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Preliminary Study of NO_x, CO, and Lean Blowoff in a Piloted-Lean Premixed Combustor Part II: Modeling

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The characteristic time model (CTM) is a semi-empirical model for gas turbine emissions and performance. The CTM represents the essence of the dominant physical subprocesses related to combustor performance in terms of characteristic times. Properly formulated, these characteristic times account for variations in combustor geometry, fuel characteristics, and operating conditions. In this work, the capability of the CTM to correlate the piloted-LP NO_x, CO and blowoff data described in part I of this paper is assessed.

INTRODUCTION

Semi-empirical models for gas turbine combustor emissions assign characteristic times, which are based on combustor geometry, fuel characteristics, and operating conditions, to the dominant subprocesses of combustion related to performance and pollutant emissions. Linear ratios of these characteristic times, or of sums of the times weighted with empirical constants, describe the emissions indices of oxides of nitrogen (NO_x) and of carbon monoxide (CO). Furthermore, equalities between these characteristic times describe the lean blowoff limit.

Tuttle et al. [1] measured local CO, NO and temperature values for diffusion flames stabilized on a simple disk flameholder with a single point probe. These workers found that CO originates in the leading edge of the shear layer which surrounds the bluff-body recirculation zone. Thermal NO formation was found to be most significant in the near-stoichiometric trailing edge of the shear layer near the burner centerline. The above information about the spatial location and thermal environment associated with CO oxidation and thermal NO formation is the basis of the conventional combustor characteristic time models (CTMs) for CO and

NO_x. Preliminary CTMs for the piloted-lean premixed Combustor A NO_x, CO, and blowoff data discussed in part I are summarized here.

MODEL FOR NO_x FROM THE COMBUSTOR A PILOT FLAME

In applying the CTM to the pilot flame in a gas-fired staged combustor (see Fig. 1) such as Combustor A, it is assumed following Tuttle et al. [2] that pilot flame NO emissions are proportional to a Damköhler number (the ratio of a fluid mechanic time to a chemical kinetic time) as follows:

$$\text{NO}_x \text{EI}|_{\phi=1} = 4.41(1-y_{fm})(\tau_{sl,NO}/\tau_{NO}) \pm 1.02 \text{ (g NO}_x\text{/kg fuel)} \quad (1)$$

$\tau_{sl,NO}$ is the characteristic fluid mechanic time for eddy dissipation in the post-flame region, and τ_{NO} is the characteristic kinetic time for NO formation in the post-flame region. The subscript $\phi=1$ denotes the pilot diffusion flame, and the correlation slope and standard deviation are from Newbury and Mellor [3]. The mass fraction of the total combustor fuel flow to the pilot flame ($1-y_{fm}$) is included to

Figure 1. Schematic of a generic piloted-LP combustor operating with y_{fm} less than one.

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account for the fact that the number of stoichiometric eddies varies with the mass flow of fuel to the pilot flame.

Following Tuttle et al. [2] the kinetic time is defined as

$$\tau_{no} = 10^{-12} \exp(135,000/RT_{\phi=1}) \text{ (ms)} \quad (2)$$

where the pre-exponential factor is selected such that the characteristic time ratio in Eq. (1) is on the order of unity and R is the universal gas constant. The global activation energy (135,000 cal/gmol) for diffusion flame NO formation was deduced empirically from Arrhenius graphs, and, following Tuttle et al. [1], the appropriate temperature associated with the NO forming eddies is the stoichiometric adiabatic flame temperature ($T_{\phi=1}$). Note that in a the piloted-LP combustor (see Fig. 1) operating with y_{fm} between zero and one, the pilot flame is supplied with hot, vitiated air from the LP flame. Therefore the stoichiometric flame temperature must be modified to account for inlet air vitiation and preheating effects.

Following Mellor and Washam [4], the characteristic fluid mechanic time for Combustor A is defined as:

$$\tau_{sl,no} = 1000 \cdot (l_{no}/V_{\phi=1}) \text{ (ms)} \quad (3)$$

where the stoichiometric flame zone velocity ($V_{\phi=1}$) is used to estimate the velocity of stoichiometric eddies convecting through the combustor:

$$V_{\phi=1} = (\dot{m}_{a,\phi=1} / \dot{m}_a) (T_{\phi=1} / T_{in}) V_{ref} \text{ (m/s)} \quad (4)$$

The ratio of air flow rates accounts for the mass fraction of combustor air flow which accelerates the stoichiometric eddies through the primary zone, and V_{ref} is the combustor reference velocity. Due to operational differences between Combustor A and previously-analyzed conventional combustors, this ratio is not known a priori.

