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Modeling curvature effects in turbulent autoigniting non-premixed flames using tabulated chemistry

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Abstract

Turbulent flames are intrinsically curved. In the presence of preferential diffusion, curvature effects either enhance or suppress molecular diffusion, depending on the diffusivity of the species and the direction of the flame curvature. When a tabulated chemistry type of modeling is employed, curvature-preferential diffusion interactions have to be taken into consideration in the construction of manifolds. In this study, we employ multistage stage flamelet generated manifolds (MuSt-FGM) method to model autoigniting non-premixed turbulent flames with preferential diffusion effects included. The conditions for the modeled flame are in MILD combustion regime. To model the above-mentioned curvature-preferential diffusion interactions, a new mixture fraction which has a non-unity Lewis number is defined and used as a new control variable in the manifold generation. 1D curved flames are simulated to create the necessary flamelets. The resulting MuSt-FGM tables are used in the simulation of 1D laminar flames, and then also applied to turbulent flames using 2D direct numerical simulations (DNS). It was observed that when the curvature effects are included in the manifold, the MuSt-FGM results agree well with the detailed chemistry results; whereas the results become unsatisfactory when the curvature effects are ignored.

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Keywords: Multistage (MuSt) FGM; Tabulated chemistry; MILD combustion; Preferential diffusion; Flame curvature

1. Introduction

Curvature (denoted as κ) is an inherent feature of turbulent flames. It either strengthens or weakens the effects of preferential diffusion depending on the Lewis numbers of species and the direction of curvature [1]. This phenomenon is depicted in Fig. 1: for the species that lie on the concave side

of the flame front (at the same side as the center of curvature), the molecular diffusion speed decreases if $Le < 1$, and increases if $Le > 1$, compared to a flat flame. On the other hand, for the species that lie on the convex side of the flame front (opposite side of the center of curvature), the molecular diffusion speed increases if $Le < 1$, and decreases if $Le > 1$, compared to a flat flame. As a result, whenever preferential diffusion effects are important in a flame, the interaction with curvature should be considered as well. These interactions have been studied extensively for both premixed [2–6] and non-premixed flames [7–13]. In this text, we define the flame

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Fig. 1. Sketch depicting the effects of flame curvature on molecular diffusion of species. When flame curvature is concave to fast diffusing species (left), it suppresses the preferential diffusion. When flame curvature is convex to fast diffusing species (right), it strengthens the preferential diffusion.

curvature to be positive when the center of curvature lies on the oxidizer side, and negative when the center of curvature lies on the fuel side.

Verhoeven et al. [14] and more recently Abtahizadeh et al. [15] have investigated the inclusion of preferential diffusion effects in FGM modeling for non-premixed flames. Even though their modeling efforts proved successful, Verhoeven et al. reported that at the tip of the flame where curvature effects are important, considerable deviations from the simulations with detailed chemistry were observed. This conclusion strengthens the hypothesis that curvature effects should be accounted for in modeling efforts whenever preferential diffusion is present.

The inclusion of curvature effects in tabulated chemistry type of modeling has been performed for premixed flames [16]. In that work, van Oijen et al. showed that stretch and curvature effects can be sufficiently modeled by increasing the dimension of the manifold. Xuan et al. [17] and Scholtissek et al. [18,19] have revised the standard flamelet equations [20] for non-premixed flames, and accounted for the curvature terms. By performing a multi-scale asymptotic analysis, Scholtissek et al. showed in [18] that depending on parameters like curvature, scalar dissipation, and flame thickness; diffusion along mixture fraction (Z) iso-surfaces can become important, and the dimension of manifold that can represent the composition space increases. Xuan et al. solved steady flamelet equations with additional curvature terms, tabulated the thermo-chemical variables using Z , scalar dissipation rate (χ) and κ , applied it to a laminar non-premixed flame and obtained reasonable results. However, they did not consider unsteady effects and used prescribed profiles for χ and κ as a function of Z . In the literature surveyed, no attempt to model curvature effects in a non-premixed autoigniting flame using a tabulated chemistry type of chemical reduction method has been found.

