Modeling MILD combustion using a novel multistage FGM method
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Abstract

Moderate or intense low-oxygen dilution (MILD) combustion is a promising concept to reduce emissions and increase efficiency. It requires high levels of dilution and preheating of reactants, which is realized by mixing reactants with products. In order to extend the application areas of MILD combustion, adequate computational models must be developed. In this study, one of the candidate models, flamelet generated manifolds (FGM), has been assessed in terms of applicability to MILD combustion. Based on the results of this assessment, a novel multistage (MuSt) FGM method has been developed. The need for developing such a method mainly stems from the existence of different combustion stages in the MILD regime, which cannot be represented by a single progress variable. In the MuSt-FGM approach, each stage of combustion is modeled using a different progress variable, without increasing the dimension of the lookup table. The MuSt-FGM approach has been tested by conducting a priori study, and simulating both 1D laminar and 2D turbulent flames. Proving successful in all three tests, the MuSt-FGM method emerges as a promising tool for modeling not only MILD combustion, but also other systems where combustion is characterized by different stages.

Keywords: Multistage flamelet generated manifolds (FGM), Moderate or intense low-oxygen dilution (MILD), Non-premixed combustion, Autoignition, Jet in hot coflow (JHC).
1. Introduction

In a combustion system, it is desirable to have high efficiency and low emissions. These goals can be achieved simultaneously with a relatively new concept; moderate or intense low-oxygen dilution (MILD) combustion. In this concept, reactants are mixed with combustion products to create a hot and diluted initial mixture. Due to the recuperation of excess heat from the products, the efficiency increases; and due to the dilution of reactants, the increase and maximum level of temperature in the combustor are kept low, hence the emissions are suppressed. When the preheating is so high that the temperature of the reactants is above autoignition temperature, and the dilution is so intense that the temperature rise in the combustion chamber is below the autoignition temperature (in Kelvin), the system is in the MILD regime [1]. MILD combustion has other beneficial characteristics like silent operation and uniform temperature distribution [2, 3]. In the literature, it is also called as flameless oxidation (FLOX) [4] or high temperature air combustion (HiTAC) [5].

Although MILD combustion has been applied to industrial furnaces for some time [5], there are still unknown aspects to be revealed in order to extend its application to other areas like gas turbines. These aspects can be explored by DNS studies as in [6, 7], but DNS is computationally prohibitive even for a lab-scale burner, let alone an industrial application. Therefore, turbulence models and chemistry reduction techniques must be utilized to perform reliable computations of real combustors so that they can be designed and improved accordingly. Among the candidate models for such a task are flamelet based chemistry tabulation techniques like flamelet/progress variable (FPV) and flamelet generated manifolds (FGM). These techniques have already been used to simulate MILD combustion of non-premixed turbulent type and the results are compared with experimental ones in an averaged manner [8–12]. However, a thorough numerical investigation using detailed chemistry simulations is still needed to assess the suitability of chemistry tabulation techniques for MILD combustion.

When modeling adiabatic non-premixed flames, the general practice in FGM is to set controlling variables (CV) as mixture fraction (Z) and reaction progress variable (Y) [13], similar to other chemistry tabulation methods like FPV and FPI [14, 15]. Y is generally chosen as a combination of mass fractions of reactants and/or products [13, 14, 16, 17], because they are either consumed or produced throughout all combustion stages. However, Medwell et al. [18] found that in an autoigniting MILD system, initially a
preignition stage takes place in which precursors form, but reactants or products do not vary much. This is partly because the products are already present in the fuel and/or oxidizer stream in MILD combustion, hence the increase in product mass fractions is very minor in the preignition stage. In some internal combustion engine studies [19, 20], mass fractions of precursors were added to the definition of \( Y \) in order to capture the preignition period. Nevertheless, this might deteriorate the prediction capabilities in the oxidation stage since the precursors are consumed during this period. Therefore, it is troublesome to find a single and unique \( Y \) which would model the progress in every stage of combustion accurately, especially in the case of an autoigniting system.