For the pilot flame in Combustor A, the length scale associated with thermal NO formation is defined as

$$l_{no}^{-1} = (d_{cb}/\cos\theta)^{-1} + (d_{cb})^{-1} \text{ (1/m)} \quad (5)$$

This modification of Mellor and Washam's l_{no} accounts for the centerbody diameter (d_{cb}) determining both the radial and axial extent of the centerline recirculation zone; the cosine of the swirl angle, θ , accounts for the augmentation of streamline lengths through the combustor primary zone due to swirl.

When Combustor A operates in the piloted-LP mode, thermal NO production in stoichiometric eddies convecting from the pilot flame region composes the dominant fraction of total NO production in the combustor (true for y_{fm} less than approximately 0.70 – compare with Fig. 5 in part I). As

shown in Fig. 2, these data are found to align with the model of Newbury and Mellor when the mass fraction of air to accelerate the stoichiometric eddies in Eq. (5) is set to 0.25. This value will be compared with STAR-CD CFD results for Combustor A in the near future.

Figure 2. Preliminary correlation for the piloted-LP NO_x data which are dominated by NO from the pilot flame.

MODEL FOR NO_x FROM THE COMBUSTOR A LP FLAME

In the most simplified case, the thermochemical environment which surrounds a given fluid element as it convects through the combustor can be visualized in one dimension. The one dimensional fluid pathway is divided up into four zones: A, B, C, and D. Zone A is the preheat zone in which significant spatial gradients in free radical concentration and temperature are first encountered. Free radicals such as O- and H-atom and CH radicals form through the various reactions associated with hydrocarbon fuel oxidation.

Zone B is the hydrocarbon reaction zone. Damköhler-Reynolds number graphs [5] made for practical LP burners suggest that this is a distributed reaction zone. It is often modeled as a perfectly stirred reactor (PSR). Due to the peak level of CH which exists in zone B, NO forms through the prompt [6] mechanism which involves the attack of CH radicals on N₂, leading to HCN and N-atom, which subsequently are converted to NO. Due to the high concentrations of O and H radicals in zone B, NO also forms through the N₂O mechanism [7] through the attack of super-equilibrium O- and H-atom on nitrous oxide. Also, NO forms to some extent through the Zeldovich [8] mechanism.

Zone C is the free radical relaxation (or recombination) zone. Because the CH radical is short-lived and only exists in the flame zone, there is a negligible contribution of prompt

NO in this region. However, NO continues to form through the nitrous oxide and Zeldovich mechanisms.

Zone D is the equilibrium zone where free radicals have relaxed to their equilibrium levels. For flame temperatures greater than approximately 1850-1900 K (and/or significant fuel/air unmixedness) and large residence times, significant NO will form through the Zeldovich mechanism in this region.

The total NO formed in an LP combustor could be represented in terms of a sum of characteristic time ratios as follows:

$$\text{NO}_x \text{EI}|_{\phi < 1} = \frac{m_1}{1.4} \left(\frac{\tau_{\text{f,pr}}}{4 \tau_{\text{f,ps}}} \right) + \frac{m_2}{1.4} \left(\frac{\tau_{\text{f,pr}}}{4 \tau_{\text{f,ps}}} \right) + \frac{m_3}{1.4} \left(\frac{\tau_{\text{f,pr}}}{4 \tau_{\text{f,ps}}} \right) \quad (\text{g/kg}) \quad (6)$$

Zone B: total NO production in the fuel reaction zone

Zone C: total NO production in the relaxation zone Zone D: thermal NO production in the post-flame zone

where the characteristic time ratios represent NO formation in zones B, C, and D, respectively, and m_1 , m_2 , and m_3 are weighting constants. $\tau_{\text{f,pr}}$ is the characteristic fluid mechanic time associated with the turbulent flame zone, and $\tau_{\text{f,ps}}$ is the kinetic time associated with NO formation through the prompt, N_2O , and Zeldovich mechanisms in the PSR region. The kinetic time could be estimated from PSR experimental/modeling studies such as those of Steele et al. [9].