In this study, the effects of flame curvature-preferential diffusion interaction are modeled using multistage flamelet generated manifolds (MuSt-FGM). The composition investigated is taken from the jet in hot coflow (JHC) experiments of The University of Adelaide [21], because it was shown that preferential diffusion effects are of utmost importance for this case [22]. The flame in consideration is an autoigniting one, operating in MILD combustion mode. For MILD combustion, predicting ignition delay is crucial and highly challenging. To meet this challenge, capturing pre-ignition chemistry is of utmost importance, as was previously demonstrated by the current authors [23]. In the tabulation procedure, in addition to the standard control variables of non-premixed combustion, namely the transported mixture fraction and progress variables, a new mixture fraction with a non-unity Lewis number is defined to include the effects of preferential diffusion. Tubular opposed flamelets are simulated in a transient manner to generate the MuSt-FGM tables, and simulations of 1D curved flames as well as 2D turbulent flames are performed. It is demonstrated that the extended 3D manifold with curvature-preferential diffusion interactions included performed very well compared to the detailed chemistry cases, whereas the simulations with a 2D manifold failed to predict the chemistry accurately.

In the following sections of this study; numerical methods used and the simulation settings are given, the results are presented and discussed, and some conclusions are drawn.

2. Numerical methods and simulation setups

In order to model the effects of curvature with MuSt-FGM, it is first necessary to create flamelets with curvature. For non-premixed flames, the flame curvature (κ) can be defined as $\kappa = \nabla \cdot \mathbf{n}$, where $\mathbf{n}$ is the normal vector of the iso-surface of mixture fraction. To create curvature in unsteady flamelets, an opposed tubular flow configuration was used, which was approximated as a counterflow flame with constant curvature. This approximation was validated in [17], and the reader is referred to that study for the details of the equations solved in an opposed tubular flow configuration. To isolate the effects of curvature from other parameters, strain rate was kept constant at 300 s^{-1} , and curvature was varied from -1 mm^{-1} to 1 mm^{-1} with increments of 0.1 mm^{-1} between each simulation. Time dependent calculations were performed with these settings and autoigniting flamelets were obtained, using the 1D code called Chem1D [24]. Transport equations solved and numerical methods employed in Chem1D can be found in the work of Somers [24]. As mentioned in Section 1, the composition used is taken from the JHC configuration from Dally et al. [21], because this case contains

Table 1

Boundary conditions used in the simulations. Y represents the species mass fraction. Adiabatic flame temperature at $Z_{t,st} = 5 \times 10^{-3}$ is 1394 K.

Fuel	Oxidizer
$T = 305 \text{ K}$	$T = 1056 \text{ K}$
$Y_{H_2} = 0.11$	$Y_{O_2} = 0.03$
$Y_{CH_4} = 0.89$	$Y_{N_2} = 0.85$
	$Y_{H_2O} = 0.065$
	$Y_{CO_2} = 0.055$

Fig. 2. Distribution of the mass fraction of H_2 at $t = 0$ ms, and new CV Z_H for all t , against transported mixture fraction, Z_t , for various curvatures from -1 mm^{-1} to 1 mm^{-1} .

a large amount of hydrogen and preferential diffusion is of utmost importance. The temperature of the oxidizer entering the primary combustion chamber in the JHC experiments is varying, and a value of 1056 K is selected in this study to provide curvature effects sufficient time to have an effect on the ignition characteristics. It was seen that when the maximum temperature of 1300 K is used, the ignition in the turbulent case is not altered by the curvature effects [25]. The composition of the fuel and oxidizer are given in Table 1.

The initial distributions of H_2 in the flamelets in mixture fraction space is shown in Fig. 2. It is seen that the profile of H_2 is affected considerably with changing curvature. As mentioned in the literature [12,17], positive curvature enhances the preferential diffusion and thus more H_2 is mixing with the oxidizer at molecular level, whereas negative curvature has the opposite effect. To demonstrate how the curvature affects ignition, the evolution of maximum temperature in the whole domain for flamelets with different curvature values is given in Fig. 3. Since the case investigated has an initial maximum temperature very close to the stoichiometric mixture fraction, the evolution of the maximum temperature in the whole field provides information on ignition delay. It is observed that while positive curvature does not alter the ignition timing significantly, negative curvature delays

Fig. 3. Evolution of maximum temperature for curved flamelet cases. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the ignition almost three-fold. The reason for this asymmetry between positive and negative curvatures can be found out by examining Fig. 2 closely. At $Z_{t,st} = 5 \times 10^{-3}$, the mass fraction of hydrogen increases two-fold going from zero curvature to $\kappa = 1 \text{ mm}^{-1}$, whereas it decreases almost six-fold when curvature becomes $\kappa = -1 \text{ mm}^{-1}$. For this configuration, at zero curvature case the hydrogen content is already too high that increasing it further does not change the ignition dynamics a lot, whereas decreasing it has a big impact.

