# Primary Zone Carbon Monoxide Levels for Gas Turbines Part I—Premixed Combustion

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The analysis of the mechanism of the carbon monoxide (CO) production reveals that its formation is strongly dependent upon the local fuel/air ratio and the fuel breakdown rate. The consumption of CO is controlled by the reaction  $CO + OH \rightleftharpoons CO_2 + H$ . For premixed combustion, the temperature and the over-all rate of the combustion process are such that chemical equilibrium is attained within the primary zone residence times. Transient peak concentrations of CO, exceeding its equilibrium levels, occur for all pressure levels and fuel/air ratios over the range from rich to lean conditions. These peak CO levels appear to be proportional to the fuel/air ratio, while the final equilibrium CO levels and the fuel/air ratio relate in an exponential manner. The difference between the peak and the equilibrium CO level is largest for the lean high pressure cases. Hence, the utilization of lean combustion to reduce the CO levels may be hindered by inadvertent quenching of the peak CO levels, e.g., within the cooling layer.

#### Introduction

THE current broadening of gas turbine applications accentuates the necessity of controlling the resultant emissions of  $NO_x$ , CO, and unburned hydrocarbons. Traditionally, the gas turbine has been an aircraft powerplant and as such the emissions have been concentrated in the vicinity of airports and at high altitude. However new applications place this engine in electric powerplants, and also its utilization in land and marine vehicles is increasing. As a result of these numerous applications, public awareness and legislation have developed to the extent that stringent controls are being imposed upon the emissions into the atmosphere.

The development of gas turbines to meet the proposed emissions standards, demands a greater understanding of the fundamental processes involved in the formation of exhaust products. The complexity of these processes, however, is such that close coordination of experimental and analytical work is needed. In the past, large experimental programs have been directed towards specific goals such as smoke reduction. Though specifically successful, these programs have provided little in the way of basic understanding of combustion/emission phenomena. The inherent complexity of the involved parameters prevents simple correlations between the causes and the effects. Hence, the present analytical approach has been undertaken with the intention to define significant trends which may be used to determine, direct, and interpret future development work.

Gaseous emissions of gas turbine exhausts are characterized at full power by relatively high  $NO_x$  concentrations as discussed in a previous paper<sup>1</sup> and at low power settings by high CO emissions which are the subject of the present work.

In general, the products of combustion can be influenced by the type of fuel/air preparation, the subsequent residence time, and the rate and degree of dilution. The typical combustor has these overlapping and occurring simultaneously. However, in the primary zone, the fuel/air conditioning, in specific, the fuel/air ratio, is the fundamental influence on the CO levels. The secondary zone, as defined by the onset of dilution modifies these CO levels by dropping the temperature and equivalence ratio.

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The present work is confined to the primary zone. In this region, the CO levels are solely controlled by chemical kinetics in the case of premixed/prevaporized combustion and by a complex coupled set of chemical kinetics, aerodynamic mixing, and vaporization mechanics in the case of liquid fuel combustion. Premixed combustion has obtained practical importance as a means for lowering NO<sub>x</sub> and unburned hydrocarbon emissions. Furthermore, the chemical kinetics, as investigated in premixed combustion, are common to all combustion systems. As a result, studies of the premixed primary zone provide the keystone to understanding the more general combustion system. The present work is directed towards establishing trends in the dependence of primary zone CO levels on fuel/air ratio, pressure, and residence time for premixed combustion. The combustor model and the chemical reaction mechanism used are described in detail in Refs. 1 and 2. The analysis was done with a Pratt & Whitney Aircraft developed program which numerically solves simultaneously the chemical kinetic, thermodynamic, and gas-dynamic equations. The resulting spectrum of reaction products and the resulting temperature are given as a function of axial location or residence time.

### **Results and Discussion**

The carbon monoxide profiles resulting from the nominal conditions of engine full power setting (23 atm pressure) and idle setting (2 atm pressure) are presented in Figs. 1 and 2, respectively. The primary zone equivalence ratios of 0.5 to 2.0 are covered. A burner inlet temperature of 1000°K was chosen. This is the lowest temperature at which self ignition of commercial jet fuel takes place. It can be argued that recirculation and mixing within the primary zone produces this effective starting temperature even though the compressor exit temperature may be considerably lower.

