HEFAT2010
7th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics
19-21 July 2010
Antalya, Turkey

PREMIXED TURBULENT COMBUSTION MODELING WITH FLAMELET GENARATED MANIFOLDS INCLUDING PREFERENTIAL DIFFUSION EFFECTS

De Goey L.P.H.*, van Oijen J.A. and Bastiaans R.J.M.
*Author for correspondence
Department of Mechanical Engineering,
Eindhoven University of Technology,
Den Dolech 2, 5600 MB Eindhoven the Netherlands,
E-mail: l.p.h.d.goey@tue.nl

ABSTRACT

The FGM technique is a new method to reduce chemical kinetics. It has already proven to be accurate for modelling (partially-) premixed flames in DNS, LES and RANS settings. Previous research has focussed on flames with unit Lewis number transport models, thereby neglecting preferential diffusion effects. High accuracy was gained using a single progress variable Y_{cv1} to describe the flame kinetics. The method is extended in the present contribution for non-unit Lewis numbers by introducing an additional mixing parameter Y_{cv2} in the manifold, describing the combined fluctuations in enthalpy and element mass fractions due to flame stretch and preferential diffusion. The resulting 2D FGM is used in 2D DNS of a circular flame and compared with detailed chemistry. The agreement is near perfect thereby opening the way to model 3D turbulent CH_4-H_2-air flames on a slot burner with realistic non-unit Lewis numbers. A significant increase in flame wrinking occurs due to local changes in burning intensity.

INTRODUCTION

Detailed numerical modelling of reacting flows has gained a continuous growth of interest in the last few decades. However, the numerical modelling of combustion systems is a very challenging task. The interaction of the fluid flow, turbulence, chemical reactions and thermodynamics in reacting flows is of exceptional complexity. At the moment it has become within reach to model the most important physical aspects in detail, but this is still limited to small academic combustion problems. The modelling of the full detail of practical combustion equipment is still prohibited in the next few decades, because of current and future limitations in computing power. This problem asks for special treatments in the modelling of flames. In the last decades two main routes have been followed in combustion science to model the detailed dynamics and structure of chemically reacting flows: chemical reduction techniques [1-3] and laminar flamelet models [4]. We recently developed the Flamelet Generated Manifold (FGM) technique, which combines advantages of chemistry reduction and flamelet models [5,6]. Current state of the art of this technique is highlighted and extension to include preferential diffusion is considered in this paper.

THE FLAMELET GENERATED MANIFOD TECHNIQUE

Most recently developed efficient modelling techniques of combustion processes make use of the multi-scale nature of flames. This idea can be exploited in different smart ways to reduce the number of equations to be solved, leading to an enormous reduction in computing effort. Chemical reduction techniques (such as conventional reduction [1], ILDM [2] and CSP [3]) are based on the idea that most of the chemical time scales in the system are very small. A time-scale analysis can be performed and the fastest time scales are considered to be in steady-state. All variables can be stored in a database as a function of a few controlling variables and during run-time only the few equations for the controlling variables are solved. Laminar flamelet methods [4] are based on the idea that flame structures are much thinner than most of the scales of the distortions in the flow, also implying that the chemical reactions are very fast compared to all other time scales. The reacting flow is modelled by using a kinematic equation for the flame front, the mixture fraction equation for the mixing and a CFD solver for the flow to model these flames [4].

In the last few years our group has proposed some new directions in these fields of combustion science. These are interesting, both because of the improvement in reduction