In zone C τ_{th} is the characteristic kinetic time associated with super-equilibrium free radical relaxation, and $\tau_{\text{nr,th}}$ is the kinetic time for NO formation through the N_2O and Zeldovich mechanisms. Note that the characteristic time ratio for zone C is composed of two kinetic times which could each be estimated with detailed chemical kinetic models.

For zone D the characteristic times are similar to those associated with thermal NO given by Eqs. (2) and (3). However, due to premixing of the fuel and air, the flame temperature associated with combustion of the premixed fuel/air ($T_{\phi,m}$) replaces the stoichiometric flame temperature ($T_{\phi=1}$). Note that there is no reason to expect m_3 to correspond to the value of 4.41 used in Eq. (1).

Of the datum sets discussed in part I, only that of Leonard and Stegmaier [10] can be considered to be perfectly premixed (as Eq. (6) implies since a single ϕ and $T_{\phi,m}$ are used). At flame temperatures less than approximately 1900 K, Leonard and Stegmaier indicate that they observed no increase in NO_x with axial sample probe position (l_{probe}) varying by a factor of ± 50 times. However, due to the fact that the kinetic time (τ_{no}) is on the order of seconds for flame temperatures less than approximately 1900 K, the zone D term in Eq. (6) is negligible with respect to the other two terms (neither of which is a function of l_{probe}). Therefore, Eq. (6) agrees with the sensitivity of NO_x to residence time

observed by Leonard and Stegmaier. Additional issues such as whether or not an expression such as Eq. (6) can qualitatively model the neutral sensitivities of NO_x to changing inlet temperature and pressure observed by Leonard and Stegmaier (see part I) cannot be examined until each characteristic time in Eq. (6) is determined via well controlled, laboratory experiments. Nevertheless, a preliminary LP NO_x correlation can be obtained by assuming the following global expression:

$$\text{NO}_x \text{EI}|_{\phi < 1} = y_{\text{f,m}} (\tau_{\text{f,pr}} / \tau_{\text{no}}) \quad (\text{g NO}_x / \text{kg fuel}) \quad (7)$$

The appropriate fluid mechanic time is assumed to be the ratio of the ignition perimeter to the premixer exit velocity [11], and following Nicol [12] the chemical kinetic time is:

$$\tau_{\text{no}} = \exp(A) \cdot T_{\text{in}}^{(B+CT_{\phi,m}+Dp_{\text{in}})} \cdot P_{\text{in}}^{(E+FT_{\phi,m}+GT_{\text{in}})} \cdot \exp\left(\frac{H + Ip_{\text{in}} + JT_{\text{in}}}{T_{\phi,m}}\right) \quad (\text{ms}) \quad (8)$$

where A through J are empirical constants. While Eq. (7) does not offer the zonal resolution of physical subprocesses associated with LP NO formation as in Eq. (6), Eq. (8) does include terms from which the apparent global activation energy and pressure sensitivity associated with LP NO formation can be deduced. The appropriate constants for Eq. (8) for a given set of LP NO_x data can be computed by performing multiple variable regression analysis.

It is possible to decrease the number of free parameters in Eq. (8) without significantly decreasing the quality of the LP NO_x correlation. The pruned correlation of the Combustor A LP NO_x is shown in Fig. 3. This correlation has a standard deviation of approximately ± 6 ppmvd, 15% O_2 . The apparent activation energy deduced from the Fig. 3 correlation constants is on the order of 70 kcal/gmol. The pressure exponent deduced from the Fig. 3 correlation ranges between slightly negative to slightly positive with increasing $T_{\phi,m}$. These trends are consistent with those in the literature.

Eqs. (1) and (7) are summed together to model the Combustor A piloted-LP NO_x CTM. Figure 4 shows the model prediction of total $\text{NO}_x \text{EI}$ as a function of $(1-y_{\text{f,m}})$. Note that the non-linear trend in the data near $y_{\text{f,m}}=1$ is predicted by fuel mass fraction weighted sum of the pilot and LP NO_x correlations. The interpretation of this trend using the staged combustion model is that it is possible to get an exponential decrease in LP flame NO with only a linear increase in pilot flame NO. Over a certain range of $y_{\text{f,m}}$ this can yield a net decrease in total NO as shown in Fig. 4 (and Fig. 10 in part I). All of the Combustor A NO_x data are correlated in Fig. 5 with a standard deviation of ± 10 ppmvd, 15% O_2 .

Figure 3. Preliminary Combustor A LP NO_x correlation.

