Investigation of preferential diffusion effects for LES of a hydrogen-enriched jet-in-hot coflow flame using the FGM tabulation technique

Ebrahim Abtahizadeh, Jeroen van Oijen, Philip de Goey
Combustion Technology, Mechanical Engineering, Eindhoven University of Technology,
5600 MB Eindhoven, The Netherlands

1 Introduction

This numerical study reports on the investigation of preferential diffusion effects in autoignition of H_2 containing fuels. Moreover, these effects are implemented in the FGM technique for LES of the H_2-enriched Delft Jet-in-Hot Coflow (DJHC) burner. This burner mimics conditions of Mild combustion in which a fuel jet is ignited due to being issued into hot burned gases of coflow. Mild combustion has the unique ability to provide high efficiency and low pollutant combustion simultaneously in industrial heating processes [1, 2]. Base fuel in the experiments is Dutch Natural Gas (DNG) and very recently it has been mixed with various amounts of H_2. It has been observed that addition of H_2 has a significant effect on the flame structure and stabilization mechanism of the lifted turbulent non-premixed flame. Our previous DNS of a mixing layer for a similar case has revealed that molecular diffusion plays an important role in autoignition of such turbulent flames. Inclusion of preferential diffusion effects in the computations reveal that these effects have a significant influence on the predicted ignition delay.

In this study, the main focus is on the modeling of autoignition using the Flamelet Generated Manifolds (FGM) technique when preferential diffusion effects are important. The FGM approach has proven to be an adequate dimension reduction and tabulation method in various combustion problems. In this technique, chemical information is tabulated with a few controlling variables that may represent mixing and chemistry processes with minimal dimensions. In this study, the tabulation procedure is performed by conducting computations of igniting counterflow laminar one-dimensional diffusion flames. Preferential diffusion effects are implemented in the FGM process by adding these effects to flamelets and scalar transport equations. Comparison of results with computations by detailed chemistry reveals that addition of these effects to flamelets are essential to adequately predict autoigniton process. However, addition of non-unity Lewis terms to the transport equations does not affect the predictions significantly.

2 Numerical Methodology and Results

Schematic representation of the studied burner is shown in Fig. 1 (more detailes can be found in [3]). The main idea behind development of such a burner is to produce a condition similar to that of Mild

Correspondence to: e.abtahizadeh@tue.nl

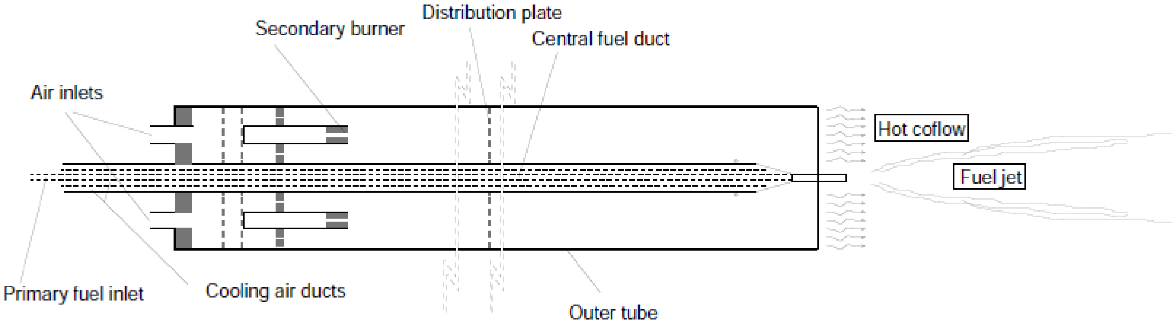

Figure 1: Schematic figure of Delft Jet-in-Hot coflow burner

Table 1: Reference values for flow rate, temperature and mass fractions of the DJHC burner

Fuel (DNG)						Coflow		
V(nl/min)	T(K)	$Y_{\mathrm{CH_4}}$	$Y_{\mathrm{C_2H_6}}$	$Y_{\mathrm{N_2}}$	Rest	V(nl/s)	T(K)	$Y_{\mathrm{O_2}}$
16.1	448	0.813	0.037	0.144	0.006	224	1540	0.084