efficiency as well as in the accuracy of the models [5,6]. These new methods are based on a detailed analysis of flames in the so-called laminar flamelet combustion regimes. The approach is based on the idea that the most important aspects of the dynamics of the internal structure of the flame fronts should be taken into account. For this reason, the system of transport equations is split in three parts: 1) a part describing the progress of the flame using a small number of transport equations for so-called progress variables, 2) a part describing the flow and mixing of chemical elements and enthalpy in the system and 3) a so-called set of flamelet equations describing the internal (flame) structure. The progress of the flame is generally described by one (or at most a few) progress variable(s) Y_{cvi} for which a transport equation is solved during run-time. The chemical source term w_Y in the transport equation for Y_{cv} is derived from the flamelet system. The flow and mixing of elements and enthalpy is described by equations for the enthalpy h and elements Z_j, which are independent of the chemical kinetics. The flamelet system is solved in a pre-processing step for each variable Y_{cv}, h and Z_j. The corresponding solution for the temperature and all species variables $T(Y_{cv},h,Z_j)$,$Y_i(Y_{cv},h,Z_j)$ and for the source term $w_Y(Y_{cv},h,Z_j)$ depend only on Y_{cv}, h and Z_j which is stored in a data-base. During run-time, i.e. when a CFD problem of a combustion process is tackled, only equations for Y_{cv}, h and Z_j are solved using the data-base to retrieve all necessary information to update the solution. In case of LES/RANS models of turbulent flames, it is necessary that transport equations are solved for the filtered/averaged quantities Y_{cv}, h, Z_j. In this case the database then has to be extended to take into account fluctuations of the quantities mentioned

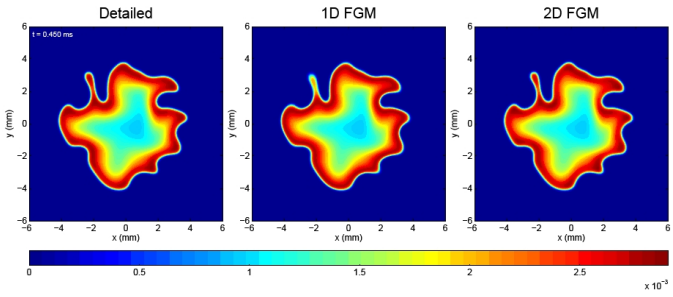

Figure 1: OH distribution in a turbulent premixed CH_4-air flame with equivalence ratio 0.7. 2D DNS computations using detailed (GRI-mech) chemistry (left), 1D FGM (middle) and 2D FGM (right); turbulence intensity $u'/s_L=8$; $Le_i=.1$

The FGM method has been developed and validated in a step-by-step approach in the recent years. At first, we focussed on 1D/2D laminar flames making detailed comparison possible with computational results using detailed chemistry [5]: burner-stabilized Bunsen flames, partially-premixed triple flames and ceramic burner stabilized flames in a furnace have been investigated with success. We subsequently focused on 2D DNS modeling of strongly stretched turbulent flame kernels using unit Lewis number transport avoiding the influence of preferential diffusion effects [6]. Furthermore, initial turbulence intensity was equal to $u'/s_L=8$, where s_L is the adiabatic burning velocity of the planar flame. Results of this study using a 1D FGM and 2D FGM are compared with computations using detailed kinetics in Figure 1. The 1D FGM is computed from a single adiabatic flamelet, while the 2D database was created from stretched flamelets without preferential diffusion effects ($Le_i=1$). DNS-FGM performs very well in this situation. A 2D manifold slightly better approaches the detailed results compared to the results for the 1D manifold, but the 1D manifold is already very accurate, even for these highly stretched flamelets. In subsequent studies, the approach has proven to be also appropriate for the (RANS and LES) computation of (partially) premixed flames. Recently, we also considered DNS of premixed CH_4-H_2-air flames described by non-unit Lewis numbers. This will be the focus of the current paper.

