MODELLING OF PREMIXED LAMINAR FLAMES USING FLAMELET-GENERATED MANIFOLDS

J. A. van Oijen and L. P. H. de Goey

Eindhoven University of Technology,
Dept. of Mechanical Engineering,
PO Box 513, 5600 MB Eindhoven, The Netherlands

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Corresponding author: J. A. van Oijen
E-mail: J.A.v.Oijen@tue.nl
Telephone: + 31 40 2473286
Fax: + 31 40 2433445

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ABSTRACT

In order to reduce the computational cost of flame simulations, several methods have been developed during the last decades, which simplify the description of the reaction kinetics. Most of these methods are based on partial-equilibrium and steady-state assumptions, assuming that most chemical processes have a much smaller time scale than the flow time scale. These assumptions, however, give poor approximations in the 'colder' regions of a flame, where transport processes are also important.

The method presented here, can be considered as a combination of two approaches to simplify flame calculations, i.e. a flamelet and a manifold approach. The method, to which we will refer as the Flamelet-Generated Manifold (FGM) method, shares the idea with flamelet approaches that a multi-dimensional flame may be considered as an ensemble of one-dimensional flames. The implementation, however, is typical for manifold methods: a low-dimensional manifold in composition space is constructed, and the thermo-chemical variables are stored in a database which can be used in subsequent flame simulations. In the FGM method a manifold is constructed using one-dimensional flamelets. Like in other manifold methods, the dimension of the manifold can be increased to satisfy a desired accuracy. Although the method can be applied to different kinds of flames, only laminar premixed flames are considered here.

Since the major parts of convection and diffusion processes are present in one-dimensional flamelets, the FGM is more accurate in the 'colder' zones of premixed flames than methods based on local chemical equilibria. Therefore, less controlling variables are sufficient to represent the combustion process. Test results of one and two-dimensional premixed methane/air flames show that detailed computations are reproduced very well with a FGM consisting of only one progress variable apart from the enthalpy to account for energy losses.
INTRODUCTION

Recently, detailed numerical simulations of flames have become within reach due to the still increasing speed of modern (super) computers. Results of multi-dimensional time-dependent flame calculations have been reported by several authors, (see e.g. [1–5].) However, computational times of these simulations often exceed days, prohibiting an extensive study on the effect of different parameters. Moreover, detailed simulations of practical systems such as in engines or furnaces will still be impossible for a long time.

In order to reduce the computational expense, several methods have been developed which simplify the description of the reaction kinetics. One way of reducing the chemical reaction mechanism is the use of ‘ad hoc’ few-step global mechanisms. In these chemical models the combustion process is described by only a few reactions, representing the conversion of fuel and oxidizer into products. Although global mechanisms have been applied in many combustion simulations (see e.g. [6–9]), their lack of accuracy causes them to be useful for global studies only.

More accurate reduction techniques are based on the observation that a typical combustion system contains many chemical processes with a much smaller time scale than the flow time scales. These fast processes can be decoupled, reducing the stiffness of the system and thus increasing the computational efficiency. The most prominent reduction methods are the systematic reduction technique by Peters and co-workers [10], the computational singular perturbation (CSP) method from Lam and Goussis [11] and the intrinsic low-dimensional manifold (ILDM) approach of Maas and Pope [12]. Each of these methods uses a different way to identify the fast chemical processes. In the systematic reduction technique partial-equilibrium and steady-state assumptions are invoked for particular reactions and species which are associated with fast processes. A detailed investigation of the reaction paths and the time scales in the chemical reaction mechanism should give information about which species are closest to steady state. For higher hydrocarbon fuels with reaction mechanisms consisting of hundreds of reactions this is a complicated task. Moreover, the steady-state assumptions invoked are also applied to ranges of compositions and temperatures in flames where they provide poor approximations.

In the CSP and ILDM method the time scale analysis is performed automatically, based on the local Jacobian of the chemical source term in the balance equations. The CSP method uses a computational singular perturbation to identify the fast time scales. Since this is done dynamically, the number and identity of the steady-state species may vary during the combustion process. Although this technique is the most accurate, its applicability on complex simulations is questionable due to its high computational cost.
The ILDM method identifies the fast processes using an eigenvalue analysis of the local Jacobian of the chemical source term. The processes represented by the eigenvectors associated with small time scales are assumed to be in steady state. The eigenvectors which represent the slow chemical processes are used to construct a low-dimensional manifold in composition space. This manifold is parametrized by a small number of variables which evolve slowly during the combustion process. For application in flame calculations the manifold is tabulated in a look-up table as a function of the parametrizing (or controlling) variables. This is done once in a pre-processing step for a given mixture and, subsequently, the look-up table can be used in a series of combustion calculations. The dimension of the look-up table is determined by the number of controlling variables which is needed to describe the slow chemical processes. For simple fuels like CO/H₂ mixtures, two controlling variables are sufficient [13, 14]. However, for an accurate reproduction of the burning velocity of premixed methane/air flames at least three degrees of freedom are needed [15]. Together with variations in enthalpy, pressure and element composition which can occur in combustion systems, this results in a high-dimensional look-up table. Therefore, the application of the ILDM method seems to be very difficult for higher hydrocarbon fuels, especially in case of premixed flames where the burning velocity plays an important role.