Previous reports<sup>1,2</sup> describe the sequence of the ignition delay time, the abrupt temperature rise during the peak chemical activity, and the gradual approach to equilibrium composition in detail. It is convenient to view the complex oxidation of hydrocarbons as occurring in three broad stages. The first stage produces light hydrocarbons and light partially oxidized hydrocarbons such as formaldehyde, acetaldehyde, formyl (HCO), organic peroxides, etc. The following sequence of reactions leads mainly to large amounts of  $H_2O$  and maximum amounts of  $H_2O + H_2O + H_2O$ 

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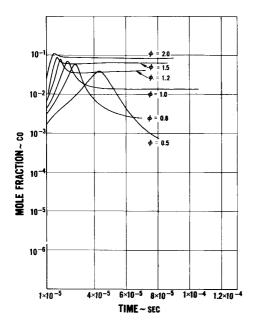


Fig. 1 CO molefraction vs elapsed time for high pressure premixed combustion at various equivalence ratios,  $T_{\rm inl\,et}=1000^{\circ}{\rm K}$ ,  $P_{\rm inl\,et}=23$  atm.

recombination and reshuffle reactions play an active role. The final stage, in particular for lean combustion cases, is largely characterized by the conversion of CO to  $\rm CO_2$ . In general, it is agreed that only the reaction  $\rm CO+OH \rightleftarrows \rm CO_2+H$  contributes significantly to the oxidation of CO.

The rate constant of the CO/CO<sub>2</sub> conversion reaction is taken from Ref. 5. Dryer et al.<sup>6</sup> have fit experimental data on this reaction by a non-Arrhenius type rate constant based on transition state theory calculations. This rate constant deviates from the rate constant used in the present study by less than a factor of three over the temperature range within the combustor primary zone. These rate differences produced no significant results in comparative studies; only the decrease in CO after the peak was slightly more rapid when the rate constant of Ref. 6 was used. However, these differences are smaller than the error limit based on the uncertainty of the reaction rates available. The present conclusions do not exclude the possibility of significant influences in the secondary zone.

The balance between the CO formation and the CO con-

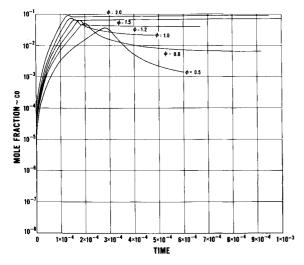


Fig. 2 CO molefraction vs elapsed time for low pressure premixed combustion at various equivalence ratios,  $T_{\rm inl\,et}=1000^{\circ}{\rm K},\ P_{\rm inl\,et}=2$  atm.

sumption rate in the case of the premixed combustion is characterized by a rapid CO production leading to a transient peak of CO which is followed by a gradual approach to equilibrium concentration.<sup>3</sup> Specifically, the initial CO formation rates increase with equivalence ratio. It has been found that the resulting CO levels of the transient peaks also increase with the fuel/air ratio in an approximately linear fashion. The very rich and the very lean cases show slightly higher CO levels than to be expected from this linearity. Subsequently, there is an approach towards equilibrium, with the composition after  $10^{-3}$  sec approximating the true equilibrium values. This effect will hold true at shorter residence times for effective inlet temperatures above  $1000^{\circ}$ K.

Experimental data<sup>7</sup> obtained from probing within a burner can confirm these analytical trends. At near stoichiometric proportions, the measured CO levels approach the equilibrium concentrations, while at lean conditions, there are large excesses of CO above equilibrium levels. Within the framework of premixed combustion, the analytical results are consistent with experimental observations, as discussed below.

Since the CO overshoots above equilibrium are smaller for stoichiometric or rich combustion at low pressure (see Fig. 2) the CO levels stay essentially unchanged with residence time as long as the condition of maximal temperature in the primary zone prevails. For an ideal lean combustion case, on the other hand, the CO level decreases within the same residence time range from the high overshoot level to the equilibrium concentration. In practice, however, the residence time within the primary zone can be effectively so short that the CO level at the end of the primary zone still exceeds the equilibrium concentration.

The transient CO peaks occur when the rates of the CO producing and of the CO consuming reactions are nominally balanced. The rate of CO production is closely linear to the hydrocarbon concentration, i.e., to the fuel/air ratio, because of the fact that the initial O2 concentration changes little for different fuel/air ratios. For a given fuel/air ratio, the rate of the CO consuming reaction is linearly proportional to the product of the CO and the OH (hydroxyl radical) concentrations. The peak concentration of OH (i.e., during its overshoot above equilibrium) is almost constant for the range of equivalence ratio from  $\phi = 0.8$  to  $\phi = 1.5$  (Ref. 1). At  $\phi = 0.5$  and at  $\phi = 2.0$ , the OH peak concentration is somewhat lower. This causes the CO peak concentration to vary almost linearily with fuel/air ratio except for the extreme cases, with higher CO peaks. Furthermore, the OH level during the CO peak condition and during the CO equilibrium condition is considerably higher for low pressure cases than for high pressure cases. Therefore, the CO consumption is faster for low pressure combustion; i.e., the absolute values of the CO peaks tend to decrease with decreasing pressure. In addition, the CO equilibrium levels at high and low pressure are about equal for very rich cases, while the lean low pressure CO equilibrium level exceeds the lean high pressure CO level. Therefore, the relative CO peaks become higher with decreasing fuel/air ratio and with increasing pressure.