RESULTS FOR NON-UNIT LEWIS NUMBERS

Earlier 2D computations of spherically expanding premixed CH_4-air flames have shown that a single progress variable Y_{cv1} was sufficient to reproduce results found with detailed chemistry if unit Lewis number are used in the transport model [6]. Enthalpy and element mass fractions are conserved in this case, thereby avoiding fluctuations in flame temperature and equivalence ratio; a single adiabatic premixed flamelet (1D FGM) describing the reaction progress (in terms of Y) is then sufficient, a 2D FGM, taking into account local distortions due to flame stretch and curvature, increases accuracy further but a 1D FGM was already quite accurate. For the case of flames with realistic non-unit Lewis numbers, e.g. necessary to model CH_4-H_2-air flames, the model has to predict fluctuations in enthalpy and element mass fractions as well. These fluctuations may lead to a local enhancement/lowering of the mass burning rate due to rising/decreasing temperature peak values and equivalence ratio fluctuations. It is known that even

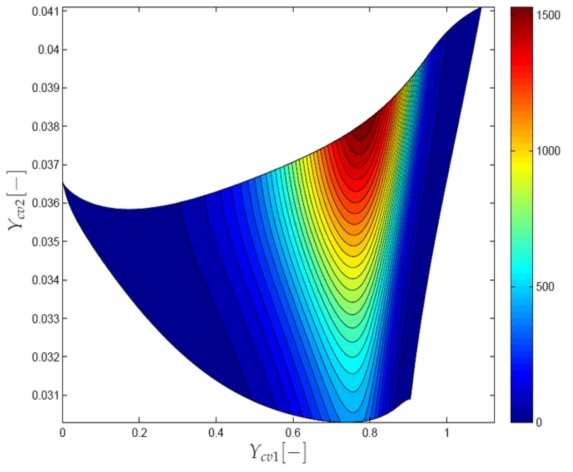

Figure 1:False color plot of source term distribution w_Y As function of Y_{cv1} and Y_{cv2}.

local flame extinction may appear at highly stretched/curved flame areas and enhanced burning in other flame areas. Cellular and other flame instabilities may appear, depending on the mixture composition.

For the FGM concept, this means that 4 additional equations have to be solved; h, Z_H, Z_O and Z_C need to be taken into account apart from Y_{cv1}. The FGM database would increase to a 5D manifold, which is very large. Earlier computations [7] of stretched flames have shown however, that fluctuations in h, Z_H, Z_O and Z_C are (roughly) linearly related to each other in the curved and stretched laminar flames, so that a single additional (mixing) progress variable Y_{cv2} (taking into account these correlations) may be sufficient. A 2D FGM manifold including variations in enthalpy and elements due to flame stretch and preferential diffusion is created and stored. For the case of methane-air is re-appeared that a 1D manifold already reproduces detailed results quite accurately. This is related to the fact that methane has Lewis numbers close to one, leading to very weak preferential diffusion effects.

In case of heavier or lighter fuels, the situation is different. For that reason we modelled hythane-air flames consisting of methane and hydrogen in the mixture, leading to significant changes in Lewis numbers and therefore highly relevant preferential diffusion effects. In the following we focus on hythane-air flames consisting of 60% (mol) methane and 40% (mol) hydrogen. For this case we followed the following procedure. As first progress variable describing the main reaction progress we used

$$Y_{cv1}=Y_{CO2}/M_{CO2}+Y_{H2O}/M_{H2O}-0.4\ Y_{H2}/M_{H2}-0.6Y_{CH4}/M_{CH4}, \quad (1)$$

subsequently scaled between 0 and 1. For second progress variable we used the combined mixing parameter

$$Y_{cv2}=Z_C+Z_H, \quad (2)$$

This choice has been made in a rather ad-hoc manner to force a strictly increasing behaviour of both Y_{cv1} and Y_{cv2}. The 2D database is created by modelling 1D adiabatic flamelet structures including flame stretch and curvature. The flame stretch rate and curvature fields are applied to the flamelets by using a step-wise increasing curvature and stretch, combined in such away by forcing the mass burning rate is constant through each flamelet. To explain this procedure, we start from the mass conservation equation [8] in the flamelet coordinate system:

$$\frac{\partial m}{\partial s} = -\rho K - mk \quad (3)$$

where m(s) is the mass burning rate as function of the flame coordinate s in the flamelet, K(s) the stretch rate en k(s) the local flame curvature. By forcing m(s) to be constant we find