In this paper a different method is presented to create a manifold. This method shares the idea with so-called flamelet approaches [16, 17] that a multi-dimensional flame can be considered as an ensemble of one-dimensional (1D) flames. This implies that the path followed in composition space in case of multi-dimensional flames will be close to the path found in 1D flames. Therefore, the chemical compositions in 1D flames are used to construct a manifold in this method. The resulting manifold, to which we will refer as Flamelet-Generated Manifold (FGM), will be a better approximation of the mixture composition in ‘colder’ zones of laminar premixed flames than the ILDM. As a result of this, less controlling variables are sufficient to represent the combustion process. Therefore, the dimension of the look-up table can be kept low, making it an interesting manifold method.

The main goal of this paper is to present the FGM method and to explain the basic ideas behind it. Although the technique can be applied to different kinds of flames, we focus here on atmospheric premixed laminar flames. A FGM will be constructed for a hydrogen/air mixture and it will be compared with the corresponding ILDM. For a methane/air mixture a FGM has also been generated, which has been used in several test simulations. The results of these simulations will be compared with results of detailed computations.

The outline of this paper is as follows. In the next section the so-called flamelet equations are derived starting from the set of three-dimensional instationary conservation equations describing the system. How a FGM is constructed for a premixed laminar flame using the set of
flamelet equations, is discussed in the following section. The main differences with the ILDM method are discussed briefly. The implementation of the FGM method in numerical simulations of laminar flames is demonstrated, subsequently. The main issues which are discussed are the implementation of the look-up table and the method used to solve the equations. Test results are reported for both one and two-dimensional (2D) laminar methane/air flames in the subsequent section. A discussion is given in the final section.

**FLAMELET EQUATIONS**

The evolution of chemically reacting flows is described by a set of differential equations representing the conservation of mass, momentum, species mass fractions, and energy. The equations are the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (1)$$

with \( \rho \) the mass density and \( \mathbf{v} \) the flow velocity, the momentum equations

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nabla \cdot \mathbf{\tau}, \quad (2)$$

where \( p \) denotes the pressure and \( \mathbf{\tau} \) the viscous stress tensor, the conservation equations for the \( N \) species mass fractions \( Y_i \)

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) - \nabla \cdot \left( \frac{1}{\text{Le}_i} \frac{\lambda}{c_p} \nabla Y_i \right) = \omega^+_i - \omega^-_i, \quad i = 1, \ldots, N, \quad (3)$$

and the balance equation for the enthalpy \( h \)

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{v} h) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) = \nabla \cdot \left( \sum_{i=1}^{N} h_i \left( \frac{1}{\text{Le}_i} - 1 \right) \frac{\lambda}{c_p} \nabla Y_i \right). \quad (4)$$

Here, the thermal conductivity \( \lambda \), the specific heat \( c_p \), and the Lewis numbers \( \text{Le}_i = \lambda/\rho D_i c_p \), with \( D_i \) the diffusion coefficient of species \( i \), have been introduced. The chemical source term is divided in a production part \( \omega^+ \) and a consumption part \( \omega^- \), consisting of the positive and negative contributions, respectively. The pressure is given by the perfect gas law

$$p = \rho R T \sum_{i=1}^{N} Y_i / M_i, \quad (5)$$

where \( R \) is the universal gas constant and \( T \) the absolute temperature. The specific enthalpy follows from

$$h = \sum_{i=1}^{N} Y_i h_i, \quad h_i(T) = h_i^o + \int_{T_0}^{T} c_{p,i}(\tau) d\tau, \quad (6)$$
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$M_i, c_{p,i}, h_i$ and $h_i^o$ being the molar mass, the specific heat, the specific enthalpy and the enthalpy of formation of species $i$, respectively.

The numerical solution of this set of equations is computationally expensive. Due to the large number of species which is involved in general, a large set of equations arises, which is strongly coupled by the chemical source terms. Furthermore, the different contributions to the chemical source terms describe processes with a wide range of time scales. This causes the set of equations to be stiff, which implies that special techniques have to be used to solve the system. In order to tackle this problem, the chemical reaction models can be simplified using reduction techniques. Most of these reduction methods are based on the assumption that a large number of species (or linear combinations of them), is in steady state. This implies that the left hand side of Equation (3) can be neglected for these species, leaving a balance between chemical production and consumption:

$$\omega_i^+ - \omega_i^- = 0, \quad i = 1, \ldots, M, \quad (7)$$

assuming the first $M$ species to be the steady-state species. The solution of this set of algebraic equations (7) forms a manifold which can be stored in a look-up table with dimension $N - M$. Due to the application of steady-state relations, both the number and the stiffness of the differential equations have been decreased.