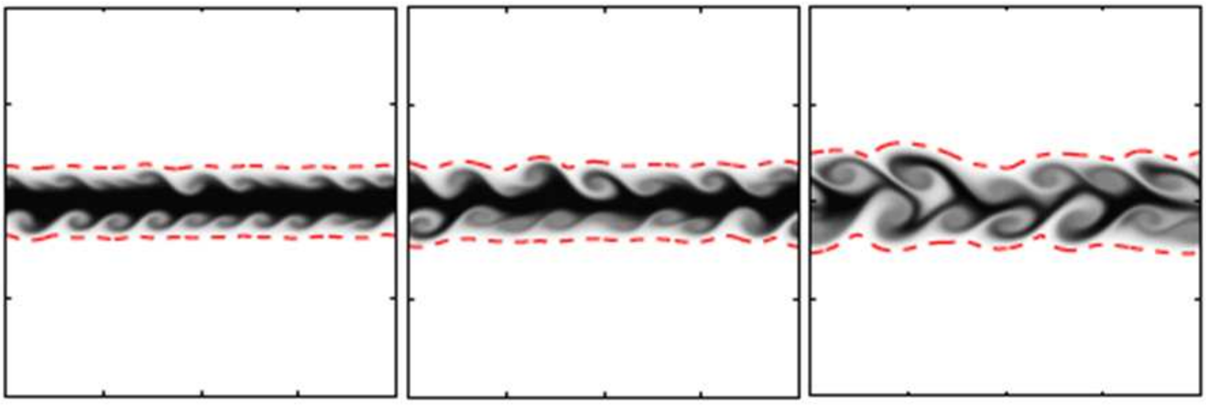

Figure 2: DNS of mixing layers, CH_4-H_2 1:1, DRM19, non-unity Lewis numbers, U_{fu} - U_{ox} = 67 m/s

combustion. The coflow is consists of combustion products of a lean premixed CH_4/air flame that is stabilized on a secondary burner. This burner is very similar to the Adelaide burner [4] with a major difference in cooling of the combustion products from the secondary burner. In the Delft burner, the heat loss is done through radiative and convective heat transfer from the burner to the surroundings which in the Adelaide one, it is done by addition of air to the combustion products. Fuel is basically Dutch Natural Gas (DNG) and a range of H_2 is added to the fuel from 2% up to 25%. A lifted non-premixed turbulent flame is created as a result of entrainment of the hot coflow into the gaseous fuel.

It has been experimentally observed that addition of H_2 affects the structure of the flame and its stabilization mechanism considerably. This observation together with similar observation of the Adelaide group was a motivation for us to study mixing and autoignition process in DNS of mixing layers as shown in Fig. 2. This DNS is basically performed for the conditions of the Adelaide setup with 50% H_2 [5]. The most reactive mixture fraction [6] of this mixture has a very small value (less than 6.7×10^{-3}) and lies in very close vicinity of the oxidizer stream away from Kelvin-Helmholtz instabilities at the mixing layer. This situation leads to a condition in which molecular diffusion has a high impact on the autoignition than turbulence transport. In this situation, preferential diffusion effects due to presence of H_2

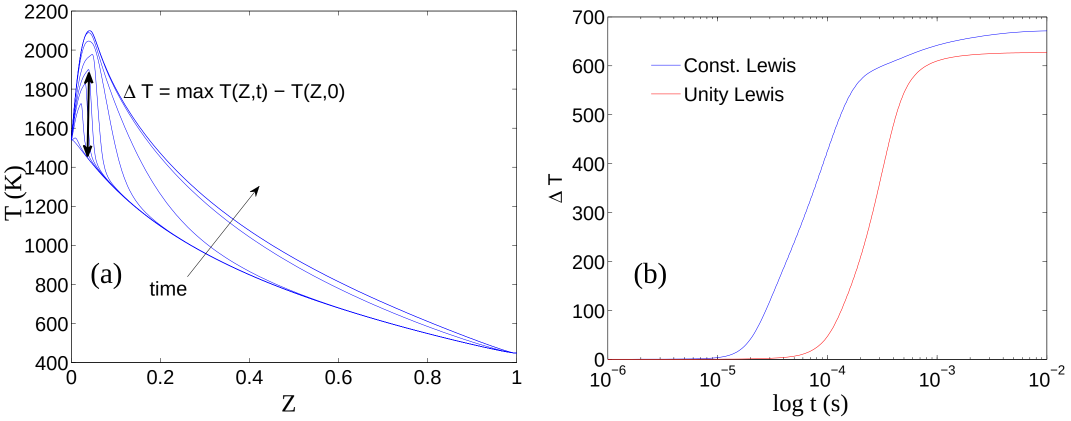

Figure 3: (a)Igniting counterflow diffusion flamelets, GRI-3.0, non-unity Lewis numbers, $25\%H_2$ (b) Effect of transport model on the autoignition time.