In this study, a detailed \textit{a priori} analysis was conducted using 1D flames in order to assess the applicability of FGM method to MILD combustion of non-premixed type. Different \( Y \) definitions were tested to evaluate the performance variation by the choice of \( Y \). Judging by the results of these tests, a multistage (MuSt) FGM technique was developed to model each stage of combustion (preignition, oxidation, post-ignition, etc.) separately and accurately. Simulations with MuSt-FGM approach were carried out and compared with the detailed chemistry results.

2. Numerical method and simulation setup

Two basic assumptions in the FGM method [21] are that there exists a lower dimensional manifold in the composition space, and a turbulent flame is an ensemble of 1D laminar flamelets [22]. Prior to actual simulation of a flame, suitable 1D flames are solved and all the thermo-chemical variables are stored in lookup tables as functions of a few CVs which represent the manifold. In a CFD simulation, only the transport equations for the CVs are solved and all the required variables are looked up from the tables. CVs are selected as \( Z \) and \( Y \) in adiabatic non-premixed combustion, where \( Z \) represents the mixing of fuel and oxidizer, and \( Y \) models reaction progress. \( Y \) must increase monotonically throughout the whole combustion process in order to express composition space as a unique function of itself. In this study, \( Z \) was calculated using Bilger’s definition [23] and normalized such that \( Z_{\text{oxidizer}} = 0 \) and \( Z_{\text{fuel}} = 1 \), and \( Y \) was selected as a linear combination of species mass fractions.

The conditions to be investigated were chosen as the HM1 case of the jet in hot coflow (JHC) experiments of Dally et al. [24]. This case was shown to be operating in MILD regime, and was studied by the current authors in DNS context [7]. The fuel is composed of CH\(_4\) and H\(_2\) equal in volume, and the oxidizer has
3% of O$_2$, 85% of N$_2$, 6.5% of H$_2$O and 5.5% of CO$_2$ by mass fractions. The temperatures of the fuel and oxidizer are 305 K and 1300 K, respectively. The temperature and species profiles in the fuel and oxidizer were assumed to be constant for the sake of simplicity.

To assess the applicability of the FGM method to MILD combustion, it is first necessary to perform computations with detailed chemistry. These computations were conducted using CHEM1D [25], which is a 1D flame simulation tool developed at Eindhoven University of Technology. Igniting mixing layers (IML), which were shown to be successful in modeling JHC conditions [17], was selected as the flamelet type. In IML; the fuel and oxidizer are initially placed side by side, mix through molecular diffusion, and react in time. DRM19 [26] was used as the reaction mechanism, which includes 21 species and 84 reversible reactions. Since the fuel contains a large amount of hydrogen, the preferential diffusion effects are crucial in predicting the ignition delay, and can be accurately modeled using constant Lewis number approach as shown in [27]. The Lewis numbers used were calculated from the results of a simulation with multi-component diffusion model. The ignition delay was determined as the time at which the source term of HO$_2$ becomes negative, and verified by checking the temperature increase in Z–space.

For the FGM modeling part, firstly an a priori analysis similar to Ramaekers et al.’s study [28] was performed. This analysis can be summarized as follows: an FGM table is created using the flamelets from the detailed simulations with a suitable choice of Y and Z; Z and Y are calculated at every grid point and time step using the species mass fractions from the detailed solutions; using calculated Z and Y data, all the species, temperature, and Y source term information are looked up from the table; and the looked up values are compared with their counterparts from the detailed solution. A relative error for each of the looked up parameter $P_i$ was computed as:

$$
\epsilon_i = \frac{1}{N} \sum_{k=1}^{N} \frac{(P_{i\,\text{Detailed}} - P_{i\,\text{FGM}})}{\frac{1}{N} \sum_{k=1}^{N} |P_{i\,\text{Detailed}}|} \tag{1}
$$

where $N$ is the number of grid points. Since the same solution was used for both the FGM table creation and a priori testing, a perfectly monotonic Y would result in error terms very close to zero. However, it is not straightforward to find such a Y, especially for MILD combustion. The calculated errors were examined as a function of time. Among all the predicted parameters, the emphasis was put on the source term of Y, since its miscalculation would lead to inaccurate Y results and thus incorrect lookup.
After the *a priori* analysis, actual FGM simulations in 1D were performed. The solutions of the detailed and FGM simulations were compared in terms of the evolution of reaction progress. Finally, the same case used in 1D simulations was investigated by performing 2D DNS in the form of autoigniting mixing layers using detailed chemistry, standard FGM, and MuSt-FGM. The details of DNS settings can be found in [7]. In the DNS calculations, unity Lewis number assumption was adopted for simplicity.

