lambda}{c_p} \frac{\partial Z}{\partial x} \right) = -\rho K Z \quad (7)$$

$$\frac{\partial (\rho \mathcal{Y})}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \mathcal{Y} - \frac{\lambda}{c_p} \frac{\partial \mathcal{Y}}{\partial x} \right) = -\rho K \mathcal{Y} + \dot{\omega}_y \quad (8)$$

The chemical source term for $\mathcal{Y}$ ($\dot{\omega}_y$) is retrieved from the FGM database using linear interpolation; when the solutions for $Z$ and $\mathcal{Y}$ have converged all species mass fractions are retrieved from the FGM database in the same way.

A. The need for using the appropriate FGM database

When premixed flamelets are computed using a premixed flamelet-based FGM and when non-premixed flamelets are computed using a non-premixed flamelet-based FGM it can be seen from figure 3 that combustion chemistry and diffusive transport are well described by the FGM database. However, if the non-appropriate type of FGM database is used, i.e. premixed flamelets are computed using a non-premixed flamelet-based FGM or non-premixed flamelets are computed using a premixed flamelet-based FGM, it can be seen from figure 4 that errors appear when predictions using FGM databases are compared to detailed chemistry. These errors are most significant for CO and H$_2$ which are formed under rich conditions but in non-premixed flamelets can diffuse towards the reaction layer near the stoichiometric mixture fraction where they are consumed again. When premixed flamelets are considered this is not possible; this results in higher CO and H$_2$ under rich conditions. In figure 4 this effect is most visible in CO and H$_2$ mass fraction predictions in non-premixed flames using a premixed flamelet-based FGM database. For OH it is observed that errors using the wrong type of FGM database are not as significant as for CO and H$_2$. It will be examined whether this can be attributed to the dominance of chemistry (convective and diffusive) transport.

It can be concluded that it is important to use the appropriate FGM database when accurate predictions of species are desired, especially when CO and H$_2$ are concerned.

B. Partially-premixed flamelets

For partially-premixed flamelets FGM databases which are based on either premixed or non-premixed flamelets are not sufficient. It will be examined whether the local
additional transport equation has to be solved.

It will be examined whether a switch function as de-

\[ \dot{\omega}_Y (Z, Y') = \alpha \dot{\omega}_Y^P (Z, Y') + (1 - \alpha) \dot{\omega}_Y^{NP} (Z, Y') \]  

(9)

To determine the weight factor \( \alpha \) several methods have been proposed starting with the flame index method proposed by Yamashita et al. [11], for which a modified version for the use with FPI-databases was introduced by Fiorina et al. [5]; nevertheless for one-dimensional flames these indices exhibit a non-continuous behavior. Another switch function formulation which will be examined reads:

\[ \alpha = \tanh \left[ \log \left( \frac{\nabla Y' \cdot \nabla Y}{\nabla Z \cdot \nabla Z} \right) \right] \]  

(10)

which should exhibit a continuous and smooth behavior throughout the entire domain.

IV. WORK IN PROGRESS

It will be examined whether a switch function as defined in the previous section yields an increase in accuracy of predictions when FGM databases are used to replace expensive detailed chemistry computations. The switch function will be compared to the use of an additional control variable, e.g. \( H_2 \) mass fraction, for which an additional transport equation has to be solved.

REFERENCES