$$K(s) = -mk/\rho(s) \quad (4)$$

By increasing k stepwise (0, 0.01, 0.02,...) and K(s) accordingly, a series of stretched and curved flamelets is produced with constant m and k. Element mass fractions and enthalpy within the flamelet solutions change accordingly as expected. The resulting changes are parametrized using Y_{cv2} as in Eq.(2). The resulting source term w_Y of Y_{cv1} as function of the two control variables Y_{cv1} and Y_{cv2} is shown in figure 2. This manifold is then used in a series of 2D DNS computations of a circular expanding flame in which Y_{cv1} and Y_{cv2} are solved, while all other data are retrieved from the 2D FGM database. Results of the H-radical distribution in this flame with a 1D

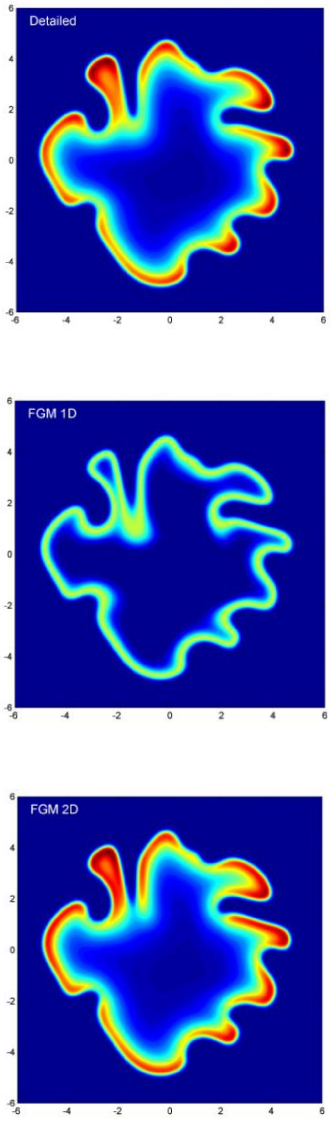

Figure 3 H-radical distribution in a turbulent premixed 60% CH_4- 40% H_2-air flame with equivalence ratio 0.7. 2D DNS computations using detailed (GRI-mech) chemistry (a), 1D FGM (b) and 2D FGM (c).

FGM (without preferential diffusion) and the 2D FGM are presented in Figure 3 and compared with detailed (GRI-mech 3.0) computations using the same non-unit Lewis number transport model. It is clear that the 1D FGM (with a fixed and constant Y_{cv2}) cannot predict the local increase/decrease of the H-radical peak values in positively/negatively curved flamelets, while the 2D FGM can. High values of H-radicals more-or-less coincide with local flame temperature increments leading to fast combustion. The figure shows that the 2D FGM is not perfect, but very well represents the behaviour. This shows that the major effects of changes in the w_Y due to preferential diffusion phenomena are reproduced well. It should be noted that Eq.(4) is not satisfied in the flamelets which appear during the computations presented in Figure 3. Apparently it does not make much difference how the flame stretch is supplied during the production of the 2D manifold. This means that it makes less difference which procedure is used to derive the source term and the rest of the manifold. The computation time is reduced by two orders of magnitude by using FGM instead of the full reaction mechanism.

APPLICATION

To investigate the effect of preferential diffusion in practical situations, 3D DNS of lean premixed turbulent Bunsen flames on a slot burner are performed. We again consider a fully premixed fuel with an equivalence ratio of 0.7 and compare a CH_4-air flame with a H_2-CH_4-air flame with a molar fractional distribution of 40% H_2 and 60% CH_4 (referred to as hythane in the following). A 1D FGM is used for the methane flame, but the 2D FGM, introduced above was used for the hythane mixture.

