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CO Emission of Premixed and Diluted Flames in a Stagnation Burner

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Abstract

Moderate or Intense Low oxygen Dilution (MILD) combustion combines low emissions with high efficiency, which has the potential to provide significant performance improvement of Gas Turbine (GT) combustors. The presence of cold walls in a GT combustor can have an effect on the produced emissions and therefore needs to be fully understood. In this paper, the emissions behaviour of premixed and MILD methane/air flames in a head-on quenching configuration have been simulated with the one-dimensional (1D) stagnation burner geometry. The level of dilution, wall temperature and inlet velocity have been varied. The results show that CO emissions increase with increasing dilution levels, until MILD conditions are reached, then decrease with the increase of dilution levels. It is also shown that increasing inert wall temperature does not have a noticeable effect on CO emissions. In addition, CO emissions decrease with increasing the inlet velocity in premixed cases, but increase for MILD cases.

Introduction

Regulations concerning emissions, along with concern for a cleaner environment have motivated combustion engineers to develop novel combustion techniques for achieving ultra-low levels of pollutant emissions from gas turbine combustors. Recently, Moderate or Intense Low oxygen Dilution (MILD) combustion has emerged as a novel promising option to achieve ultra-low emissions of nitrogen oxides (NOx) and carbon monoxide (CO) in addition to significantly improved pattern factor, combustion stability, and low noise emission for gas turbine combustion application [3].

MILD combustion has been applied to industrial burners for some time, but the complex physical mechanisms are yet to be resolved to extend the application to Gas Turbines (GTs). To this end, de Joannon et al. [5] defined MILD combustion based on the Perfectly Stirred Reactor (PSR) simulation results, and Evans et al. [7] broaden the definition in a non-premixed case. Sidey et al. [17] performed numerical simulations of methane (CH_4) flames with hot combustion products in a laminar counterflow configuration. The results show that the transition to the MILD regime is accompanied by the transformation of the ignition/extinction S-shaped curve becoming monotonic. Practical research on MILD gas turbines have been performed, using FLameless OXidation (FLOX) [15] and Colorless Distributed Combustion (CDC) [9]. They focused on the methods to achieve MILD combustion under different working conditions, such as the mixing type of fuel and oxidizer, pressure and heat intensity.

Flame Wall Interaction (FWI) can play a key role in the formation of pollutants, such as unburned hydrocarbons or CO, even though FWI takes place in only a small fraction of the combustion chamber [10]. FWI is generally classified into two types: Head-On Quenching (HOQ), which occurs when the propagation direction of the flame front is perpendicular to the wall surface [13]; and Side-Wall Quenching (SWQ), when a flame propagates along a wall surface [13]. The effect of FWI for the unburned hydrocarbons emissions has been studied theoretically, experimentally and numerically [6]. Singh et al. [18] measured the stationary, wall-normal CO concentration, gas phase temperature simultaneously as well as wall surface temperatures on an impinging jet burner. Their experimental results show that in lean and stoichiometric flames the CO profiles follow a similar trend and CO is mainly consumed in the hot post-flame region. Mann et al. [12] conducted experimental study on the evolution of temperature and CO mole fraction in stagnation-stabilized, atmospheric CH_4/air flames under a transient FWI. They reported that in the quenching zone, the CO oxidation path changed because of heat losses to the wall, and CO emissions remain high at a low temperature. Approaching FWI from an experimental point of view is particularly difficult due to small length and time scales in the process and complex interaction between wall, flow field and chemistry [6]. Therefore, most FWI studies have been performed theoretically and numerically. To model the FWI in laminar flow, two flow fields are often used: the stagnation or impinging flow, and the boundary layer flow where the flame interacts with the wall [1]. Vlachos et al. [21] simulated CO emissions for conventional premixed CH_4/air impinging on a flat surface with the stagnation flow geometry. They reported that high strain rates, which is an increasing function of inlet velocities, favour unburned CH_4 and CO.

This paper focuses on the limitations of MILD, specifically the effect of FWI. To the authors' knowledge, there is no literature about FWI under MILD combustion. However, the literature shows that FWI has a significant effect on emissions. Therefore, to apply MILD combustion in GTs, it is necessary to investigate FWI under MILD combustion. For this purpose, 1D axisymmetric premixed burner-stabilized stagnation flames are used to study the impinging flow. This model is verified with experimental data by Bergthorson [2]. Drawing on an approach from Sidey et al. [16], the effect of dilution ratio, inlet velocity and wall temperature are investigated.

