Numerical studies of the Influence of Turbulence and Coherent Structures on Flame and Emission Characteristics in Lean Premixed Combustion

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Abstract

In this work we present the numerical investigation of a lean premixed methane-air flame under turbulent conditions, as it may occur in a gas turbine combustor, using the one-dimensional Linear Eddy Model (LEM). We study the influence of turbulent conditions on flame behavior and pollutant formation of CO and NO by varying the turbulent diffusivity and the integral length scale. Increasing the turbulent diffusivity leads to higher burning velocities and larger flame width. CO emissions are increasing whereas NO is decreasing which is closely related to the flame width and corresponding temperature fields. When the integral length scale is increased the flame width, the burning velocity and CO emissions slightly decrease whereas NO production slightly increases. The analysis shows that small scale eddies have a more significant effect on the flame and emission characteristics than large scale eddies. Furthermore, we compute the influence of fluctuations in equivalence ratio on flame characteristics as well as on CO and NO formation. Harmonic perturbations and harmonic perturbations with superposed stochastic fluctuations are investigated. Generally, oscillations in the fuel concentration lead to oscillations of flame temperature and emissions. Thereby, the forcing with the superposed stochastic fluctuations shows a much more distinct effect than the harmonic forcing alone. Stochastic perturbations are much stronger and last much longer without decreasing significantly downstream of the flame. The averaged concentrations of NO and CO are higher with stochastic perturbation and slightly lower with pure sinusoidal forcing.

1 Introduction

Modern gas turbines operate under lean premixed combustion to comply with emission standards which are especially strict concerning NO_x and CO. One major drawback of this kind of flames is their susceptibility for combustion instabilities which may be induced by coherent flow structures [1, 2]. As combustion instabilities have counterproductive and destructive effects, mechanisms behind them have to be understood. Many works deal with the influence of swirl number, Reynolds number, and/or oscillation on instabilities and NO_x emissions [3–5]. However, more fundamental studies varying single turbulence parameters and studies on CO emission dealing with these effects in lean premixed combustion are rare.

Fundamental parameter studies are difficult to realize experimentally; it is merely impossible to regard the effect of one parameter without influencing others; numerical methods are reasonable for these investigations. Since the turbulent premixed gas turbine combustion processes are strongly time dependent an unsteady approach has to be used. Furthermore, detailed chemistry is necessary to conduct studies on the interaction of turbulent structures and pollutant emissions and all physical scales have to be resolved because combustion processes are strongly influenced by small scale eddies.

DNS which includes all necessary characteristics is very time consuming and often constrained to two spatial dimensions. The Linear Eddy Model (LEM) [6, 7] resolves all turbulent length and time scales on a one-dimensional line and is less time (and memory) consuming than DNS. Although, it is a one-dimensional model, it has demonstrated to capture many characteristic features of turbulence and turbulent combustion and allows parameter studies which are usually not feasible with a DNS.

In this paper we investigate the influence of turbulent diffusivity and integral length scale on flame structure and NO and CO emissions with LEM using a skeletal mechanism in a lean premixed air-methane flame under atmospheric conditions. Furthermore, we study effects of fluctuations in equivalence ratio – purely sinusoidal and superpositions with higher harmonic and stochastic signals – on flame characteristics.

