Modeling of CO Formation in Turbulent Premixed Combustion

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In turbulent premixed flames, the interaction of random eddies and flame significantly affects the inner structure of the flame and leads the flame front to intrinsically wrinkled. The flame stretch, a combination effect of aerodynamic strain rate and flame curvature, particularly with differential diffusion of heat and chemical species, modifies the burning velocity and may even cause local flame extinction. Several studies on the response of the flame burning velocity and extinction to the flame stretch, have been carried out [1]-[5]. In the limit of large activation energy and low stretch, the flame burning velocity was shown to be linearly dependent on the flame stretch [1, 2]. This subject has been further studied later using a rate-ratio asymptotic analysis with reduced chemistry [4] and recently DNS with a detailed chemical kinetic mechanism [5].

The present work concerns with another important effect of flame stretch, the influence of the flame stretch on the intermediate combustion products such as CO, in a turbulent propane/air flame. The work was motivated by previous findings in modeling an experimental flame constructed and measured by VOLVO Aero AB. Although the major species and temperature field were reasonably well simulated using different models such as fast chemistry models based on simple Eddy-Dissipation Concept or detailed chemistry based flamelet library approach [10], the important pollutant species CO was calculated poorly in comparison with the experimental data.

Asymptotic and numerical analyses of hydrocarbon/air flame structures indicate that the competition among the elementary reaction rates and mass and heat transfer rates in the inner layers strongly affects the formation of intermediate species such as CO. To demonstrate the effect, we chose the VOLVO experimental flame - a lean-burn flame in a model gas turbine afterburner, in which the flame is stabilized by a triangular prism. The fuel/air equivalence ratio is 0.6, unburned mixture temperature 600 K and pressure of 1 atm.

Figure 1 shows the influence of the aerodynamic strain rate on the laminar burning velocity and flame structures of the VOLVO lean propane/air premixed flame. The laminar flamelet structures under different strain rates are calculated on a model 'back-to-back' twin-flame configuration (studied in [4]), using an in-house code [7], with detailed chemical kinetic mechanism [8]. In the figure s_L^0 denotes the unstretched laminar flame burning velocity, which is $0.743 m/s$ from the numerical calculation. As seen at low strain rate the burning velocity is approximately linearly dependent on the strain rate. As the strain rate increases, the laminar burning velocity decreases. At high strain rate (about 2200 s^{-1}) the slope of s_L vs. K profile tends to infinity. Further increasing the strain rate (K) leads to flame extinction.

The flame extinction can be further understood from the CO and O_2 profiles shown in Fig.1. As seen, at the inner layer a high super-equilibrium CO peak is found. At large positive G (post-flame zone) a low CO concentration is found. In the case of zero strain rate, the CO mole fraction at far post-flame zone reaches its equilibrium, which is very low ($< 20 ppm$) in this lean flame. Increasing the strain rate leads to a decrease in the flow residence time, therefore the CO mole fraction at the post-flame zone can not reach to its equilibrium. Instead a rather high CO is found, indicating an incomplete combustion. It is interesting to note that the super-equilibrium CO peak in the inner layer is only slightly affected by the strain rate. The O_2 mole fraction follows similar trend. As the strain rate becomes high, the flow residence time becomes short and there is a higher O_2 leakage to the post-flame zone, as a result of the incomplete combustion.