## Conclusions

Over the range of equivalence ratios investigated (from  $\phi=0.5$  to  $\phi=2.0$ ), the final equilibrium CO levels vary by more than two orders of magnitude. In comparison to the equilibrium CO concentrations, however, the peak CO levels vary in the same range of fuel/air ratios by less than a factor of three; i.e., the peak CO levels for premixed combustion are less sensitive to stoichiometry than are the final levels. Therefore, for a given fuel/air ratio at the exit of a combustor, rich and lean burning are distinguished by the fact that in the lean burning case, the main conversion of CO to CO<sub>2</sub> takes place in the primary zone, while in the rich burning case, the main CO conversion is caused by air added in the secondary zone. For lean combustion, inhomogeneity in the primary zone would produce excessive amounts of CO. Rich combustion with poor

mixing (inhomogeneity) in the secondary zone would also result in excessive CO formation.

In general lean combustion should be employed, if homogeneity with respect to the local fuel/air ratio can be obtained within the primary zone. However, there is no advantage of lean over rich combustion, if initial maldistribution causes inhomogeneity in the primary zone and the secondary zone improves the uniformity. For this condition, low  $NO_x$  production might make rich combustion preferable. Many conventional burners are of this type.

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# Part II—Liquid Fuel Combustion

The effect of the fuel droplet vaporization rate on the production of carbon monoxide (CO) during combustion in a gas turbine has been evaluated. The temporary CO concentrations exceeding the equilibrium values, observed for premixed combustion, are reduced or eliminated by the gradual introduction of fuel via droplet vaporization. Staged fuel addition is demonstrated as a means of avoiding the excessive initial CO formation associated with premixing at low equivalence ratios.

#### Introduction

AS turbines of the present generation rely upon liquid fuel as the prime energy source. This fuel is conventionally prepared for combustion by pressure or air assisted atomization. Howev..., the fuel droplets do persist within the active combustion zone. As a result, the influence of the vaporization/mixing process is superimposed on the chemical kinetics which were the sole control of premixed combustion. The vaporization/mixing rate can under certain conditions become a significant factor in liquid fuel combustion emissions.

The preceding work<sup>1</sup> presented a discussion of the CO production and consumption within the primary zone of a gas turbine combustor for premixed combustion. The present effort extends this to combustion of vaporizing fuel droplets. This work is also confined to the primary zone of a gas turbine combustor. The combustor model and chemical reaction mechanism applied have been described in detail in Ref. 2. Following the arguments in Ref. 2, the liquid fuel vaporization and mixing has been simulated by a fuel availability rate process. Comparison with the results from a more complete treatment of the droplet vaporization mechanism<sup>4</sup> shows that the availability rate used corresponds to droplet sizes of about  $20\mu$ ,  $40\mu$ , and  $105\mu$ .<sup>2</sup>

In reality, the primary combustion zone has fuel being sprayed into the hot combusting gas mixture. Some of the initial drops are small and vaporize immediately; others enter the hottest active zone and are at once vaporized. This part of the fuel is immediately available for combustion. The remainder of the fuel enters the recirculation zone as droplets, and vaporizes and combusts in a continuous fashion. Hence, a continuous distribution of droplet sizes may be viewed as a two part system, where smaller drops are represented by premixed combustion and larger drops as liquid fuel combustion.

In effect, there is an immediate introduction of vaporized and mixed fuel followed by a period where the remaining fuel vaporization predominates. In order to simulate this effect, a fraction of the fuel is premixed and the remainder is introduced by the aforementioned fuel vaporization mechanism, This ratio of premixed fuel to liquid fuel has to be estimated because of a lack of detailed experimental information. The condition of 25% premixed/75% liquid initial fuel has been used as a base. However, the limiting case of 100% initial liquid fuel combustion has also been investigated.

Emphasis has been given to high pressure conditions, since the carbon monoxide (CO) levels for high pressure premixed combustion<sup>1</sup> showed the largest excursions above equilibrium. The pressure dependency is deduced from comparison with results of low pressure combustion. For large droplets, vaporization/mixing becomes the rate determining step in the combustion process. Therefore, the early parts of rich combustion with large droplets resemble lean conditions if one adjusts for different ignition delay times. This makes the results for rich combustion more encompassing.

#### Results

The rate of carbon monoxide production and consumption is a function of a number of parameters such as temperature, fuel/air ratio, degree of premixedness, fuel droplet size, and pressure. For comparison, all cases are for an effective air inlet temperature of 1000°K.

For the more realistic combustion type with 25% premixed/75% liquid initial fuel, the response of the temperature and CO levels to droplet size is demonstrated in Figs. 1 and 2, respectively. The case of completely premixed combustion is added in Figs. 1 and 2 for comparison. Premixed combustion can be