These steady-state relations give, however, poor approximations in the 'colder' regions of a flame where convection and diffusion play an important role. In the cold region of a flame, where chemical reactions are negligible, bad manifold data will not hurt too much. However, there is an important region in flames where reaction and diffusion are in balance. A better approximation of the mixture composition in these regions can be found if we take the most important transport processes also into account. Since the major parts of convection and diffusion processes are also present in 1D flames, the compositions in 1D flames will be representative for the compositions in more general flames as well.

In order to explain this idea, we consider a part of a premixed flame as displayed in Fig. 1, and follow a curve $x(s)$ through the flame, locally perpendicular to isosurfaces of a certain species mass fraction $Y_j$, and parametrized by the arc length $s$. The evolution of all species mass fractions $Y_i$ along this curve may be described approximately by a one-dimensional equivalent of Equation (3)

$$m \frac{\partial Y_i}{\partial s} - \frac{\partial}{\partial s} \left( \frac{1}{Le_i c_{p,i}} \frac{\partial Y_i}{\partial s} \right) = \omega_i^+ - \omega_i^- + P_i, \quad i = 1, \ldots, N, \quad (8)$$

with $m$ taken to be a constant mass-flow rate. Since $x(s)$ is perpendicular to the isosurfaces of $Y_j$, the most important (1D) transport and diffusion phenomena are represented by the left-hand side of Equation (8). Multi-dimensional and transient effects — due to flame
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stretch, i.e. variations of the mass-flow rate along the curve, and curvature — are gathered in the perturbation term $P_i(s, t)$. This perturbation includes terms due to flame stretch, i.e. variations of the mass-flow rate along the curve, and curvature effects. For instance, a (most likely small) diffusion term associated with the curvature of the flame is included in $P_i$. Furthermore, the isosurfaces of $Y_{i \neq j}$ generally don’t coincide with the isosurfaces of $Y_j$, resulting in extra transport terms which are included in $P_{i \neq j}$.

It is expected that in most situations $P_i$ is small compared to the other terms in Equation (8), although this might not be justified under extreme circumstances, such as near local flame extinction and in regions with strong flame stretch. Therefore, the next step is to neglect the perturbation $P_i$, yielding a set of one-dimensional differential equations

$$m \frac{\partial Y_i}{\partial s} - \frac{\partial}{\partial s} \left( \frac{1}{Le_i} \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial s} \right) = \omega_i^+ - \omega_i^-, \quad i = 1, \ldots, N. \quad (9)$$

This resulting balance equation (9) between convection, diffusion and reaction can be considered as a steady-state relation just like Equation (7). Note that in conventional reduction techniques not only $P_i$ is neglected, but also the left-hand side of Equation (8). The set of equations (9), completed with a similar one-dimensional equation for the enthalpy, is referred to as a set of flamelet equations.

A solution of these equations $(Y_i(s), h(s))$ is called a flamelet and forms a curve in composition space which can be regarded as a one-dimensional manifold parametrized by $s$. In order to be able to use the manifold in further calculations it can be parametrized by a single controlling variable $Y_{cv}$. This controlling variable (or progress variable) may be the mass fraction of any (linear combination of) species which results in a unique mapping $Y_i(Y_{cv})$ for all $i$. This implies that $Y_{cv}(s)$ should be either a continuously increasing or decreasing function of $s$.

**FGM’s for Premixed Flames**

In this section it is described how the set of flamelet equations (9) is used to create a manifold. As in the ILDM method a distinction is made between variables which are conserved by chemical reactions (element mass fractions $Z_j$, pressure $p$ and enthalpy $h$) and variables which are changed by reactions: the species mass fractions. Note that the chemical composition of the burnt mixture is determined by the conserved variables, while the combustion process from unburnt to burnt is described by the reactive controlling variables, which are often called progress variables. Following Maas and Pope [12] we will first consider the case of constant pressure, enthalpy and element mass fractions.

In order to construct a manifold for premixed flames, the set of flamelet equations (9) can be solved treating the system as a freely-propagating premixed flame. This implies that the
boundary conditions at the unburnt side are of Dirichlet type

\[ Y_i(s \to -\infty) = Y_{u,i}, \quad (10) \]

\[ h(s \to -\infty) = h_u, \quad (11) \]

and at the burnt side of Neumann type

\[ \frac{\partial Y_i}{\partial s}(s \to \infty) = 0, \quad (12) \]

\[ \frac{\partial h}{\partial s}(s \to \infty) = 0, \quad (13) \]

and that the mass-burning rate \( m \) is an eigenvalue of the system. The resulting curve \( Y_i(s) \) is determined by its starting point \( (Y_{u,i}, h_u) \). The one-dimensional manifold in composition space is simply the flamelet starting at the point which represents the unburnt mixture for which the manifold is created. In this way the manifold connects the two most distinguished points in composition space: the point corresponding to the unburnt mixture and the equilibrium point.