Numerical Model

CHEMKIN PRO software package [4] was used to perform the simulations. The governing equations for the stagnation-flame reactor model were identical to those used in the Opposed-Flow Flame Model [8]. The axisymmetric geometry consisted of a nozzle and a stagnation plane normal to the flow. The computational domain was 2 cm long. The wall was considered to be inert with a constant temperature. For the inert wall the species boundary condition on the wall satisfies a zero species flux. The simulations were run on adaptive grids to ensure an adequate resolution.

To calculate the exhaust composition, a cylindrical control volume which extends from the nozzle exit up to the end of the computational domain was used [20]. As a result, the mass flux $\dot{m}_{exh,j}$ of a species j exiting the cylinder is:

$$\dot{m}_{exh,j} = \sum_{i=1}^{N} [2\rho_i \left(\frac{v}{r}\right)_i Y_{i,j} \Delta x_i] , \tag{1}$$

where N is the total number of cells, ρ_i is the mixture density at the i^{th} cell, $Y_{i,j}$ is the mass fraction of a species j, Δx_i is the length of the i^{th} cell, and v/r is the scaled radial velocity by the radius r, which is a function of x alone.

The mole fraction $X_{exh,j}$ of a species j at the outlet is:

$$X_{exh,j} = \frac{\dot{m}_{exh,j} / MW_j}{\sum_{i=1}^{N} [2\rho_i \left(\frac{v}{r}\right)_i \Delta x_i / MW_{mixture,i}]} , \tag{2}$$

where MW_j is the molecular weight of a species j and $MW_{mixture,i}$ is the mixture molecular weight at i^{th} cell.

Chemical Kinetics Model

Methane was used as the fuel for this study. The gas-phase oxidation of methane was described by GRI 3.0 [19] with its corresponding thermodynamic and transport databases. This mechanism has been optimized at lean-to-stoichiometric fuel mixtures, over a wide range of pressures and residence times, and is representative of the most recent and comprehensive methane combustion mechanism. All simulations were performed at atmospheric pressure with mixture averaged transport properties, with the Soret effect considered.

Dilution Method

The homogeneous mixtures with different levels of dilution are prepared in the same manner as Sidey et al. [16]. Hot products of premixed methane/air were produced with the freely propagating premixed flame model at 298K inlet temperature and stoichiometric conditions. The domain length was large enough (4cm) so that at the outlet the hot products of the premixed burner are in chemical equilibrium at the adiabatic flame temperature. These hot products were then mixed with cold reactants which is a stoichiometric mixture. The degree of mixing is given by the "dilution level," k , which is the ratio of hot products mass flow rate to the fresh mixture as described in Sidey et al. [16]. Undiluted cold reactants are defined as k=0, which is conventional premixed stoichiometric combustion, while pure hot products at the adiabatic flame temperature correspond to k = 1.0. As a result of this mixing, enthalpy of the final mixture remains the same for different values of k. The final mixture temperature was then calculated using the mixture enthalpy. The mixture temperature and oxygen concentration are shown in Figure 1. As expected, the mixture temperature increases with increasing the dilution level, but decreases for the oxygen mole fraction.

Verification of the Numerical Model

To verify the numerical model, simulation results from Sidey et al. [16] and Bergthorson [2] were reproduced showing good agreements. The simulation results in a Plug Flow Reactor (PFR) model are shown in Figure 2. The temperature gradient in the flame zone decreases with increasing the dilution level, leading to a widening of the reaction zone, and therefore inducing the decrease of the peak CO emissions and the increase of the CO pre-ignition. Note that all exhaust CO emissions are presented in a dry basis, corrected to 15% O_2 (see Equation (3)) according to established industrial practice (e.g. [11]).

$$CO(ppmvd, 15\% O_2) = 10^6 \frac{0.059 X_{CO}}{0.209(1 - X_{H_2O}) - X_{O_2}} , \tag{3}$$