play a very important role. Importance of these effects on autoignition of igniting counterflow diffusion flames are illustrated in Fig. 3. These flamelets are computed using compositions according to Table 1 by addition of 25% H_2 to the fuel. Two transient flamelets are computed based on unity and non-unity Lewis numbers and autoignition times are compared. Predictions demonstrate approximately an order of magnitude difference in the ignition delay of these two sets of flamelets. Interpretation of this observation in a laminar (or even turbulent) coflow diffusion flame configuration suggests two flames with a significant difference in the predicted flame lift-off height. Therefore, preferential diffusion effects have to be considered for simulations of this flame based on tabulation techniques.

Solutions of igniting counterflow flamelets at an applied strain rate of 100 s^{-1} are used for tabulation of chemistry. These solutions are mapped on two controlling variables: mixture fraction Z and progress variable $\mathcal{Y}$ to account for mixing and reactions chemistry, respectively. Since preferential diffusion is present, redistributions of elements have to be considered in the definition of mixture fraction. For this purpose, a definition proposed by Barlow et al. [7] is used:

$$Z = \frac{2M_C^{-1}[Z_C - Z_{C,2}] + 0.5M_H^{-1}[Z_H - Z_{H,2}]}{2M_C^{-1}[Z_{C,1} - Z_{C,2}] + 0.5M_H^{-1}[Z_{H,1} - Z_{H,2}]} \tag{1}$$

where M_j and Z_j denote to the molar mass and mass fraction of elements j (say hydrogen and carbon), respectively. Subscripts of 1 and 2 refer to quantities in the fuel and oxidizer streams. The reaction progress variable, in general, has the form of:

$$\mathcal{Y} = \sum_i \alpha_i Y_i \tag{2}$$

in which α_i denotes a weight factor for mass fraction of each species Y_i present in $\mathcal{Y}$. This variable should be defined in such way that it can capture chemical processes from the very beginning to the end of the process. A possible choice leading to a unique mapping is:

$$\mathcal{Y} = \frac{Y_{CO_2}}{W_{CO2}} + \frac{Y_{H_2O}}{W_{H_2O}} - X_{H_2}\frac{Y_{H_2}}{W_{H_2}} - (1 - X_{H_2})\frac{Y_{CH_4}}{W_{CH_4}} \tag{3}$$

where X_{H_2} is mole fraction of H_2 in the fuel stream. It can be seen that H_2 is only present in this definition when it is added to the fuel stream. Fig. 4 shows the manifold for two arbitrary quantities of temperature T and source term of the progress variable $\dot{\omega}_{\mathcal{Y}}$. In this Figure, we have normalized $\mathcal{Y}$