3. Standard FGM

In an FGM study, the first action is to select a suitable $Y$ which would monotonically increase throughout the process. In this study, we made a few selections based on different approaches. Firstly, we followed the traditional approach and selected $Y$ as $Y_{H_2O}$. This is because the flame in consideration is dominated by hydrogen chemistry and H$_2$O is the main product of the hydrogen combustion. As a second candidate, $Y_{HO_2}$ was chosen as $Y$ following the findings of Medwell et al. [18], where they mention that in a MILD system, firstly the preignition chemistry takes place and the precursor species like HO$_2$ and CH$_2$O are produced, while the final products are not formed in considerable quantities. Finally a combination of H$_2$O and HO$_2$ was selected as $Y$ in an effort to include the effects of both the preignition and oxidation chemistries, as was done in engine related studies [19, 20]. The weight of $Y_{HO_2}$ was selected as 1000 times that of $Y_{H_2O}$ to make the mass fractions and the source terms of the two species comparable.

FGM tables were created using the abovementioned $Y$ selections and the *a priori* study was performed for each selection. The errors in computing the source term of each $Y$ are shown in Fig. 1. It is seen that the standard selection of $Y = Y_{H_2O}$ fails to predict its source term by a factor of 100 in the beginning of the simulation. The error gradually drops below 1% and stays very low after the autoignition. On the other hand, $Y_{HO_2}$ performs very well until the ignition, but becomes quite unsuccessful afterwards. The compromise selection of $Y = Y_{H_2O} + 1000 \times Y_{HO_2}$ behaves somewhere in between, as expected. It produces a substantial error of 35% in the very beginning of the simulation. The error decreases afterwards until the ignition and keeps moderate during the ignition, but increases during the oxidation period and exceeds 100%. It should be noted that other combinations of $Y_{HO_2}$ and $Y_{H_2O}$ have been tried, but they either failed in the beginning of the simulation, or through the end. These trials are not presented here for the sake of brevity.

The reason for the large error terms was investigated for each $Y$ definition. Firstly, the evolution
of each $\mathbf{Y}$ at $Z_{st} = 6.7 \times 10^{-3}$ was examined to check if there are any non-monotonicities. As seen in Fig. 2a, $\mathbf{Y}_2 (Y_{HO_2})$ decreases after the ignition takes place, which explains why it fails as a $\mathbf{Y}$ in that region. Although $\mathbf{Y}_1 (Y_{H_2O})$ does not exhibit any non-monotonicity, its growth is extremely slow in the beginning of the simulation, while its source term increases exponentially in the same region (not shown here). This means that a slight miscalculation of $\mathbf{Y}$ will lead to an enormously large error in the look-up of $\omega_{\mathbf{Y}}$, which will eventually cause the solution to diverge. Addition of $1000 \times Y_{HO_2}$ to $Y_{H_2O}$ seems enough to overcome this problem as $\mathbf{Y}_3 (Y_{H_2O} + 1000 \times Y_{HO_2})$ exhibits a large enough growth in the beginning of the simulation. In addition, $\mathbf{Y}_3$ is monotonic throughout the simulation at $Z_{st}$ as well, which means that its failure to predict its source term cannot be explained by examining only the stoichiometric conditions.

The changes in $\mathbf{Y}$ were further analyzed at the lean ($Z = 4 \times 10^{-4}$) and rich ($Z = 0.6$) conditions, and are also presented in Fig. 2. It is noticed that at lean condition, the values of $\mathbf{Y}_2$ and $\mathbf{Y}_3$ drop after the ignition, and thus become non-monotonic. Even though the amount of decrease is small, any non-monotonic behavior of $\mathbf{Y}$ is excluded from the FGM table, and therefore the oxidation phase cannot be covered at all by $\mathbf{Y}_2$ and $\mathbf{Y}_3$ at the lean conditions. This situation explains why the performance of $\mathbf{Y}_3$ deteriorates as the simulation proceeds. At $Z = 0.6$, $\mathbf{Y}_1$ and $\mathbf{Y}_3$ exhibit non-monotonic behaviors right from the beginning, which explains their high error terms at the start of the simulation (see Fig. 1). Although $\mathbf{Y}_3$ performs better than $\mathbf{Y}_1$ in the sense that it starts to increase earlier, it cannot resolve the issue all together.