The second step is to select a suitable control variable (CV) that would represent the effects of curvature accurately. The instinctive selection would be curvature itself, as was implemented in the work of Xuan et al. [17]. However, curvature is an instantaneous parameter, and hence it lacks the information regarding what happens in time before that particular instance. Using curvature as a CV would be analogous to using strain rate or scalar dissipation rate instead of progress variable to represent the chemical progress. Therefore, to be able to simulate a transient case properly, it is essential to select a CV which can reflect the history effects of curvature, while being distinct from other CVs, i.e., mixture fraction and progress variables. For this purpose, a new mixture fraction was defined, which varies between 0 and 1 from oxidizer to fuel when normalized like the standard mixture fraction, but has the diffusivity equal to that of H_2 . Therefore, it can be considered as the normalized non-reacting mass fraction of H_2 . This new CV is named Z_H and will be called so throughout the text. The diffusivity of Z_H is chosen the same as H_2 because it is a species which shows strong preferential diffusion, and is present in the current configuration in large quantities. Due to its preferential diffusion, Z_H would feel the effects of curvature; while it will be independent of progress variable(s) because it is a passive scalar. For convenience, its initial value is selected as equal to Y_{H_2} ; but unlike

Y_{H_2} , distribution of Z_H in Z_t space does not change throughout the flamelet simulation. Therefore, the profiles of Z_H shown in Fig. 2 are dependent only on the prescribed curvature values, which demonstrates that Z_H correlates well with flame curvature.

In order to represent the pre-ignition and oxidation stages of combustion accurately, the multistage (MuSt) FGM method is utilized [23]. In this method, combustion is divided into appropriate stages such as pre-ignition, oxidation, and post-oxidation (emission) stages, and each stage is represented with a different progress variable ($\mathcal{V}$) and a corresponding MuSt-FGM table. Each $\mathcal{V}$ is solved throughout the whole combustion process, but the table to be used in the retrieval process is changed depending on the combustion stage. The active combustion stage during calculation is determined based on the calculated values of $\mathcal{V}$ s. Required combustion stages to be modeled for this case were determined based on our experience with the case simulated. In the future, this process can and should be automated. The reader is referred to [23,25] for more information.

Using transported mixture fraction (Z_t), Z_H , $\mathcal{V}_1 = Y_{HO_2}$, and $\mathcal{V}_2 = Y_{H_2O}$ as CVs, MuSt-FGM tables are generated. Z_t is a passive variable, which is 0 at the oxidizer side and 1 at the fuel side, and a transport equation is solved with $Le_{Z_t} = 1$ to calculate the values in between. Therefore it is not directly calculated using species or elemental mass fractions. Z_t was used instead of Bilger's definition to keep the distribution of Z_H constant in Z_t space. Z_t at the stoichiometric composition is found to be $Z_{t,st} = 5 \times 10^{-3}$, which is slightly lower than $Z_{B,st} = 6.7 \times 10^{-3}$, where Z_B is Bilger's definition of mixture fraction. Y_{HO_2} and Y_{H_2O} were chosen as $\mathcal{V}_1$ and $\mathcal{V}_2$ because the case is dominated by hydrogen chemistry, and these species are a precursor and a product of hydrogen autoignition, thus representing the pre-ignition and oxidation stages well. The MuSt-FGM tables generated are 3D tables with $100 \times 21 \times 100$ grid points in Z_t , Z_H , and $\mathcal{V}$ directions for each table. The grid points in Z_t direction are clustered around $Z_{t,st} = 5 \times 10^{-3}$.