Figure 4. Prediction of the non-linear trend in piloted-LP NO_x near $y_{fm} = 1$.

MODEL FOR CO FROM THE COMBUSTOR A LP FLAME

The temperature of the outer portion of the shear layer, in which CO oxidation is quenched, may be approximated as the average of the fuel/air mixture temperature (T_{nm}) and the exhaust gas temperature (T_e) after Mellor [13]. By selecting a quench length so that the characteristic times corresponding to the Combustor A data are within the range of characteristic times reported in Connors et al. [14], and using the CO CTM developed there, it was found that the appropriate CO quench location for Combustor A is associated with the dome cooling slots.

Figure 5. Preliminary correlation of all Combustor A NO_x data.

Figure 6 shows a comparison between Combustor A and the natural gas data found in Connors et al. for a conventional, heavy-duty combustor. Using the length scale definition described above for Combustor A, the data from Combustor A fall within the range of characteristic time ratios corresponding to the natural gas data in Connors et al. In this figure, the data for Combustor A align according to combustor residence time (squares versus other data).

Following Tuttle et al. [2], Fig. 7 shows the variation of COEI with characteristic time approximated as linear. The slope corresponding to the Combustor A data is larger

Figure 6. Comparison between Combustor A and the natural gas data in Connors et al. [14]. It is assumed that cooling air quenches CO in the dome for Combustor A.

than the slope associated with the data of Connors et al. because the range of equivalence ratios corresponding to Combustor A is small compared to the range for the data of Connors et al. and much closer to the lean blowoff limit (see Part I). Apart from having a large slope compared to the natural gas data found in Connors et al., the lack of correlation of the Combustor A data in Fig. 7 suggests that the ultralean emissions for the LP combustor will require more significant modification to the diffusion flame CO CTM of Connors et al. than attempted to date.

Figure 7. Same as Figure 7 except the linear model for COEI with $\tau_{co}^*/\tau_{sl,co}$ is shown.

MODEL FOR COMBUSTOR A LEAN PREMIXED BLOWOFF

For each set of operating conditions reported for Combustor A, the fuel flow to the combustor was decreased slowly until the flame was extinguished. The air and fuel mass flow rates, along with the combustor inlet conditions, at the point of extinction are then used to calculate the fluid mechanic time (τ_u) and the chemical kinetic time (τ'_{hc}) using the lean blowoff model for a tube-and-disc flameholder of Plee and Mellor [15].

To estimate the increased residence time in the shear layer surrounding the centerline recirculation zone due to swirl, the length scale in the fluid mechanic time (τ_u) defined in Plee and Mellor is modified as in Eq. (5):

$$\tau_{sl} = 1000 \cdot \frac{l_{co} / \cos \theta}{V_{lip}} \quad (\text{ms}) \quad (9)$$

where l_{co} is the sum of d_{ab} and step height (see Fig. 1). Also, in this analysis, the temperature at the sudden expansion of Combustor A is approximated as the average of the inlet air

temperature (T_{in}) and the adiabatic flame temperature based on the primary zone air (T_{qz}).

If the model of Plee and Mellor is rearranged to determine the appropriate activation energy for the ignition delay time of natural gas, the overall activation energy for the Combustor A data is determined to be 21 kcal/gmol (this value excludes the flagged datum in Fig. 8). This is the same activation energy used in Plee and Mellor for C_3H_8 and higher order hydrocarbons. Spadaccini and Colket [16] also found the larger alkanes present in natural gas lead to overall ignition delay activation energies less than that for pure CH_4 .

Figure 8 shows the lean blowoff model of Plee and Mellor [15] applied to Combustor A. If the flagged datum is excluded, the slope of the best-fit is 1.85 with a y-intercept that is on the order of a standard deviation from the origin. Also included is the predictive equation recommended by Plee and Mellor for cases in which fuel-penetration effects are negligible. Although the Combustor A blowoff data appear to be closely modeled by the correlation of Plee and Mellor for negligible fuel-penetration effects, more data would further validate this agreement and confirm the exclusion of the flagged datum in Fig. 8.

The universality of the NO_x , CO, and blowoff models discussed above will be assessed in the future with respect to 1) additional experiments which are planned for Combustor A, 2) the Combustor B data discussed in part I and 3) data from experiments with laboratory flameholders.

Figure 8. Lean blowoff limit of Combustor A compared to the negligible fuel-penetration correlation in Plee and Mellor [15].

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