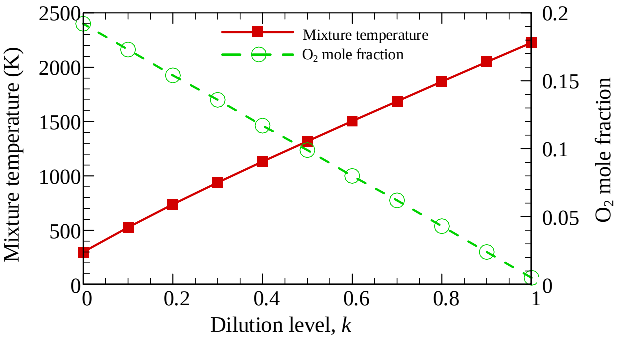

Figure 1. Mixture temperature and O_2 molar fraction profiles under different dilution levels.

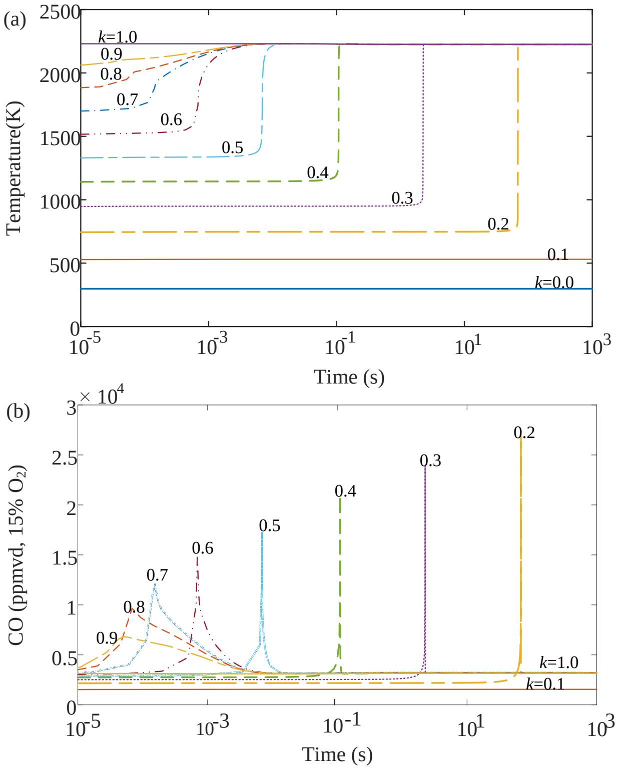

Figure 2. Temperature (a) and CO evolution on a dry basis, corrected to 15% O_2 (b) of mixtures diluted with hot products at different dilution levels (marked on the plots) in a PFR.

Results

Effects of dilution level

The temperature profile for different dilution levels at 300K wall temperature is shown in Figure 3 (a). The inlet velocity is 10m/s for all cases. There is no ignition for k = 0.0, 0.1 and 1.0 cases, as the residence time of the k= 0.0 and 0.1 cases is too short, and there is only pure hot products for the k=1.0 case. For lightly diluted mixtures (k = 0.2 to 0.5) ignition events are characterized by a sharp jump from the preheat temperature to the adiabatic flame temperature, similar to a conventional premixed flame. At higher levels of dilution (k = 0.6 to 0.9), there is a gradual change in temperature. As can be seen, the ignition of the k=0.6 case is significantly advanced compared to k=0.5 case, which suggests that between k=0.5 and 0.6, there is a transition to MILD combustion. In addition, for k=0.6, the inlet temperature is above 1650K, and the oxygen mole fraction is less than 8%, also indicating that the flame is in MILD combustion region, matching the observations of Sidey et al. [17].

It can also be seen from Figure 3 (a) that the peak temperature is almost the same from k=0.6 to 0.9 cases. The diluents in this paper are hot combustion products at 2226K adiabatic temperature. For cases with low level of dilution (k < 0.5), the post-flame reactions do not have sufficient time to reach equilibrium due to the quenching at the wall. From the CO mole fraction profile as shown in Figure 3 (b), the peak CO mole fraction decreases with increasing dilution levels, due to the increasing post-flame zone, the main region where CO emissions are oxidised [11]. Near the wall, the CO emissions for all cases drop dramatically due to the quenching of the flame at the wall [12].