As an example we have shown the one-dimensional ILDM and FGM for a stoichiometric hydrogen/air mixture in Fig. 2 together with a scatter plot of the chemical state at different positions in a 2D stationary premixed Bunsen flame stabilized on a cold burner rim computed using detailed chemical kinetics. The detailed reaction mechanism is a subset of the mechanism used in the Maas and Pope papers and includes 7 species and 7 reversible reactions. The mass fraction of H\(_2\)O is used as controlling variable, because it is continuously increasing during the combustion process from \( Y_{H_2O} = 0 \) at the unburnt mixture to the chemical equilibrium value \( Y_{H_2O} \approx 0.24 \). Generally, Lewis-number effects cause local enthalpy and element mass fraction variations in flames and thus also in the FGM database. In the ILDM method, however, the element composition and the enthalpy of the mixture are constant throughout the manifold and variations in the conserved variables can only be accounted for using additional controlling variables. Therefore, to make a fair comparison of the methods in Fig. 2, unit Lewis numbers are assumed in the computation of both the FGM and the 2D flame so that the element mass fractions and the enthalpy are constant in both manifolds. An example of a FGM computed using non-unit Lewis numbers, is presented in the following section. Note that the composition is determined by chemical processes in the high temperature range \( (Y_{H_2O} > 0.19, T > 1600K) \) and that the results of the ILDM and FGM method are therefore equivalent. However, in the ‘colder’ zone \( (Y_{H_2O} < 0.19) \) diffusion processes disturb the balance between chemical production and consumption, which causes the FGM to lie much closer to the detailed computation than the ILDM. In the ILDM method the number of controlling variables in this region should be increased to get accurate results. The addition of extra dimensions to the ILDM in order to satisfy accuracy requirements is described in [18].
The accuracy of the FGM method can be increased by increasing the number of progress variables as well. When the different terms in the perturbation $P_i$ cannot be neglected compared to the other terms in the flamelet equations, the number of progress variables should be increased. This can be done by increasing the dimension of the manifold in such way that the vector $P_i$ lies in the manifold so that its component perpendicular to the manifold can be neglected again.

A two-dimensional FGM can be constructed from a set of flamelets starting at different points on a 1D curve in composition space with constant conserved variables. This set of 1D flamelets forms a 2D surface in composition space: the 2D FGM. This method to generate multi-dimensional manifolds has been introduced by Pope and Maas [19]. A unique choice of the starting curve — manifold generator in [19] — cannot be given, although it should include the unburnt mixture and must be chosen in such way that the resulting manifold covers an as large as possible range of the controlling variables.

A projection of a 2D FGM on the CO$_2$–CO plane for a stoichiometric methane/air mixture is shown in Fig. 3. The origin in the plot corresponds to the unburnt mixture, which consists of CH$_4$, O$_2$ and N$_2$ only, and is connected with the equilibrium point by the 1D manifold. The projection of the starting curve coincides with the $x$ and $y$-axis in Fig. 3. Along the $x$-axis CO$_2$ and H$_2$O are added to the unburnt mixture, while along the $y$-axis CO and H$_2$ are added. Along the whole starting curve the enthalpy and the element mass fractions are kept constant, which causes all flamelets to end up in the same chemical equilibrium. The different flamelets rapidly converge to a one-dimensional manifold, which indicates that, apart from the conserved variables, one progress variable might be enough to describe the chemical state.

The choice of the starting curve determines the resulting manifold, but it may not be crucial. If we assume that two controlling variables are sufficient to represent the chemical composition in a premixed flame satisfactory, then the flamelets would rapidly relax towards a 2D attracting manifold. Therefore, however the starting points are chosen, the resulting manifold will be close to the underlying manifold except near the starting curve itself, where chemistry is negligible anyhow. This method to generate multi-dimensional manifolds can be extended to the general case of $d$ dimensions by choosing a $(d - 1)$-dimensional starting ‘plane’.

So far we only considered the case of constant conserved variables $p$, $h$ and $Z_j$. In general, one or more of these quantities vary in space or time. For instance, in burner-stabilized flames the enthalpy changes due to non-adiabatic effects resulting from flame stabilization. Furthermore, cooling due to radiation or walls may cause the enthalpy to decrease. To account for these enthalpy changes, the FGM can be extended with $h$ being an additional
parameter. To extend the manifold, the flamelet equations (9) are solved for different values of the initial enthalpy $h_u$. Corresponding to the $d$-dimensional manifold, we then obtain a $(d + 1)$-dimensional manifold parametrized by $d$ progress variables and $h$. Changes in the other conserved variables can be treated similarly, yielding a $(d + n_c)$-dimensional manifold, $n_c$ being the number of additional controlling variables. Note, $n_c$ has a maximum value of $n_c + 1$, the number of independent conserved variables with $n_e$ being the number of elements. However, for most applications only a small number of additional controlling variables is needed.