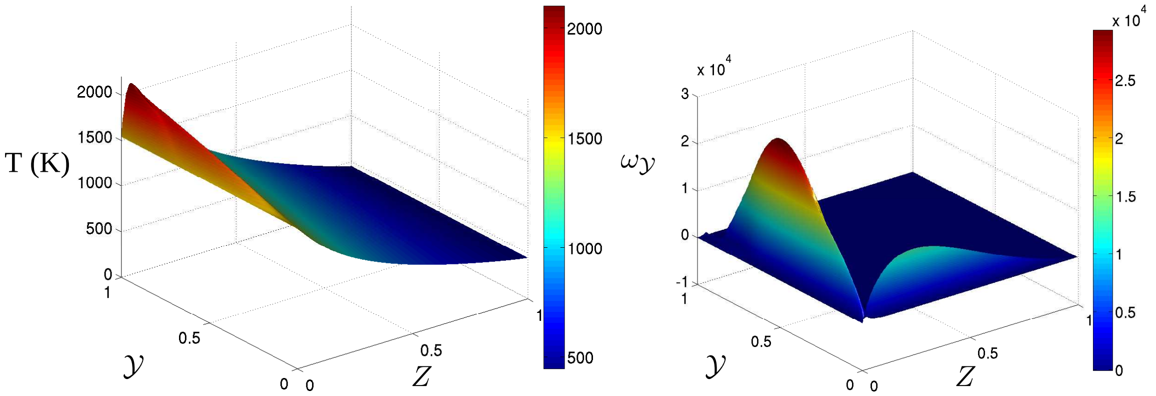

Figure 4: Temperature and Source term of progress variable as a function of two controlling variables

between 0 and 1 to visualize clearly the plotted quantities. However, the actual value of $\mathcal{Y}$ has been used in the computations. Both values have their maximum value close to the stoichiometric mixture fraction. $\omega_{\mathcal{Y}}$ has an initial rise at $\mathcal{Y} = 0$ that happens in a very small time scale. This rise is due to some residual source terms due to initial mixing of fuel and oxidizer with frozen chemistry assumption.

During flame simulations, two transport equations should be solved for the same controlling variables. These transport equations are defined in such a way that they incorporate non-unity Lewis effects and in general form they read:

$$\frac{\partial \rho Y_{cv}}{\partial t} + \nabla \cdot (\rho u Y_{cv}) - \nabla \cdot (\frac{\lambda}{C_p} \nabla \cdot Y_{cv}) = \nabla \cdot (\Lambda_1 \nabla \mathcal{Y} + \Lambda_2 \nabla Z) + \rho \dot{\omega}_Y \tag{4}$$

where Y_{cv} is the relevant quantity for each controlling variable (Z or $\mathcal{Y}$). Λ_1 and Λ_2 represent diffusion coefficients related to non-unity Lewis effects:

$$\Lambda_1 = \frac{\lambda}{c_p} \sum_{i=1}^{Nsp} \gamma_i (\frac{1}{Le_i} - 1) \left(\frac{\partial Y_i}{\partial \mathcal{Y}} \right)_Z \tag{5}$$

$$\Lambda_2 = \frac{\lambda}{c_p} \sum_{i=1}^{Nsp} \gamma_i (\frac{1}{Le_i} - 1) \left(\frac{\partial Y_i}{\partial Z} \right)_{\mathcal{Y}} \tag{6}$$

where γ_i is computed based on the relevant weight factors for Z and $\mathcal{Y}$. It should be noted that coefficients of Λ_1 and Λ_2 have different values for various controlling variables. These coefficients are precomputed and stored in table in order to be retrieved during simulations.

Initial verification of the solution procedure has been performed using unity Lewis assumption for generation of flamelets and in the scalar transport equations which is compared with detailed chemistry in Fig. 5. Results demonstrate that with unity Lewis assumption, the FGM table is capable to reproduce ignition process from the beginning of the process to the steady-state solution accurately. This also means that there are almost no numerical errors in the tabulation process.

Effect of Λ_1 and Λ_2 in the scalar transport equations has been illustrated in Fig. 6. For these computations flamelets are computed with non-unity Lewis numbers. Fig. 6(a) shows comparison of predicted autoignition by detailed chemistry and FGM with and without Λ_1 and Λ_2 in the scalar transport equations at applied strain rate of 100 s^{-1}. It is observed that Λ_1 and Λ_2 have a negligible effects on the predicted autoignition process. There are some discrepancies close to the stationary solution that is related to the definition of $\mathcal{Y}$ which is unable to yield a monotonically increasing flamelets close to the

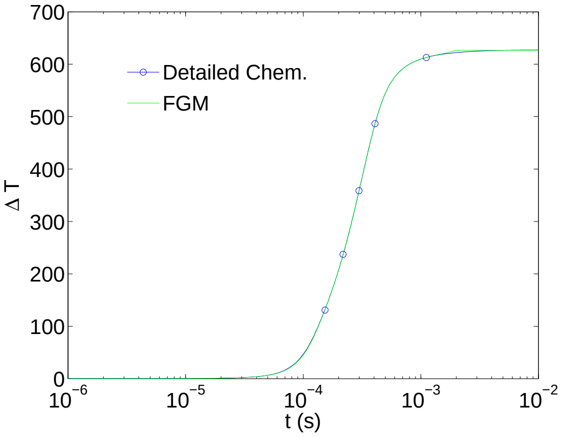

Figure 5: Predictions of autoignition by detailed chemistry GRI30 and FGM with unity Lewis number assumption for flamelets and zero diffusion terms in transport equations.