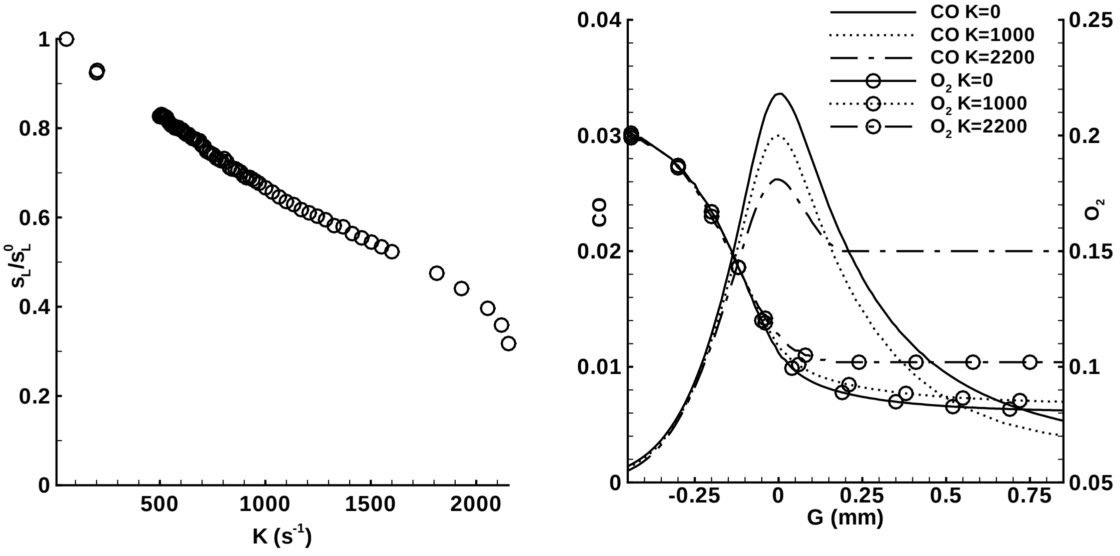

Figure 1: Burning velocity (left) as a function of strain rate (K) and distributions of O_2 and CO in the flamelet coordinate (right), at different strain rates, calculated using a detailed chemical kinetic mechanism [8] in a back-to-back, counter flow configuration

From the above figure it is obvious that to simulate CO emissions in turbulent flames, one should include the flame stretch effect and relatively detailed chemical kinetics in the modeling. For this purpose, different approaches may be employed, e.g. the level-set flamelet library approach [6], or other high order methods.

The flame surface in turbulent flows is a complex 3-D configuration. In the flamelet regime, the flame thickness may be assumed much thinner than the radius of the curvature. Therefore the local flamelet may be assumed to be subjected to a single well defined flame stretch. Several authors [3, 9] have argued that because the flame surface changes its shape to concave and convex alternatively, the time averaged mean curvature in a flame situation considered here is close to zero. For simplicity, the effect of curvature on the flame structure is neglected and only the strain rate effect on the flame structure is considered.

Based on the flamelet library approach, the influence of flame stretch is explicitly modeled in two ways: The effect of flame stretch on the burning velocity, and therefore the tracking of the turbulent flame position, is modeled in the level-set G-equation [10], and the effect of flame stretch on the flamelet structure (chemical species and temperature profiles) is stored in a so-called flamelet library, which is used in an ensemble average to obtain the mean statistical quantities.

The basic idea of ensemble average of stretched flamelet can be briefly described as below. If the joint PDF, $\wp(\xi, K)$, is known at the flow field (x, y, z), the Favre averaged mean quantities at that point can be computed via, e.g. for the mass fraction of species i:

$$\widetilde{Y}_i(x,y,z) = \frac{1}{\overline{\rho}} \int \int_{-\infty}^{\infty} \wp(G,K) Y_i(\overline{G}(x,y,z) - G, K) \rho(\overline{G}(x,y,z) - G, K) dG dK, \tag{1}$$

where the mean density is calculated by

$$\overline{\rho} = \int \int_{-\infty}^{\infty} \wp(G,K) \rho(\overline{G}(x,y,z) - G, K) dG dK \tag{2}$$

The joint PDF $\wp(G,K)$, is presumed here as the product of a Gaussian distribution for the flame distance function (G) and a log-normal distribution of stretch rate (K), following [11].

In Eq.1, $\overline{G}(x,y,z)$ is the distance function at flow field point (x,y,z). If $\overline{G}(x,y,z) = 0$, the mean flame surface is then at (x,y,z). The mean flame position in the turbulent flow field is traced with a mean G-equation, together with the Reynolds averaged Navier-Stokes (RANS) equations and two-equation $k-\varepsilon$ model. More discussions of level-set flamelet library approach can be found in [6] and our previous publication [10].