In the remaining part of this paper we will discuss the application of a FGM to laminar premixed burner-stabilized flames. Since in these flames only variations in the enthalpy and no large multi-dimensional perturbations are expected, a manifold will be used with two controlling variables: one progress variable and the enthalpy ($d = 1$, $n_c = 1$).

**IMPLEMENTATION OF FGM’S IN A REACTING-FLOW CODE**

The implementation of FGM’s in a reacting-flow code can be divided in roughly two parts: the first part exists of the generation and storage of the flamelet data and the second part is the coupling of a FGM with a multi-dimensional combustion computation.

The data to be stored are the solutions of the adiabatic flamelet equations for different values of $h_u$. The first flamelet is solved for an unburnt mixture with a relatively high temperature, say $T_u = T_{u,max} = 390$ K. For the following flamelets the enthalpy is decreased by lowering the temperature of the unburnt mixture in steps of approximately 30 K. The flamelet equations are solved using a Newton method, where the previous flamelet is used as the initial guess of the solution. Since the difference between two succeeding flamelets is small, a few iterations is sufficient to reach a converged solution. When an unburnt temperature of about $T_{u,min} = 240$ K is reached, another method to lower $h_u$ is applied, because lower temperatures would not be realistic. From this point the enthalpy is decreased by converting a fraction of the fuel with oxygen into products ($CO_2$ and $H_2O$), keeping the element composition constant and the temperature of the mixture at $T_{u,min}$. This process is continued until the flame temperature becomes too low and the flame extinguishes. As mentioned before, the exact way how the unburnt mixtures are chosen, influences only the unburnt side of the manifold, where chemistry is not important.

The resulting data set is shown in Fig. 4 for a stoichiometric methane/air mixture, where $Y_{O_2}$ and $h$ have been appointed as controlling variables. Note that, due to non-unit Lewis-number effects the enthalpy changes in each flamelet, but that the initial and equilibrium
value are the same. In literature several techniques to store manifold data have been proposed, ranging from artificial neural networks and *in situ* adaptive tabulation to orthogonal polynomials [20–22]. The most important criteria by which these storage techniques can be judged are the memory required for the storage of the table, the CPU time required to retrieve a value, and the accuracy of the retrieved value. In the following a method will be explained which exploits the geometry of the data set, resulting in a fast, accurate, and stable look-up procedure.

The manifold is stored as follows. For each separate flamelet all dependent variables, $\varphi$, which are needed in combustion simulations and the enthalpy are stored as a function of the progress variable. To realize this, the $Y_{cv}$ range is divided into equal-sized regions, and a cubic polynomial is fitted through the data points in each region. The resulting fit, consisting of the separate cubic polynomials, and its first derivative are forced to be continuous at the region boundaries. Moreover, the fit should match the data set exactly at both the unburnt and equilibrium composition. The accuracy of the fit can be improved by increasing the number of regions or the order of the polynomials.

To retrieve data from the manifold for given values of the controlling variables ($Y_{cv}^*, h^*$) the following procedure is followed. First it is determined where the entry ($Y_{cv}^*, h^*$) is located. Therefore, the enthalpy is evaluated in two succeeding flamelets at $Y_{cv} = Y_{cv}^*$, yielding $h^i$ and $h^{i+1}$ for flamelets $i$ and $i + 1$ (see Fig 4) such that $h^{i+1} < h^* < h^i$. In the next step, intermediate values for the dependent variables are evaluated in both flamelets: $\varphi^i$ and $\varphi^{i+1}$. The final value $\varphi^*$ is obtained using a linear interpolation between these values:

$$\varphi^* = \frac{h^* - h^{i+1}}{h^i - h^{i+1}} \varphi^i + \frac{h^i - h^*}{h^i - h^{i+1}} \varphi^{i+1}.$$  (14)

Due to this linear interpolation as a function of $h$, the first derivative of $\varphi$ with respect to $h$ is discontinuous at the flamelets, which may be a problem in gradient-based solvers. However, since the dependent variables change very smoothly in the direction of $h$, this imperfection has no consequences in our case.