2 The numerical methods

2.1 The Linear Eddy Model

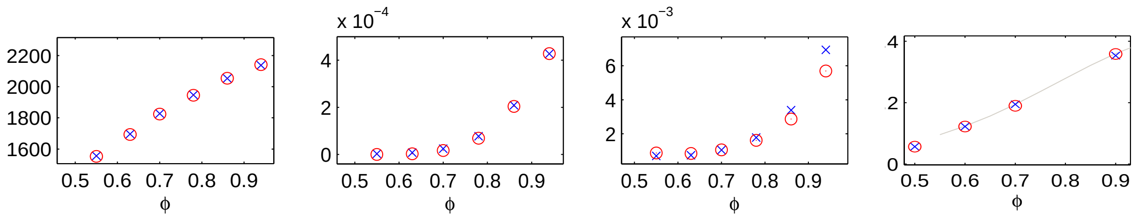
The Linear Eddy Model (LEM) of Alan Kerstein, e.g. [6, 7], resolves all physically relevant length (Kolmogorov scale, η, to integral length scale, L) and time scales on a one-dimensional domain. The main idea behind this approach is to treat molecular diffusion processes and turbulent advection separately. Molecular diffusion is implemented deterministically whereas turbulent stirring is represented by a sequence of statistically independent rearrangement events. The rearrangement events are expressed by triplet maps, which compress the scalar field within a chosen segment by a factor of three and the original field is then replaced with three adjacent copies of the compressed field, with the middle copy mirrored. Each event, representing an eddy, is governed by three random variables: the time when the eddy occurs, the location and the size of the eddy. The location is chosen randomly. The size of the eddy is chosen from a distribution of domain sizes which is obtained by applying Kolmogorov scaling laws. Identifying that the rearrangement events induce a random walk of one particle on a line, a rate parameter, λ, with dimensions $[l^{-1}t^{-1}]$ and a pdf describing the length distribution, $f(l)$, can be determined. The diffusivity of the random walk is thereby interpreted as the turbulent diffusivity D_t:

$$\lambda = \frac{54}{5} D_t L^{-3} \frac{\left[1 - (\eta/L)^{-5/3}\right]}{\left[(\eta/L)^{4/3} - 1\right]}, \qquad f(l) = \frac{-5/3}{L^{-5/3} - \eta^{-5/3}} l^{-8/3}.$$

The time when an eddy occurs is calculated from a Poisson process. The model reproduces important key features of turbulent mixing [7] and proved itself to be a valid model in studies on various research fields, amongst them LEM simulations on turbulent premixed combustion and pollutant formation by Menon et al. [8, 9].

2.2 The combustion mechanism

Detailed combustion mechanisms are necessary to investigate dynamic processes in combustion. The GRI-mechanism [10] is a standard mechanism for natural gas and ignition processes which has been validated against a huge number of data sets but turns out to be relatively slow regarding spatial and temporal resolved calculations. Reduced mechanisms have been provided for various kinds of combustion conditions.



(a) T in K (b) NO (c) CO (d) s_L in m/s

Figure 1: Validation of the considered mechanism ($\odot$) with the Gri-3.0-mech ($\times$) for different values of equivalence ratio ϕ; the gray line (–) is a correlation for laminar burning velocity of methane-air combustion by Abu-Orf [11]

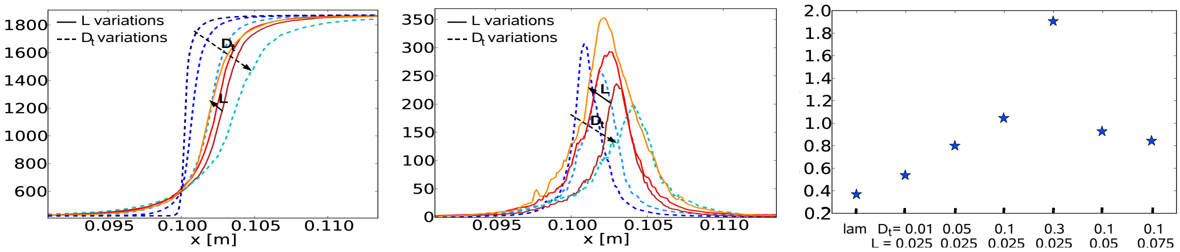
The mechanism used here is a combination of a skeletal mechanism for methane-air combustion by Peters [12] and a NO_x decomposition mechanism suggested by Volkov [13]. With some adjustments it includes 20 species and 54 reactions. It was tested amongst other mechanism [14, 15] under the present conditions and was found being fast and at the same time sufficiently accurate.

Figure 1 shows temperature, NO and CO mass fractions for different values of equivalence ratio in comparison with the GRI3.0-mech calculated with Cantera and 0-D-combustion. Furthermore, the laminar burning velocities, calculated from the reaction rates of an one-dimensional code [16] is compared to a correlation suggested by Abu-Orf [11]. Species and temperature distributions from laminar one-dimensional calculations where considered as well. They also give good agreement comparing the GRI3.0-mech with the considered skeletal mechanism (not shown here). The mechanism reproduces the NO_x and CO emissions in the relevant lean region accurate enough for the considered studies as only trends are regarded.