It can be deduced that the combination of the mass fractions of HO$_2$ and H$_2$O to find a suitable $\mathbf{Y}$ is a trade off: as the weight of HO$_2$ is increased, the preignition chemistry is better represented and the non-monotonicity at the rich side is eased; but the oxidation chemistry is missed and the non-monotonicity in

Figure 1: Relative error terms for the prediction of the source term of each progress variable definition, calculated through *a priori* analysis. The vertical black line indicates the start of ignition.
Figure 2: Evolution of normalized progress variables at $Z_{st} = 6.7 \times 10^{-3}$ (a), $Z = 4 \times 10^{-4}$ (b) and $Z = 0.6$ (c). Normalization was done using the global extremes at the corresponding mixture fractions. The vertical black lines indicate the start of ignition.
the lean side is amplified. With the selection of \[ \mathcal{Y} = Y_{H_2O} + 1000 \times Y_{HO_2}, \] the error terms are quiet large both in the very beginning of the simulation and through the end, therefore increasing or decreasing the weight of HO\(_2\) will make it worse for either of the boundaries. \( \mathcal{Y} \) might be made monotonically increasing for all the \( Z \) values through a careful inspection of the evolution of all the species instead of just \( H_2O \) and HO\(_2\), and by fine tuning species weights; or better yet through an optimization study as in [29–31]. However, the purpose of this study is not to perform such an optimization procedure, but to propose an alternative approach; multistage FGM, which is discussed in detail in the next section. It is worth mentioning that all of the \( \mathcal{Y} \) definitions discussed in this section are tried in \textit{a posteriori} sense to compute the flame using FGM. The calculations with \( \mathcal{Y}_1 \) and \( \mathcal{Y}_3 \) either numerically failed to converge or did not result in ignition, and the results with \( \mathcal{Y}_2 \) are highly inaccurate for the oxidation region, as presented in the next section.

4. Multistage FGM

The concept of multistage (MuSt) FGM was inspired by the findings of the standard FGM; in an autoigniting MILD system, precursors like HO\(_2\) represent the preignition region accurately, while the products like \( H_2O \) is successful in capturing the ignition-oxidation region. The basic idea is to use two \( \mathcal{Y} \)s; one until the autoignition and another afterwards, without increasing the dimension of the manifold. Although the basic idea is simple, the implementation is not straightforward. One option might be to create a single scaled \( \mathcal{Y} \) out of the two \( \mathcal{Y} \)s. This can be achieved by calculating \( \mathcal{Y}_1 \) using the flamelets only until the ignition and \( \mathcal{Y}_2 \) using those after the ignition, and then attaching two \( \mathcal{Y} \)s back to back to create a single FGM table. The continuity of the \( \mathcal{Y} \)s can be ensured by tuning the weight coefficients, but there would be a jump in the source term since two different definitions of \( \mathcal{Y} \) are used. Therefore, two separate FGM tables are created for two \( \mathcal{Y} \)s, and each one of the tables is used for a different stage of combustion.

When there are two different \( \mathcal{Y} \)s with two separate tables, the problem is to determine for which \( \mathcal{Y} \) to solve a transport equation and/or from which table to lookup. We adopted the strategy to solve transport equations for both of the \( \mathcal{Y} \)s simultaneously at all times, and make the lookup selection based on some threshold variable. For this method to work, the source terms of both of the \( \mathcal{Y} \)s must be stored in both of the tables. Since HO\(_2\) is rapidly consumed when the oxidation reactions start, the point when \( Y_{HO_2} \) reaches its maximum in \( Z \)–space can be used as an indication of the end of the preignition phase and the beginning
of the oxidation phase. However, the value of $Y_{\text{HO}_2}$ itself cannot be used as a threshold variable since it will decrease after reaching its maximum and this makes it impossible to determine whether the process is in preignition or oxidation stage. On the other hand, $Y_{\text{H}_2\text{O}}$ will always increase once the fast oxidation reactions start and thus can be used as the threshold parameter. Therefore, it was decided to create the second table using the points after $Y_{\text{HO}_2}$ reaches its maximum in $Z$–space, and then use the minimum values of $Y_{\text{H}_2\text{O}}$ in the second table as the threshold parameter to decide on which table to lookup during MuSt-FGM calculations.