Figure 4 shows the chemical source term of the progress variable Y for the hythane case at some time instance. The simulation clearly shows an enhanced reaction rate in regions convex toward the reactants and reduced reaction rate in concave regions, which was not visible in the methane flame. Extinction occurred occasionally in the latter regions. The effect of preferential diffusion was quantified by comparison with a simulation with the 1D FGM. Thus this computation did not incorporate preferential diffusion effects in the 3D transport equations, although the 1D FGM was obviously calculated using the appropriate Lewis numbers in one dimension. The comparison showed that inclusion of a second independent variable W into the manifold was quite important, otherwise effects of preferential diffusion were not captured in the flame. Effects of preferential diffusion were shown to enhance curvature, and thereby to increase the turbulent burning velocity and reduce the mean flame height considerably. Compared to 0% hydrogen, the case of 40% hydrogen increased the burning velocity by approximately 80%. When 3D preferential diffusion was ignored an increase of only 30%, primarily due to the increase of laminar burning velocity, was found.

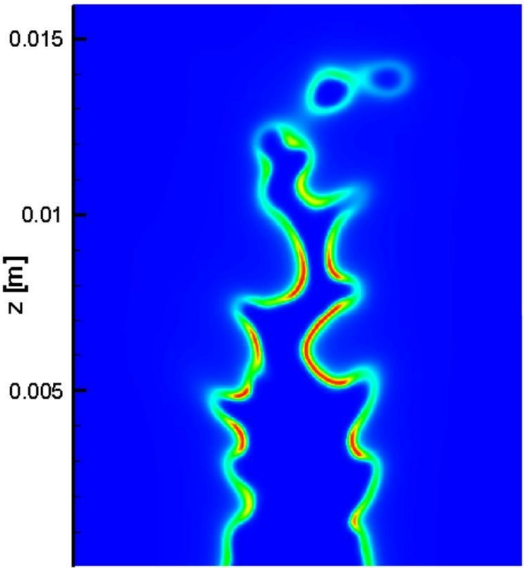

Figure 4 Source term of Y in a turbulent fully premixed 60% CH_4- 40% H_2-air flame with equivalence ration 0.7. 3D DNS computations using 2D FGM.

CONCLUSIONS

The FGM technique is one of the most promising techniques to model turbulent combustion accurately using detailed chemistry. In the present contribution, we successfully extended FGM for the modelling of premixed flames with DNS including non-unit Lewis numbers to predict preferential diffusion effects. Local fluctuations in combustion rate due to flame curvature and fow straining along the flame surface are predicted appropriately. Lean CH_4-H_2-air flames with realistic Lewis numbers thereby exhibit a significantly larger flame wrinkling and higher turbulent burning rate than similar flames with unit Lewis numbers.

REFERENCES

[1] Peters, N., Reducing mechanisms, S48-67. In M.D. Smooke, editor, Reduced kinetic mechanisms and asymptotic approximations for methane-air flames, Berlin, Springer Verlag, 1991.
[2] Maas, U. and Pope, S.: Simplifying chemical kinetics: Intrinsic low-dimensional manifolds in composition space. Combust. Flame, 88 (1992) 239-264.
[3] Lam, S. and Goussis, D., Conventional asymptotics and computational singular perturbation for simplified kinetics modeling, S 227-242. In M.D. Smooke, editor, Reduced kinetic mechanisms and asymptotic approximations for methane-air flames, Berlin, Springer Verlag, 1991.
[4] Peters, N., Laminar flamelet concepts in turbulent combustion, Proc. Combust. Inst. 21 (1986) 1231--1250.
[5] van Oijen, J. and de Goey, L.: Modelling of premixed laminar flames using flamelet-generated manifolds. Combust. Sci. Technol. 161, (2000) 113-131.

[6] van Oijen, J.,Bastiaans, R. and de Goey, L.: *Low-Dimensional Manifolds in Direct Numerical Simulations of Premixed Turbulent Flames*. Proc. Combust. Inst., **31** (2007) 1377-1384.
[7] van Oijen J. and de Goey, L.: Preferential diffusion effects in stretched methane-hydrogen-air flames, Combust. Flame (2009) submitted.
[8] de Goey, LPH and ten Thije Boonkkamp, JHM, *A Flamelet description of premixed laminar flames and the relation with flame stretch*, Combust. Flame, **119**, 253-271, (1999)