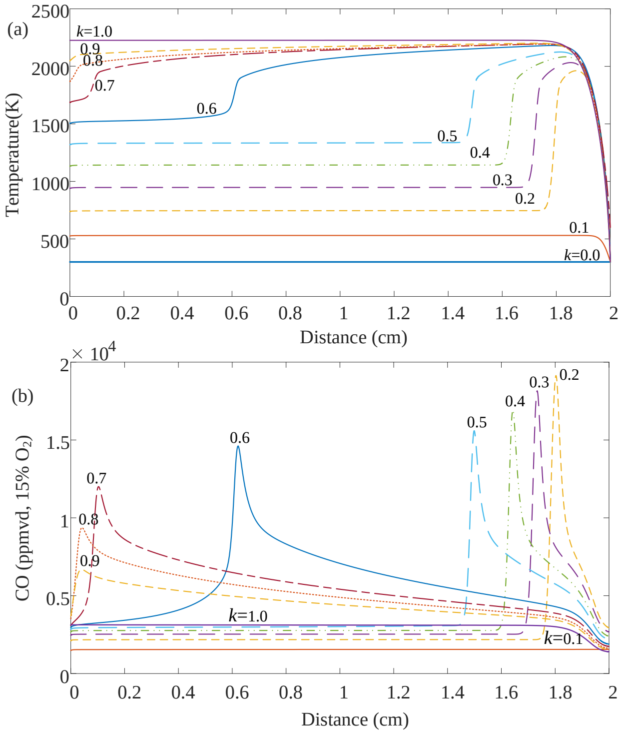

Figure 3. Temperature (a) and CO emissions (b) on a dry basis, corrected to 15% O_2 profiles from nozzle exit (0mm) to the wall (2mm) at different dilution levels (marked on the plots) and 300K wall temperature, 10m/s inlet velocity.

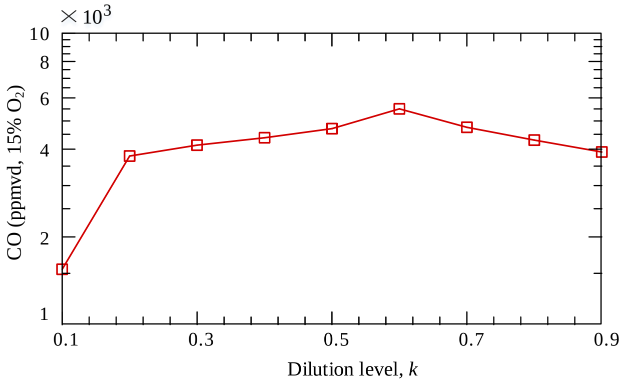

Figure 4. Exhaust CO emissions on a dry basis, corrected to 15% O_2 with different dilution levels at 300K wall temperature, 10m/s inlet velocity.

Using Equation (2), the exhaust CO emissions at different dilution levels are shown in Figure 4. It shows that the CO emissions increase with the dilution level from 0.1 to 0.6. Since the ignition delay time decreases with increasing the dilution level, the residence time of the products in a high temperature regime increases with the dilution level. This may promote the dissociation of CO_2 into CO. In addition, by increasing the dilution level, the CO_2 mole fraction increases and the O_2 mole fraction decreases, which reduces the net rate of CO oxidation. However, the trend changes direction from the premixed to MILD combustion. This is because the residence time of products under high temperature for MILD cases is nearly the same as shown in Figure 3, but the peak CO generated in the flame front decreases with increasing the dilution level.

Effects of wall temperature

The stagnation wall is an inert wall, which means there is no surface reactions. The wall temperature (T_w) was set to 300K, 600K and 900K. The dilution level was varied from 0.1 to 0.9. The exhaust CO mole fraction at different wall temperatures is shown in Figure 5. The CO emissions increase with increasing dilution levels in premixed cases, and decrease in MILD cases, which is the same trend as shown in Figure 4. At each dilution level, the CO mole fractions are almost identical, apart from the strain-extinguished solutions at $k = 0.1$. At the inlet velocity of 10 m/s, the $k = 0.1$ case is strain-extinguished for $T_w = 300$K and 600K, but has an ignited solution for 900K. This may be induced by the decrease of the near wall temperature gradient so that the reactant can accumulate the minimum ignition energy. These results might be different if we do not assume inert wall boundary conditions. As reported by Popp and Baum [14], at a higher T_w, the surface reaction and thermal diffusion play a significant role.