To illustrate how the tables are created in the MuSt-FGM approach, the parts of the flamelet solution used in generating the first and the second table are shown in Fig. 3a. The segments that are drawn in red are used in the table generation, and the parts drawn in black are discarded. It is seen that at $Z_{st}$, $Y_1$ reaches its maximum around the autoignition time and thus only the points before that are used in the first table generation, and only the points after that are used in the second table generation. At $Z = 0.6$ on the other hand, $Y_{1,max}$ and therefore switch occurs around 0.6 ms. Figure 3b shows how the table to be looked-up during a MuSt-FGM simulation is determined. If the value of $Y_2$ is lower than $Y_{2,min}$ in the second table (shown with the black line), lookup from the first table; else, lookup from the second table. The red line in Fig. 3b shows the initial value of $Y_2$ in the detailed simulations.

Overall, the steps of the MuSt-FGM approach can be summarized as follows:

- Select a precursor species as $Y_1$, and a product species as $Y_2$. $\text{HO}_2$ and $\text{H}_2\text{O}$ were selected in the current case.
- Generate the first table until the maximum of $Y_1$ is reached in the $Z$–space, and create the second table from there on.
- Store the source terms of both of the $Y$s in both of the tables.
- Solve two transport equations for two $Y$s, in addition to a $Z$ equation, during the actual CFD calculations with FGM.
- In the CFD calculations, if the value of $Y_2$ is below the minimum $Y_2$ from the second table, lookup from the first table; else, lookup from the second table.
Figure 3: MuSt-FGM method clarification: Table generation details (a) and lookup table determination during simulations (b). The red segments in (a) show the parts of the detailed solution used in table generation, and the black segments are the parts discarded. The black line in (b) is the threshold value of $\mathcal{Y}_2$ to determine the table to be looked up during a simulation with MuSt-FGM. The red line in (b) shows the initial value of $\mathcal{Y}_2$ from the detailed simulations, and the colors represent $\omega_{\mathcal{Y}_2}$ in kg/m$^3$s.
These steps are listed here as a two-stage strategy since it is sufficient for the current case. However, it can easily be extended to N-stage whenever necessary. For example, a third stage for the post-oxidation emission phase can be added to the current case in the future.

As in standard FGM, firstly a priori test was conducted for the MuSt-FGM approach. The error terms for the source terms of both \( Y_1 \) and \( Y_2 \) are shown in Fig. 1. It is seen that the error for the source term of \( Y_1 \) is very small in the beginning of the computations, reaches a maximum of 2% right after the autoignition due to the transition between two FGM tables. For \( Y_2 \), the error term is below 1% during the preignition and oxidation periods, and it peaks at 2.5% around autoignition with the same reason as \( Y_1 \). In overall performance, the MuSt-FGM approach seems promising with error terms staying low all the time and substantially smaller than those of the standard FGM cases.

An actual 1D simulation using the MuSt-FGM approach was successfully performed as well for the current case. The FGM tables for \( \text{HO}_2 \) as \( Y_1 \) and \( \text{H}_2\text{O} \) as \( Y_2 \) were generated as described earlier. Figures 4a-4c show the maximum of \( Y_1 \) and \( Y_2 \) in the whole domain, and the maximum temperature increase in Z–space from the detailed chemistry and MuSt-FGM results. Figure 4a also includes the result of standard FGM calculation with \( Y = Y_{\text{HO}_2} \). It is seen that the evolution of all the three parameters is captured perfectly during the preignition, autoignition and oxidation periods using MuSt-FGM method; whereas standard FGM is successful in the preignition period but fails considerably in the oxidation region. These results demonstrate the success of the MuSt-FGM method in modeling autoigniting MILD flame in a 1D setting.