One of the main advantages of this storage technique is that the boundaries of the tabulated domain are known very accurately. Therefore, effective measures can be taken if an entry is outside this domain, resulting in a robust look-up method. Such a measure is needed, for instance, when burnt gases are cooled intensively, e.g. due to a local heat sink. The enthalpy of the mixture then drops below that of the 'coldest' flamelet, and the composition enters the so-called low-enthalpy region, which is shown in Fig. 5. Since no flamelet data is available there, the manifold must be continued into this region. A similar problem occurs in the ILDM technique: at low temperatures the ILDM method doesn’t yield a solution and the manifold is continued into the cold region by linear extrapolation (see Fig. 1 in [13]). In
the FGM method the manifold is prolonged into the low-enthalpy region as follows. First
the low-enthalpy region is mapped onto the unit square \((\eta, \zeta) = [0, 1] \times [0, 1]\) using

\[
\eta = \frac{Y_{cv} - Y_{cv,b}}{Y_{cv,u} - Y_{cv,b}} \quad \text{and} \quad \zeta = \frac{h - h_{\text{min}}}{h^L - h_{\text{min}}},
\]

(15)

where \(h^L(Y_{cv})\) is the enthalpy at the coldest flamelet and \(h_{\text{min}}\) the enthalpy of the chemical
equilibrium with \(T = T_{\text{min}}\) (point \(A\) in Fig. 5). The dependent variables are denoted by
\(\varphi(Y_{cv}, h) = f(\eta, \zeta)\). The profiles of the dependent variables along the coldest flamelet and
along the chemical equilibria are known and given by \(f(\eta, 1)\) and \(f(0, \zeta)\), respectively. The
values in the low-enthalpy region are approximated by interpolation using these profiles:

\[
f(\eta, \zeta) = f(0, 1) - f(0, 0) \left\{ f(\eta, 1) - f(0, 0) \right\} + f(0, 0).
\]

(16)

Note that, since in most practical cases extensive cooling takes place in the burnt gases after
the flame front, most entries in the low-enthalpy region are very close to chemical equilibria
(\(\eta = 0\)), where almost no interpolation error is made. Although this procedure to continue the
manifold in the low-enthalpy region is rather ‘ad-hoc’ and might need some more attention,
it appears to work quite well.

Once the FGM is stored in a database, it can be linked to a standard flow field solver in
the same way as an ILDM. This means that the CFD code solves the conservation equations
for the controlling variables, together with the momentum and continuity equations. Once
a manifold is introduced, the conservation equations for the controlling variables are derived
by a projection of the governing equations onto the manifold. In the ILDM technique the
different terms in the governing equations are projected using the eigenvectors corresponding
to the fast chemical processes (see e.g. [13]). Due to the definition of the ILDM the convection
and the chemical source terms are not affected. Only the diffusion term contains a component
pointing out of the manifold, which must be projected. Although the eigenvector projection
is mathematically the only correct one, other (simplified) projection techniques have been
used successfully [14, 23, 24].

The projection in the FGM method is shown schematically in Fig. 6. In this figure it
can be seen how the different terms in Equation (8) are projected onto the manifold. Due
to the definition of the FGM, the convection \(C\), diffusion \(D\) and chemical reaction terms \(R\)
balance. Therefore, their projections will also balance independent of the projection used.
The only term which is affected by the projection is \(P\), representing the multi-dimensional
effects. However, since the perturbation \(P\) is much smaller than the other terms in (8), its
projection is not important, unless the flame is extremely stretched or curved locally. Note
again that if the perturbation cannot be neglected, the dimension of the manifold must be
increased in such way that the component of \(P\) pointing out of the manifold is small again.
Since the projection can be omitted, the conservation equation for \( Y_{cv} \) is given by Equation (3) with \( i = cv \):

\[
\frac{\partial \rho Y_{cv}}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_{cv}) - \nabla \cdot \left( \frac{1}{\text{Le}_{cv}} \frac{\lambda}{c_p} \nabla Y_{cv} \right) = \omega_{cv},
\]

with \( \omega_{cv} \) the net chemical source term. The balance equation for the enthalpy follows from Equation (4):

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{v} h) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla h \right) = \nabla \cdot \mathbf{F},
\]

where \( \mathbf{F} \) represents the enthalpy flux due to preferential diffusion:

\[
\mathbf{F} = \sum_{i=1}^{N} h_i \left( \frac{1}{\text{Le}_i} - 1 \right) \frac{\lambda}{c_p} \nabla Y_i,
\]

being a function of the species mass fraction gradients. Due to the introduction of a manifold, all species mass fractions \( Y_i \) are a function of the controlling variables \( Y_{cv} \) and \( h \). Therefore, the enthalpy flux can be written as

\[
\mathbf{F} = \sum_{i=1}^{N} h_i \left( \frac{1}{\text{Le}_i} - 1 \right) \frac{\lambda}{c_p} \left( \frac{\partial Y_i}{\partial Y_{cv}} \nabla Y_{cv} + \frac{\partial Y_i}{\partial h} \frac{\partial h}{\partial Y_{cv}} \nabla Y_{cv} \right).
\]

We now see that \( \mathbf{F} \) depends on the gradient of \( h \), which may lead to non-realistic energy fluxes. For instance at inert walls, where \( \frac{\partial Y_i}{\partial n} = 0 \) but \( \frac{\partial h}{\partial n} \neq 0 \), a non-realistic energy flux \( \mathbf{F} \) through the wall would occur. This problem is caused by the introduction of a manifold and is thus present in all manifold techniques. In the FGM method this problem can be circumvented by a substitution of the 1D manifold relation \( h = \mathcal{H}(Y_{cv}) \) in Equation (20).