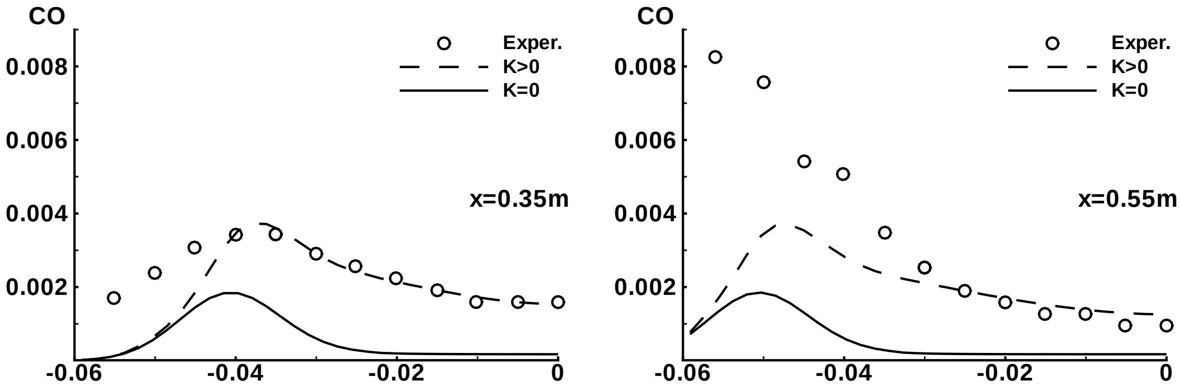

Figure 2: Mean CO mole fraction along cross flow direction (y, horizontal axis, unit in m), measured and calculated using the unstretched laminar flamelet models and stretched ones (the stretch rate is between 1000 s^{-1} and 2000 s^{-1})

Figs.2 shows the mean mole fraction of CO along y (cross flow) direction at two different positions downstream of the flame holder. In the figures, $y = 0$ represents the symmetry plane and $y = -0.06m$ represents the combustion chamber wall. The influence of flame strain rate is not very important in calculations of the O_2 profiles. The major change of O_2 mass fraction is found at the postflame (about 10% increase by including the flame strech effect). Other major species (unburned fuel, CO_2, H_2O and N_2) as well as temperature are found to agree well with the measurement and not sensitive to the flame stretch.

Fig.2 demonstrates the importance of aerodynamic strain rate on the formation of CO in turbulent flames. At noted, the unstretched flamelet structure (denoted by $K = 0$ line) yield lower CO mole fractions than the experimental data, particular in the post-flame zone (near $y = 0$ and for large x positions). The mean strain rate in the flow field is between 1000 s^{-1} and 2000 s^{-1}. With the current stretched flamelet model, the CO profiles are clearly better predicted than that with the unstretched flamelet model. It can be concluded that the experimentally observed high CO concentration in the current lean flame is mainly due to the influence of flame strain (stretch) on the local laminar flamelet structures.

The largest difference between the calculated CO and measured data is found in the near wall region. In the sections ($x = 0.35m$) it is shown that the CO peak locations calculated and measured agree well. It is reasonably accurate to assume that the mean flame position locates at the CO peak position [10]. So the near wall region is in the preheat zone at section ($x = 0.35m$). In the numerical result, the preheat zone ($y < -0.04m$, $x = 0.35m$) has much lower CO compared to the measured data. The higher CO mass fraction found in this preheat zone may be due to the turbulent diffusion of CO from the its high concentration flame zone. In addition, history effect that accounts for the transport of upstream high CO concetration to the downstream may also contribute to the high CO mass fraction found near the wall at both sections in the figure. In the current model the turbulent diffusion of high CO from the flame zone to upstream preheat zone is modeled by the fluctuations of the G-function and the history effect is not explicitly modeled. It is treated implicitly through the increase of the G-function fluctuation at down streams. These issues required further investigation.

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