Using the generated tables, MuSt-FGM calculations were performed first to simulate 1D laminar flames, using the same tubular opposed configuration as in the flamelet generation. Then 2D DNS calculations were performed in the form of autoigniting mixing layers. In the DNS, a fuel slab is placed in between two oxidizer layers initially in y-direction, and a relative initial velocity is given between the fuel and the oxidizer in x-direction, as shown in Fig. 4. Periodic boundary conditions are given in x-direction, whereas non-reflective outflow boundary conditions are applied in y-direction. To accelerate the shear layer development between the fuel and oxidizer, some turbulent fluctuations are imposed initially. 257×1025 grid points in the x and y-directions are used, respectively. The reader

Fig. 4. Not to scale sketch of the DNS domain.

is referred to [22] for a more elaborate description of the DNS code, solved transport equations, and simulation setup. In addition to MuSt-FGM calculations with a 3D table, the same calculations are performed with 2D MuSt-FGM application without the inclusion of curvature effects, and also with detailed chemistry. Detailed chemistry computations are performed using DRM19 reaction mechanism [26], and the results are used as a reference for the MuSt-FGM cases.

3. Results

3.1. 1D Results

The evolution of maxima of the progress variables is given in Fig. 5 for $\kappa = -1 \text{ mm}^{-1}$ case. 2D MuSt-FGM, which does not take curvature effects into account, completely misses the ignition delay, and does not predict the oxidation region well either. Maximum value of $\mathcal{V}_2$ for this case overshoots so much that the maximum limit of the y-axis in Fig. 5b is clipped to show the comparison of the detailed chemistry and 3D MuSt-FGM better. On the other hand, 3D MuSt-FGM captures the ignition delay perfectly, and can reproduce the later decrease of $\mathcal{V}_1$ as well. These results clearly show that when the curvature has a crucial effect on the flame mechanism, it is compulsory to include these effects in the manifold construction.

Simulations for $\kappa = 1 \text{ mm}^{-1}$ case were performed as well, and the results are presented in Fig. 6. In this case, the 2D MuSt-FGM results match better with the detailed chemistry case in terms of ignition delay, because the $\kappa = 1 \text{ mm}^{-1}$ case has a very close ignition delay to the zero curvature case, as seen in Fig. 3. However, in the oxidation stage, the effects of curvature prevail, and the results of the 2D MuSt-FGM case deviate from the detailed chemistry case. The 3D MuSt-FGM approach once again predicts the ignition delay and the evolution of maximum $\mathcal{V}_2$ almost perfectly. For

(a)

(b)

Fig. 5. Evolution of max. Y_1 (a) and Y_2 (b) in 1D calculations for $\kappa = -1 \text{ mm}^{-1}$ case with detailed chemistry, 3D MuSt-FGM, and 2D MuSt-FGM.

Y_1 , there occurs a shift in the spatial location of maximum value around $t = 3.3 \text{ ms}$, which is why the behavior changes so suddenly. Although the value of Y_1 at the main ignition site continues to decrease, another peak in the oxidizer side remains constant (not shown here for the sake of brevity). This behavior is also well captured by the 3D MuSt-FGM approach, while the absolute value is slightly under-predicted.

3.2. DNS Results

After validating 3D MuSt-FGM approach with curvature effects in 1D, it is necessary to assess the prediction capabilities in turbulent flow. As mentioned in Section 2, 2D DNS calculations are performed in the form of mixing layers, again using detailed chemistry, 3D MuSt-FGM, and 2D MuSt-FGM. Firstly, to give the reader an idea on how the DNS field looks like, temperature fields at different time instances from the detailed chemistry case are given in Fig. 7. As can be seen, first the Kelvin–Helmholtz instabilities occur due to the shear layer between the fuel and the oxidizer streams, these then grow into larger vortices as time passes, due to the lack of vortex stretching effects in 2D. Around 2 ms the ignition occurs, which is visible in the right-most image in Fig. 7.

(a)

(b)

Fig. 6. Evolution of max. Y_1 (a) and Y_2 (b) in 1D calculations for $\kappa = 1 \text{ mm}^{-1}$ case with detailed chemistry, 3D MuSt-FGM, and 2D MuSt-FGM.

Fig. 7. Temperature fields for the detailed chemistry case at $t = 0.0, 0.1, 1.0$ and 2.5 ms from left to right. Temperature ranges from 305 K to 1210 K from dark blue towards light yellow color. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In addition to maximum value of Y_2 , the cases are also compared using the average heat release rate in the whole computational domain to demonstrate the effects of curvature on the reaction rates. The results are shown in Fig. 8. It is observed again that 3D MuSt-FGM method can predict the ignition delay successfully, and the initial increase and later decrease in the average heat release rate are also well captured. 2D MuSt-FGM case predicts an earlier ignition, and over-predicts the values of maximum Y_2 and average heat release rates.