This yields

\[
\mathbf{F} \approx \sum_{i=1}^{N} h_i \left( \frac{1}{\text{Le}_i} - 1 \right) \frac{\lambda}{c_p} \left( \frac{\partial Y_i}{\partial Y_{cv}} \nabla Y_{cv} + \frac{\partial Y_i}{\partial h} \frac{\partial \mathcal{H}}{\partial Y_{cv}} \nabla Y_{cv} \right).
\]

After some rearrangement and the introduction of a coefficient \( \alpha \), the enthalpy flux \( \mathbf{F} \) can be written as a function of the gradient of \( Y_{cv} \) only:

\[
\mathbf{F} = \alpha \nabla Y_{cv}.
\]

The coefficient \( \alpha \) is stored in the FGM database together with the variables needed to solve the conservation equations, i.e. \( \rho, \lambda, c_p \) and \( \omega_{cv} \). This is obviously much more efficient and accurate than storing the species mass fractions and computing the values of \( \alpha, \rho, \lambda, c_p \) and \( \omega_{cv} \) at run-time.
TEST RESULTS FOR METHANE/AIR FLAMES

To demonstrate the performance of the FGM method, two test cases of premixed laminar methane/air flames have been simulated using a manifold with two controlling variables, i.e. $Y_{O_2}$ and $h$. Results will be shown for one and two-dimensional burner-stabilized flames, and will be compared to results obtained with the full kinetics mechanism, which consists of 16 species and 25 reversible reactions [25].

One-dimensional validation

Apart from numerical inaccuracies, the most elementary premixed flame – the freely-propagating flat flame – would be reproduced exactly by the FGM technique. Burner-stabilized 1D flames, however, are subjected to non-adiabatic effects due to heat losses to the burner and are therefore more challenging. The burner outflow is positioned at $x = 0\,\text{cm}$ and the burner area $x < 0\,\text{cm}$ is kept at a constant temperature of $T_{\text{burner}} = 300\,\text{K}$. Stationary solutions are computed for different values of the mass-flow rate $m$ ranging from 0.005 to 0.040 $\text{g/cm}^2\,\text{s}$. The adiabatic mass-burning rate of this stoichiometric methane/air flame is $m = 0.0421\,\text{g/cm}^2\,\text{s}$ which corresponds to a laminar burning velocity of $s_L = 37.5\,\text{cm/s}$.

For $m = 0.030\,\text{g/cm}^2\,\text{s}$ the profiles of the controlling variables $Y_{O_2}$ and $h$ are shown in Fig. 7. It can be seen that the FGM method is in excellent agreement with the detailed reaction mechanism. Together with the enthalpy drop in the burner, the large gradients in the flame front due to lewis-number effects ($0 < x < 0.1\,\text{cm}$) are reproduced very well. The mass fractions of CH$_2$O and H are displayed as function of $x$ in Fig. 8. Even for these species, which are very difficult to reproduce accurately using ILDM, the resemblance between the FGM and detailed results is striking.

In Fig. 9 two global observables of 1D burner-stabilized flames are presented as function of the mass-flow rate. These global observables are the non-adiabatic flame temperature $T'_b$ and the stand-off distance $\delta$, here defined as the position where the absolute value of the chemical source term $|\omega_{O_2}|$ reaches its maximum. The flame temperature is measured in the burnt mixture at $x = 10\,\text{cm}$, and is presented in the form of an Arrhenius plot. The differences in the flame temperature are smaller than 5 K and, therefore, almost invisible in the figure. Even if the results for the stand-off distance is somewhat poorer, the deviation is within 1 percent of the flame thickness. Since at low mass-flow rates the deviation from an adiabatic flamelet increases, the difference between the FGM and detailed computations also increases, but it remains less than a few percent.
Two-dimensional validation

The potential of the FGM method is demonstrated by a calculation of a 2D burner-stabilized laminar premixed flame. In this test case almost all the features found in premixed laminar flames — such as flame cooling, stretch and curvature — are present. We have simulated a methane/air flame with an equivalence ratio of 0.9 which stabilizes on a 2D slot burner in a box. The burner configuration is shown in Fig. 10. The burner slot is 6 mm wide, while the box is 24 mm wide. The burner and box walls are kept at a constant temperature of $T_{\text{burner}} = 300 \text{K}$. The velocity profile at the inlet is parabolic with a maximum velocity of $v_{\text{max}} = 1.0 \text{m/s}$. Isocontours of $T$ and the mass fractions of CH$_2$O and H are shown in Fig. 11 on a portion of the computational domain for both the detailed and reduced computations.