3 Results

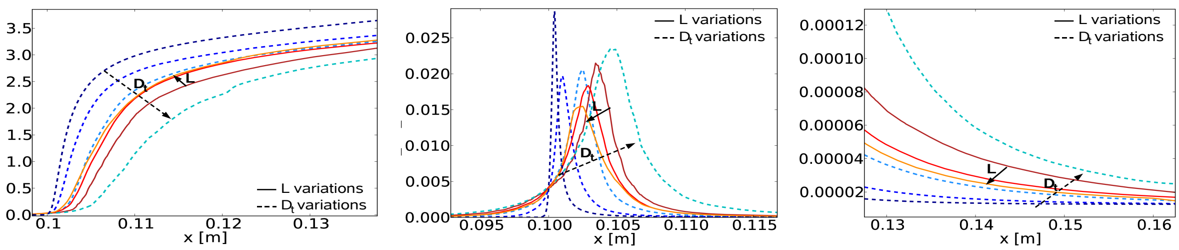
3.1 Influence of turbulence on flame structure and pollutant formation

In this section a parameter study of turbulent diffusivity, D_t, and integral length scale, L, on flame characteristics and NO and CO formation is described. D_t and L are input parameters to the LEM model giving information on turbulence and mixing behavior which are important characteristics in technical premixed gas turbine combustion. We investigate a methane-air mixture with an equivalence ratio of 0.661 preheated to 425 K. The Kolmogorov length and the initial integral length were taken from measurements in an atmospheric single burner test rig under the same conditions [17]; their values are 1e-4 m and 0.025 m, respectively. The turbulent diffusivity was varied in a physically reasonable range ($D_t = 0.01, 0.05, 0.1, 0.3$ m^2/s). In addition, two further integral length scales were considered: $L = 0.05$ and 0.075 m at $D_t = 0.1$ m^2/s. The computational LEM domain had an extend of at least five integral length scales and the turbulent data was averaged over a time of at least 20 integral time scales obtaining statistically stationary mean distributions.



(a) T_{mean} in K (b) T_{rms} in K (c) s_t in m/s

Figure 2: Mean (a) and RMS (b) temperature profiles and mean burning velocities (c) for different values of D_t and L; bluish broken lines (- -): distributions for changing D_t (laminar, 0.01, 0.05, 0.3 m^2/s; $L = 0.025$ m); reddish solid lines (—): distributions for changing L (0.025, 0.05, 0.075 m; $D_t = 0.1$ m^2/s)



(a) NO in ppm (b) CO (c) CO

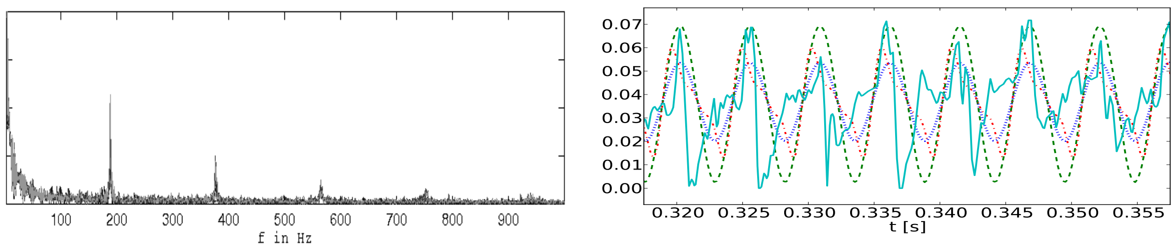
Figure 3: Mean NO (a) and CO (b), (c) mass fraction profiles for different values of D_t and L, (c) is a zoom-view of (b); line styles and colors as in Fig. 2

The results given in Fig. 2 show the mean and rms temperature distributions and the burning velocities. It can be observed that the flame thickness grows with D_t, which was expected as there are more eddies per time and area ($\lambda \uparrow$). On the other hand, it decreases with L; this is due to increasing time between eddy events. With the eddy size getting bigger as well the flame is not much affected: there is enough time between the eddies allowing the flame to return to a less turbulent state. This implies that the structure of these kind of flames are primarily driven by small scale eddies. The burning velocities were calculated from reaction rates of the main species. The displayed values are mean values over time and species. Generally a similar behavior to the flame thickness is detected.