Fig. 8. Evolution of $\max Y_2$ (a) and average heat release rate (b) in DNS calculations with detailed chemistry, 3D MuSt-FGM, and 2D MuSt-FGM.

These results show that the curvature variations in a turbulent flow affect the ignition dynamics, and 3D MuSt-FGM approach with curvature effects included can model these variations adequately.

It is also worth mentioning that even though 2D MuSt-FGM case does not include the curvature effects in the manifold construction, ignition is still more delayed compared to the flamelet with $\kappa = 0 \text{ mm}^{-1}$. This observation shows that the effect of turbulence is not limited to the flame curvature, and these extra effects can influence the results of a tabulated chemistry case with a 2D manifold. Possible candidates for the extra effects are varying stretch rates and turbulent eddy-molecular diffusion interactions. In the detailed chemistry and 3D MuSt-FGM cases, the ignition delay is somewhere between $\kappa = 1 \text{ mm}^{-1}$ and $\kappa = -1 \text{ mm}^{-1}$ flamelet cases. This is reasonable since the iso-surfaces of mixture fraction experience both positive and negative curvatures throughout the simulation, and while negative curvatures delay the ignition considerably, positive curvatures do not alter it much, as seen in Fig. 3.

The effects of curvature-preferential diffusion interaction are observed in the distribution of species in the composition space as well. In Fig. 9, distribution of Y_{H_2} in mixture fraction space at $t =$

Fig. 9. Distribution of Y_{H_2} in DNS at 0.15 ms with detailed chemistry (a), 3D MuSt-FGM (b), and 2D MuSt-FGM (c).

0.15 ms is given for all DNS cases. At this time instance, the effect of chemistry is minimal, therefore the distribution is mostly due to the transport. As can be seen, curvature effects cause the species to diffuse at different speeds, and as a result there is a large scatter in the distribution. This behavior is well captured in the 3D MuSt-FGM case because the effects of curvature are included in the manifold, whereas in the 2D MuSt-FGM case it is completely missed.

It is also worth mentioning that, because $Z_{t,\text{st}} = 5 \times 10^{-3}$ is so small for this case, stoichiometric iso-surfaces, and thus the flame front lie outside of the shear layer interaction between the fuel and the oxidizer streams. As a result, the curvature values as

well as scalar dissipation are low at the location of the flame. For a case where Z_{st} is higher, or the shear layer is more intense (i.e., higher Reynolds number), the effects of curvature-preferential diffusion interaction on the ignition dynamics could be even more prominent.

4. Conclusions

In this study, it is aimed to develop a method to capture the curvature-preferential diffusion interaction using tabulated chemistry. To this end, firstly curved flamelets were created using an opposed tubular flow configuration, and then a new CV which can represent the curvature effects was defined. Using this newly defined CV (Z_H), transported mixture fraction (Z_I) and two progress variables for pre-ignition and oxidation stages ($\mathcal{V}_1 = Y_{HO_2}$, and $\mathcal{V}_2 = Y_{H_2O}$), 3D MuSt-FGM tables were generated. Using these tables, both 1D and 2D DNS validations were performed by comparing the results to the detailed chemistry ones. In addition, calculations with 2D MuSt-FGM tables, which ignore the effects curvature, were performed as well to verify if the additional efforts to include curvature effects had any impact. The following conclusions can be drawn from the results of these simulations:

- In the presence of preferential diffusion, curvature effects alter the molecular diffusion speed of species. In turbulent flames, this interaction causes large scatters in the distribution of species in mixture fraction space.
- The changes in the species diffusion due to curvature affect the flame dynamics as well. Therefore, for tabulated chemistry approaches, curvature effects need to be included in the manifold construction whenever the preferential diffusion effects are important.
- In the MuSt-FGM context, representing curvature-preferential diffusion interaction with a passive CV which has a non-unity Lewis number (Z_H) works well and curvature effects can be captured successfully in 1D simulations.
- Even in a turbulent flame where the flame curvature varies in a transient manner, 3D MuSt-FGM application gives satisfactory results compared to the detailed chemistry case.
- Ignoring curvature effects and using a 2D manifold completely miscalculates the ignition characteristics when curvature is prominent.

In the future, the same modeling strategy for the curvature-preferential diffusion interaction should be applied to large eddy simulations (LES) to see if this interaction is still effective in the presence of turbulence modeling.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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