It may be seen that the results obtained with the FGM method are in excellent agreement with the detailed computations: not only the position of the flame front is predicted very well, but the absolute values of the mass fractions are reproduced as well. Flame cooling governing the stabilization of the flame on the burner is captured very well by the FGM, although one can hardly speak of flamelets in this cold region. Also in the flame tip, where stretch and curvature are very important, the reduced computations appear to coincide with the detailed calculations.

Computation time

Besides the accuracy, the efficiency is another important aspect of reduction methods. In order to give an indication of the efficiency of the FGM method, the computation times of detailed and reduced simulations are compared. For both models we determined the time needed to perform a time-dependent 1D flame simulation for a period of $10^{-3}$ seconds under the same conditions. To solve the equations we used a fully implicit solver with varying time steps. The FGM method has also been used with an explicit time stepper using constant time steps. The computations are performed on a Silicon Graphics workstation and the computation times are shown in Table 1. The CPU time per time step reduces approximately a factor 8 when the FGM is applied. This speed up is caused by the reduction of the number of differential equations to be solved and a faster evaluation of the chemical source terms. Another advantage of the reduced model is that larger time steps can be taken, because the smallest time scales have been eliminated. Therefore, the total CPU time of the reduced computation is 20 times less than the detailed simulation. An even higher efficiency is reached if an explicit solver is used for the reduced computations. For more complex reaction mechanisms and multi-dimensional systems the speed up will be even larger.

The computation of the FGM database used in this paper involved approximately 30
minutes, which is quite long compared to the CPU times mentioned in Table 1. Obviously, it is not efficient to construct a FGM for a single 1D flame simulation. However, the computation time which can be gained using a FGM in a series of multi-dimensional flame simulations is orders of magnitude larger than the time needed to construct the database.

DISCUSSION

In this paper a new method has been presented to create low-dimensional manifolds and it has been applied to premixed laminar flames. Since in this method a manifold is constructed using one-dimensional flamelets, it can be considered as a combination of a manifold and a flamelet approach. The FGM method shares the assumption with flamelet approaches that a multi-dimensional flame may be considered as an ensemble of one-dimensional flames. The implementation, however, is typical for a manifold method, which means that the reaction rates and other essential variables are stored in a look-up table and are used to solve conservation equations for the controlling variables. Therefore, the local mass-burning rate follows from the balance between chemical reaction and multi-dimensional convection and diffusion. In classical flamelet approaches, however, a kinematic equation for the scalar $G$ is solved [17]. In this so-called $G$-equation the burning velocity enters explicitly and the influence of flame stretch and curvature on the mass-burning rate has to be modelled. Moreover, while the conservation equations for the controlling variables are valid throughout the complete domain, the $G$-equation is only valid at one value of $G = G^*$, which denotes the position of the flame sheet. Everywhere else $G$ is simply defined as the distance to the flame sheet, resulting in a flame of constant thickness. In the FGM method the flame thickness follows from the conservation equations and is in general not constant.

Another advantage of the FGM method is that the number of progress variables is not limited to one as in existing flamelet approaches. Although the test results of laminar premixed burner-stabilized methane/air flames show that one progress variable and the enthalpy are sufficient to reproduce detailed simulations very well, more progress variables can be added to increase the accuracy of the method. Addition of progress variables might cause problems in the look-up procedure as described in this paper, because the different flamelets rapidly converge to form a lower-dimensional manifold (see Fig. 3). However, this problem can be solved using a modified storage and retrieval technique, based on the lower-dimensional manifold.

There is no difficulty in adding further conserved controlling variables. For instance, to treat non-premixed flames the manifold can easily be extended so that variations in the mixture fraction can be accounted for. In order to generate a manifold for non-premixed flames, the flamelet equations are solved for different stoichiometries and an element mass
fraction can be used as extra conserved controlling variable.

In turbulent flames the perturbations (unsteady effects, flame stretch and curvature) will probably not be small compared to the other terms in the governing equations (1D convection, diffusion and reaction). Therefore, the dimension of the manifold should be increased in such way that the perturbation vector $P$ lies in the manifold. This can be done by adding an additional progress variable as described earlier, but also by including more of the physics in the flamelet equations. For instance, if flame stretch is expected to be important, a (constant-)stretch term can be included in the flamelet equations (9). Then the equations are solved for different stretch rates, which results in an extra dimension for the manifold.

The enormous reduction of computation time due to application of a FGM allows us to perform more extensive studies of realistic flames. More tests and experience will clarify the influence of unsteady effects, flame stretch and curvature.

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Flamelet-Generated Manifolds

\[ \eta = \text{const} \]

Equilibria

\[ \eta = 0 \]

Unburnt

\[ \zeta = 1 \]

Coldest flamelet

\[ h \text{ (J/kg)} \]

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