Figure 3 shows the influence of D_t and L on pollutant emissions NO and CO. NO decreases with D_t and increases slightly with L. CO behaves the other way round. This behavior is closely related to the flame structure and temperature distribution. As temperature needs longer to reach its equilibrium value for higher values of D_t so do NO and CO.

3.2 Influence of perturbations in equivalence ratio on flame structure and pollutant formation

The investigations were conducted for the same conditions as in the previous section but under preliminary laminar considerations. Turbulent simulations for $D_t = 0.1$ m^2/s and $L = 0.025$ m show the same tendencies as the laminar results. Equivalence ratio oscillations were studied as they occur in gas turbines under combustion instabilities. Figure 4(a) shows spectra of concentration fluctuations measured in a single burner water test rig converted to air conditions. The input signals of methane fluctuations used for the analysis shortly upstream of the flame are given in Fig. 4(b). Four different signals were considered: i) a sinusoidal signal, ii) a signal including the dominant frequency and the first two higher harmonics, iii) a signal including the dominant frequency and higher frequency oscillations/stochastic superposition, called hereafter 'pseudo-stochastic' signal, (directly taken from measurements), and iv) a sinusoidal signal with twice the amplitude of the first signal. The temporal averaged signals correspond to an equivalence ratio of about 0.661 for all four cases.

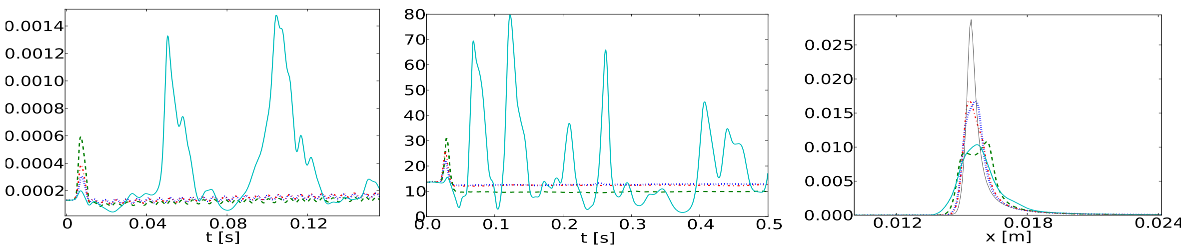


(a) spectrum of measured concentration fluctuations

(b) CH_4 fluctuation

Figure 4: (b): Different investigated fluctuation signals shortly upstream of the flame: ·· sinusoidal signal, - - sinusoidal signal with higher amplitude, -· sinusoidal signal with higher harmonics, – stochastic signal

The flame is located at a position x of approximately 0.015 m. Figures 5 and 6 represent the temporal evolution of the signal shortly downstream, further downstream of the flame and the time-averaged (over 0.5 s $\sim$ 100 1/dominant frequency) distribution for NO and CO, respectively.



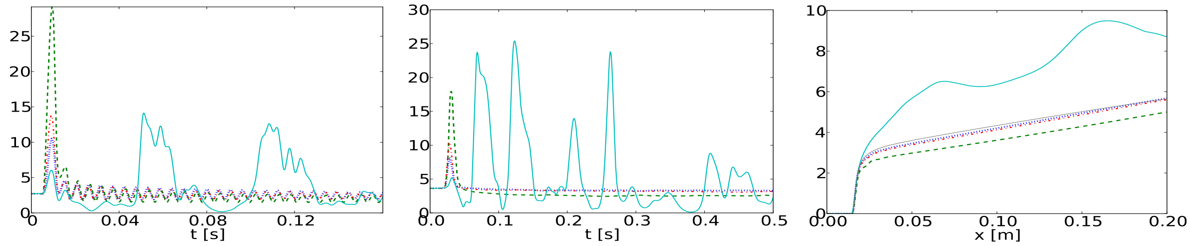
(a) CO at $x = 0.02$ m

(b) CO at $x = 0.05$ m in ppm

(c) CO_{mean}

Figure 5: Temporal evolution of CO mass fraction at position (a) $x = 0.02$ m and (b) $x = 0.05$ m; (c) mean CO distribution; colors as in Fig. 4(b), gray line (–): distribution without oscillating input

