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 flameletbased 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 partiallypremixed and non-premixed flamelets. A flame-index was introduced to distinguish between premixed and nonpremixed 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 nonpremixed combustion mode. From these two references it can be concluded that a premixed flamelet-based FGM



Fig. 1. Two flamelet types used for this study: premixed (left) and partially-/non-premixed (right) flamelets.

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 isocontours.

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

$$\psi = \psi\left(Z, \mathcal{Y}\right) \tag{1}$$

in which ψ 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:

$$\mathcal{Y} = \frac{Y_{\rm CO_2}}{M_{\rm CO_2}} + \frac{Y_{\rm H_2O}}{M_{\rm H_2O}} + \frac{Y_{\rm H_2}}{M_{\rm H_2}} \tag{2}$$

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:

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

$$\frac{\partial \left(\rho Y_{i}\right)}{\partial t} + \frac{\partial}{\partial x} \left(\rho u Y_{i} - \frac{\lambda}{c_{p}} \frac{\partial Y_{i}}{\partial x}\right) = -\rho K Y_{i} + \dot{\omega}_{i} \quad (4)$$

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

in which x, ρ , u, K denote the physical coordinate perpendicular to the flame, the mixture density, the velocity of the gas mixture and the flame stretch [7] respectively. Y_i , \mathbf{V} , $\dot{\omega}$, λ , c_p , μ and h denote the mass fraction of species i, the diffusion velocity, the chemical production rate, the thermal conductivity, the specific heat at constant pressure, the dynamic viscosity and the total enthalpy, respectively. N_s denotes the total number of species present in the used reaction mechanism and subscript 2 refers to the oxidizer stream. The low-Mach approximation is applied to the equation of state to prohibit acoustic waves propagating though the computational domain. For counterflow diffusion flames an additional transport equation for the unknown stretch field K has to be solved:

$$\frac{\partial \left(\rho K\right)}{\partial t} + \frac{\partial}{\partial x} \left(\rho u K - \mu \frac{\partial K}{\partial x}\right) = -\rho K^2 + \rho_2 a^2 \quad (6)$$

in which *a* denotes the applied strain rate at the oxidizer side. This transport equation has been derived by Dixon-Lewis [4]; here the formulation for two-dimensional cartesian geometries has been adopted. The set of governing equations describing either premixed or non-premixed flamelets is solved by the fully implicit solver CHEM1D [9] developed at TUE.

B. Boundary conditions for the flamelet equations

When FGM databases are to be constructed from unstrained steady premixed flamelets, equations 3, 4 and 5 are solved. K equals zero everywhere and equation 6 thereby is redundant. The equation of state closes the system of equations. Boundary conditions for premixed flamelets are:

$$u(x \to -\infty) = s_{\mathsf{L}}(Z_u)$$

$$Y_{\mathsf{i}}(x \to -\infty) = Z_u Y_{\mathsf{i},1} + (1 - Z_u) Y_{\mathsf{i},2}$$

$$h(x \to -\infty) = Z_u h_1 + (1 - Z_u) h_2$$

in which subscript u denotes the unburnt mixture, s_{L} denotes 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_u . 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:

$$\begin{array}{rcl} Y_{\mathrm{i}}\left(x\rightarrow-\infty\right) &=& Y_{\mathrm{i},1}\\ h\left(x\rightarrow-\infty\right) &=& h_{1}\\ Y_{\mathrm{i}}\left(x\rightarrow+\infty\right) &=& Y_{\mathrm{i},2}\\ h\left(x\rightarrow+\infty\right) &=& h_{2}\\ K\left(x\rightarrow+\infty\right) &=& a\left(t\right) \end{array}$$

in which subscripts 1 and 2 again refer to the fueland 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- \mathcal{Y} 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 CH₄/air (21% O₂ and 79% N₂ 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, \mathcal{Y} 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 \mathcal{Y} direction. For the FGM database based on non-premixed flamelets, 600 flamelets with increasing strain rate have been used. The unsteady



Fig. 2. OH mass fraction, which is a function of Z and \mathcal{Y} , originating from the non-premixed flamelet-based Flamelet Generated Manifold database. OH is a typical indicator of combustion chemistry activity.

flamelet equations, equation 3, 4, 5 and 6 are solved while the strain rate at the oxidizer side is increased by $1 \ s^{-2}$ 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 a 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:

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

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

The chemical source term for $\mathcal{Y}(\dot{\omega}_{\mathcal{Y}})$ 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 flameletbased 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



Fig. 3. Results for steady premixed flamelets using a premixed flameletbased FGM (left) and steady non-premixed flamelets using a nonpremixed flamelet-based FGM (right). For the premixed flamelets black lines with circle markers denote a flamelet with $Z = 0.67Z_{\rm st}$, blue lines with square markers denote a flamelet with $Z = 1.5Z_{\rm st}$. For the non-premixed flamelets black lines with circle markers denote a flamelet with $a = 10 \ s^{-1}$, blue lines with square markers denote a flamelet with $a = 10 \ s^{-1}$. In all figures solid lines denote detailed chemistry solutions while the markers (circles, squares or triangles) denote solutions using FGM databases. Figures from top to bottom represent CH₄ mass fractions, O₂ mass fractions, CO mass fractions, H₂ mass fractions and OH mass fractions.

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 over (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



Fig. 4. Results for premixed flamelets using a non-premixed FGM (left) and non-premixed flamelets using a premixed FGM (right). Identical symbols have been used as in figure 3.

source term for \mathcal{Y} can be defined as a linear combination of the source term in premixed and non-premixed flamelets for the same values for Z and \mathcal{Y} :

$$\dot{\omega}_{\mathcal{Y}}(Z,\mathcal{Y}) = \alpha \dot{\omega}_{\mathcal{Y}}^{\mathrm{P}}(Z,\mathcal{Y}) + (1-\alpha) \, \dot{\omega}_{\mathcal{Y}}^{\mathrm{NP}}(Z,\mathcal{Y}) \qquad (9)$$

To determine the weight factor α 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:

$$\alpha = \tanh\left[\log\left(\frac{\vec{\nabla}\mathcal{Y}\cdot\vec{\nabla}\mathcal{Y}}{\vec{\nabla}Z\cdot\vec{\nabla}Z}\right)\right] \tag{10}$$

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

[1] R.W. Bilger, "The structure of diffusion flames," *Comb. Sci. Tech.*, vol. 13, pp. 155–170, 1976.

- [2] R.W. Bilger, "On reduced mechanisms for methane-air combustion in non-premixed flames," *Comb. Flame*, vol. 80, pp. 135–149, 1990.
- [3] H. Bongers, J.A. van Oijen and L.P.H. de Goey "The Flamelet Generated Manifold method applied to steady planar partiallypremixed counterflow flames," *Comb. Sci. Tech.*, vol. 177(12), pp. 2373–2393, 2005.
- [4] G. Dixon-Lewis, "Structure of laminar flames," Proc. Comb. Inst., vol. 23, pp. 305–324, 1990.
- [5] B. Fiorina, O. Gicquel, L. Vervisch, S. Carpentier and N. Darabiha, "Approximating the chemical structure of partially premixed and diffusion counterflow flames using FPI flamelet tabulation," *Comb. Flame*, vol. 140, pp. 147–160, 2005.
- [6] O. Gicquel, N. Darabiha and D. Thevenin, "Laminar premixed hydrogen/air counterflow flame simulations using Flame Prolongation of ILDM with differential diffusion," *Proc. Comb. Inst.*, vol. 28, pp. 1901–1908, 2000.
- [7] L.P.H. de Goey and J.H.M. Ten Thije Boonkkamp, "A mass based definition of flame stretch for flames with finite thickness," *Comb. Sci. Tech.*, vol. 122, pp. 399–405, 1997.
- [8] J.A. van Oijen and L.P.H. de Goey, "Modelling of premixed laminar flames using Flamelet Generated Manifolds," *Comb. Sci. Tech.*, vol. 161, pp. 113–137, 2000.
- [9] L.M.T. Somers, *The simulation of flat flames with detailed and reduced chemical models*. PhD Thesis: Eindhoven University of Technology, 1994.
- [10] G.P. Smith, D.M. Golden, M. Frenklach, N.W. Moriarty, B. Eiteneer, M. Goldenberg, C.T. Bowman, R.K. Hanson, S. Song, W.C. Gardiner Jr., V.V. Lissianski and Z. Qin, *GRImech 3.0 reaction mechanism.* Sandia National Laboratories, 2000.
- [11] H. Yamashita, M. Shimada and T. Takeno, "A numerical study on flame stability at the transition point of jet diffusion flames," *Proc. Comb. Inst.*, vol. 26, pp. 27–34, 1996.