The MuSt-FGM approach was further tested in turbulent conditions by conducting a 2D DNS of the same configuration in the form of autoigniting mixing layers. Calculations with detailed chemistry, MuSt-FGM, and standard FGM were performed and the results were compared. \( Y \) definitions for the MuSt-FGM case were kept the same as in 1D simulations, and \( Y_3 \) was used for the standard FGM case. The details of the DNS settings can be found in [7]. The evolution of temperature field is given in Fig. 5 to provide an idea on how the mixing layers develop.

The average heat release rate and source term of \( Y_2 \) are calculated from the DNS results and presented in Fig. 6. The increase in the heat release occurs earlier in the MuSt-FGM case than the detailed one, as a result the ignition delay is shorter in the former by 8%. The trend of first increasing and then decreasing heat release is consistent in both cases, which demonstrates the success of MuSt-FGM in modeling the
Figure 4: Evolution of the maximum values of $Y_1$ (a) and $Y_2$ (b), and maximum temperature increase in $Z$-space (c). The vertical black line indicates the start of ignition.

Figure 5: Temperature field from the DNS with MuSt-FGM at $t = 0.1, 0.3, 0.5$ ms from left to right.
Figure 6: 2D DNS results: average heat release rate in W/m$^3$ (a) and average $\omega Y_2$ in kg/m$^3$s

autoignition and oxidation periods. Although standard FGM predicts the ignition delay with a reasonable accuracy, it completely fails to capture the oxidation region. Consistent with heat release rate, $\omega Y_2$ exhibits an earlier increase in the MuSt-FGM case, but agrees well the detailed case later on. These results verify that the MuSt-FGM method can model a turbulent flame which includes stretch and curvature effects. Standard FGM results are not shown in Fig. 6b because it does not solve for $Y_2$.

5. Conclusion

In this study, we have performed an *a priori* analysis using 1D flames to evaluate the applicability of FGM method to non-premixed MILD combustion. Performance of different progress variable selections has been tested. Based on the results of the *a priori* analysis, multistage (MuSt) FGM method has been developed. Using MuSt-FGM approach, the *a priori* analysis has been repeated, and actual 1D MuSt-FGM calculations have been performed. Finally, 2D DNS of the same configuration has been conducted using detailed chemistry, standard FGM and MuSt-FGM. The main conclusions are as follows:

- Standard FGM with single progress variable cannot model an autoigniting MILD system. This is
because there are different stages of combustion in this system such as preignition, autoignition, and oxidation; and finding a single $\mathcal{Y}$ which represent them all is very difficult, if not impossible.

- It is feasible to represent different stages of combustion using a unique $\mathcal{Y}$ for each stage without increasing the dimension of the FGM table. This idea is formulated as MuSt-FGM approach and used in the calculations.

- MuSt-FGM successfully captures all the stages of combustion in a 1D flame, as shown in both \textit{a priori} and \textit{a posteriori} manner.

- Even in a 2D turbulent environment, MuSt-FGM reproduces the detailed solution reasonably well, demonstrating its success in modeling a flame including curvature and stretch effects.

Storing two tables instead of one might seem like a disadvantage of MuSt approach in terms of memory requirement. However, since two tables represent two different stages of combustion, the number of grid points in a MuSt table can be half of what it would be in a standard FGM table with the same resolution. Therefore, no extra memory is requested in the MuSt-FGM approach. In addition, resolution of two tables can be set differently to meet different needs of each combustion stage, which is an advantage over standard FGM. The only extra computational cost of MuSt approach is the additional transport equation(s) to be solved for additional $\mathcal{Y}(s)$. Nevertheless, this is a tiny cost which can certainly be tolerated considering the accuracy MuSt-FGM method provides.

MuSt-FGM can be useful in other application areas like diesel combustion to capture autoignition and two-stage ignition. It can also be used to calculate emissions like NO$_x$ and CO by representing the slow chemistry of post-combustion zone with a suitable additional $\mathcal{Y}$ like the mass fraction of the emitted species itself. It is also worth mentioning that although MuSt method was introduced as an alternative to $\mathcal{Y}$ optimization techniques, it can actually be combined with those methods to optimize the $\mathcal{Y}$ definition of each stage.

In the future, MuSt method will be further tested using 3D DNS calculations, both in \textit{a priori} manner and by conducting actual calculations, to investigate its success in modeling MILD combustion in a 3D turbulent environment.
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