The sinusoidal signals only cause small fluctuations of NO and CO mass fractions whereas the pseudo-stochastic signal induces significantly higher oscillation amplitudes in CO and NO. Furthermore, the harmonic fluctuations

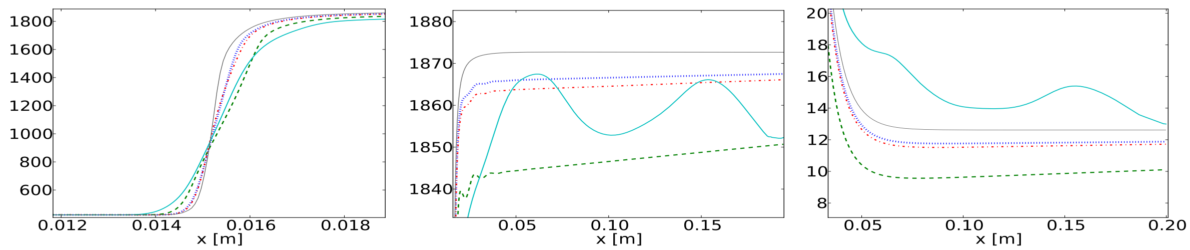


(a) NO at $x = 0.02$ m in ppm (b) NO at $x = 0.05$ m in ppm (c) NO_{mean} in ppm

Figure 6: Temporal evolution of NO mass fraction at position (a) $x = 0.02$ m and (b) $x = 0.05$ m; (c) mean NO distribution; line styles and colors as in Fig. 4(b), gray line (–): distribution without oscillating input

quickly decrease though the fluctuations induced by the pseudo-stochastic signal are still evident further downstream of the flame.

The mean values of NO as well as CO concentration increase with pseudo-stochastic forcing although the temperature slightly decreases. In addition, a steady state is not reached. The pseudo-stochastic perturbations in the CH_4 mass fraction upstream of the flame are less damped than the sinusoidal fluctuations due to diffusion effects which in turn induce the stronger fluctuations in the temporal distribution of CO and NO mass fraction. The mean levels of the NO and CO concentration are increased since NO and CO are convex functions of the equivalence ratio in the lean combustion regime.



(a) T_{mean} in K (b) T_{mean} in K, zoom view (c) CO_{mean} in ppm, zoom view

Figure 7: (a), (b): Mean total, exhaust temperature distributions; (c) mean exhaust CO distribution); line styles and colors as in Fig. 4(b), gray line (–): distribution without oscillating input

The coherent forcing on the other hand reduces the emissions slightly. This could be related to the flame width which increases with the amplitude of the sinusoidal forcing. The increased flame width causes a slight reduction of the mean equivalence ratio of the forcing signal which is inserted into the CH_4 distribution at the same position shortly upstream of the flame for all calculations.

4 Conclusion and outlook

We investigated the effect of varying turbulence parameters and equivalence ratio oscillations on lean premixed methane-air flames.

With increasing turbulent diffusivity CO emissions are increasing whereas NO is decreasing which is closely related to the increasing flame width and corresponding temperature fields. When the integral length scale is increased NO/CO production slightly increases/decreases due to a decreasing flame width. This indicates that small scale eddies have a more significant effect on the flame and emission characteristics than large scale eddies.

Harmonic perturbations with stochastic superposition cause strong overshoots of CO and NO mass fractions that are still dominant further downstream of the flame and increase the mean emissions. Sinusoidal oscillations do not show major effects. This behavior is explained with a stronger damping of the sinusoidal than the pseudo-stochastic fluctuations upstream of the flame and the increased mean formation of CO and NO is related to the convex dependency of NO and CO on the equivalence ratio in the lean combustion regime.

Further studies are planned on conducting simulations using LEM as a subgrid model in 3D-LES. We will investigate a flame in a flame regime similar to that of gas turbine combustion with perturbations in mass flow rate, respectively equivalence ratio to gain further insight into mechanisms driving the formation of CO and NO during combustion instabilities. The LEM-subgrid model has the distinct advantage over other subgrid and combustion models that flame turbulence interactions are resolved (in a 1D domain) on all scales directly and require only limited modeling.

Acknowledgment

The authors would like to thank Alan Kerstein and David Lignell for their support and the German Science Foundation (DFG) for financial aid.

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