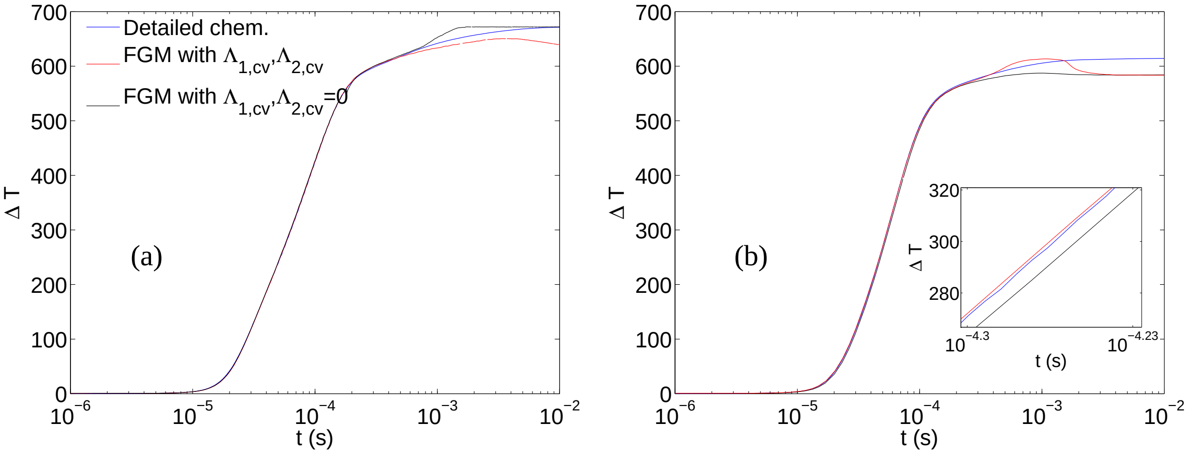

Figure 6: Predictions of autoignition by detailed chemistry GRI30 and FGM with non-unity Lewis numbers for flamelets and zero and non-zero values for diffusion terms in transport equations.

steady-state. In this situation, flamelets are discarded from the tabulation process due to crossing with other flamelets as a result of presence of preferential diffusion. We tried different ways e.g. Principal Component Analysis to define a suitable progress variable to overcome to this problem. However, it appears that with a fixed definition for progress variable, it is almost impossible to find a suitable definition for both the autoignition process and the steady state. Since we are interested mostly in the autoignition part to investigate mixing and autoignition process of the lifted turbulent flame, the current definition remained unchanged. In order to investigate importance of Λ_1 and Λ_2 at higher scalar dissipation rates, we contrast predictions at the applied strain rated of 600 s^{-1} in Fig. 6(b). At this strain rate autoignition times are predicted slightly different. This difference is lower for the case where Λ_1 and Λ_2 is present in the formulation which indicates a slightly higher importance of these coefficients at higher mixing levels.

3 Conclusions

Preferential diffusion effects have been investigated in autoignition of H_2 containing fuels in Mild combustion using 1D counterflow igniting flamelets. It is revealed that ignition delay of such flamelets is changed by an order of magnitude by including these effects. Tabulation of chemistry has been performed by defining a mixture fraction and progress variable. These controlling variables have been defined in such a way that they can describe the autoignition process adequately where preferential diffusion effects are present. Initial verification of the FGM table is performed with unity Lewis assumption for flamelets and transport equations. It turns out that the FGM table is capable to reproduce the predicted time-dependent solution by detailed chemistry. Implementation of preferential diffusion effects in the FGM has been performed by generating flamelets with non-unity Lewis numbers and adding extra terms to the scalar transport equations. Results demonstrate that generating flamelets with non-unity Lewis numbers are essential for an accurate prediction of autoignition. The extra terms in the scalar transport equations have a negligible effects which become slightly important at higher mixing levels.

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