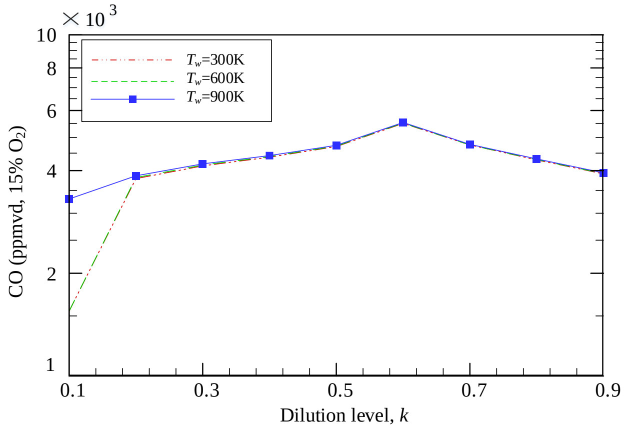

Figure 5. Exhaust CO emissions on a dry basis, corrected to 15% O_2 with different wall temperatures at 10m/s inlet velocity.

Effect of inlet velocity

To study the effect of the inlet velocity on MILD combustion and FWI, the inlet velocity was set to 10m/s, 15m/s and 20m/s at a constant 300K wall temperature with dilution levels from 0.1 to 0.9. The exhaust CO mole fractions with different inlet velocities at 300K wall temperature are shown in Figure 6. It can be seen that all solutions are strain-extinguished at k=0.1. The 10 m/s case has an ignited solution from $k = 0.2$, the 15 m/s case has an ignited solution from k = 0.3, and the 20m/s case has an ignited solution from $k = 0.4$. The CO emissions decrease with increasing inlet velocity in premixed cases, but then for the MILD cases it increases with the inlet velocity. For premixed cases, increasing the inlet velocity forces the flame close to the cold wall, leading to the decrease of the peak temperature which inhibits the dissociation of CO_2 into CO. For MILD cases, the flame font is far away from the wall, so the peak temperature changes little at different inlet velocities. However, the width of the CO profile increases with increasing the inlet velocity, which induces the increase of CO emissions.

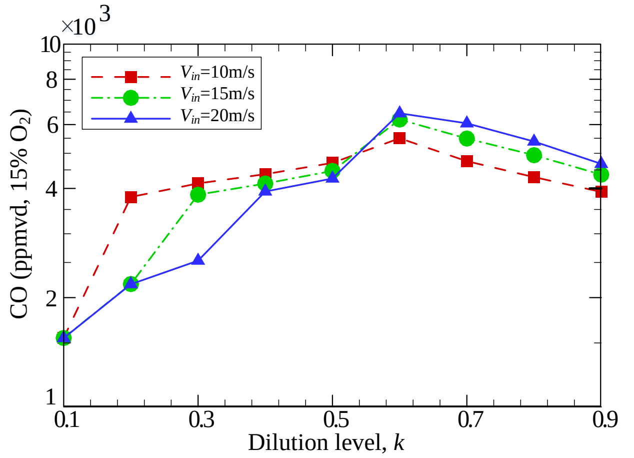

Figure 6. Exhaust CO emissions on a dry basis, corrected to 15% O_2 with different inlet velocities at 300K wall temperature.

Conclusions

The CO emissions behaviour of premixed and MILD flames have been investigated using the CHEMKIN stagnation burner geometry. The effects of the level of dilution, wall temperature and inlet velocity were studied. It was observed that the CO emissions increase with dilution levels up to k = 0.6, then slowly decrease beyond that point. Wall temperature does not significantly affect CO emissions. This is likely due to the assumption of the inert wall. As the simulations neglect the wall chemistry, the inert walls do not significantly affect the CO emissions, however increasing the wall temperature does stabilise the low dilution level cases. This effect of surface reaction on the wall will be the subject of further studies. The inlet velocity can decrease the CO emissions in premixed cases, but then for the MILD cases the CO emissions increase with the inlet velocity.

Acknowledgements

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