PREDICTION MODEL OF NO\textsubscript{x} FOR GAS TURBINE COMBUSTOR WITH DIFFUSION AND LEAN PREMIXED FLAMES

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Abstract

In order to predict the NO\textsubscript{x} concentration etc., it is necessary to carry out 3-D reacting flow analysis in the combustion zone. However, regardless of improved numerical scheme, and physics-based modeling of flow phenomena and combustion reaction, these techniques not yet reached to a level to be applied to practical combustor problem, because of vast computation time and consequently high computation costs, etc.. To improve NO\textsubscript{x} characterization of new Dry Low NO\textsubscript{x} Combustor (DLNC) and optimum fuel scheduling for DLNC operations, a NO\textsubscript{x} prediction method to be applicable for practical combustor problems needs to be developed.

In this paper has been proposed a simple semi-empirical model for predicting DLNC NO\textsubscript{x} emissions that formed from lean premixed combustion flames and diffusion flames. This model comprised of experimental coefficients for adjusting or incorporating effects of practical combustion liner configurations and effects of flow conditions in combustion zone, etc.. Also, the present model is applied to newly designed and redesigned DLNC for estimating NO\textsubscript{x} emission levels and its variation with gas turbine operating conditions, which are compared with the experimental data of full pressure combustion with Natural Gas (NG) fuel.

Nomenclature

- \(G_{ad}\): Air used for diffusion combustion in reactor 1
- \(G_{ad} = \beta G_{fd} / (\alpha_{ih} \times \phi_{d})\)
- \(G_{ai}\): Combustion air of reactor i
- \(G_{f1}\): Fuel of reactor 1
- \(G_{f2}\): Fuel of reactor 2
- \(G_{fd}\): Diffusion fuel to be reacted in reactor 1,
- \(G_{fd} = \beta G_{f1}\)
- \(G_{fi}\): Fuel of reactor i
- \(G_{g1}\): Combustion gas in reactor 1,
- \(G_{g1} = G_{fd} + G_{ad}\)
- \(G_{g2}\): Combustion gas in reactor 2
- \(G_{gi}\): Combustion gas in reactor i
- \((NO\textsubscript{x})_{1}\): NO\textsubscript{x} generated from reactor i (1.23 MPa)
- \(P\): Internal pressure of the combustor
- \(\sigma_{ih}\): Theoretical fuel/air ratio
- \(\beta\): Ratio of diffusion fuel to be reacted in reactor 1
- \(\phi_{1}\): Equivalence ratio in reactor 1
- \(\phi_{2}\): Equivalence ratio in reactor 2
- \(\phi_{i}\): Equivalence ratio in reactor i

Introduction

From the view point of improving cycle efficiency and environmental counter measure on combined cycle power generation, constant progress has been made on the development of high temperature gas turbine Dry Low NO\textsubscript{x} Combustor (DLNC). In spite of combustion at high temperature, NO\textsubscript{x} emission level DLNC has been lowered considerably year by year. In order to lower the NO\textsubscript{x} emission level while maintaining stable flame, in these DLNC it is necessary to define the
optimum combustion conditions and the operating conditions. In recent years, in the DLNC, operated at high temperatures in particular, there is growing trend towards considerably reducing the amount of film cooling air to be used for liner cooling, since the efficient wall cooling technique as well as reducing NOx emission level are important problem to be paid attention. In order to lower the temperature of combustion flame it is necessary to set the premixed equivalence ratio to around 0.6 to 0.5, also under this condition, most of air fed to the combustor can be used as combustion air as shown in Figure 1. As a result, the amount of the air used for the purpose other than combustion such as dilution, film cooling etc., can be reduced substantially.

Various wall cooling techniques, namely the reduction of the area to be cooled and adoption of new cooling technique are under progress in terms of lowering the amount of film cooling air. This shows that the selection of such combustion conditions that reduces NOx emission level is closely linked with the cooling technique and combustor configuration. In the conceptual designing stage of a new low NOx combustor, it is necessary to combine diffusion flame and premixed flame of various equivalence ratios by taking into consideration of combustion stability as well as the NOx level. Therefore, accurate prediction of NOx emission characteristics corresponding to the combustion conditions and operating conditions are desirable.

A most common way of predicting the NOx emission characteristics is 3-dimensional reacting flow analysis in the combustor. Although, recently based on the improved numerical scheme, physics based modeling of turbulence and chemical reaction, etc., prediction accuracy of some computation codes have been improved to a great extent, however, due to limitation on total number grid points, high computation cost, lack of knowledge to model properly some of the physical phenomena, etc., none of them have reached to a level to be used in the practical combustion problems.

However, as an alternative way of predicting NOx emission level based on various practical machine operation data, there exist some methods for comparative evaluation using empirical formula of Sullivan(1976), which correlates data based on diffusion combustion and the Lewis(1981) correlation between flame temperature and NOx emission level. In the case of using these prediction technique for some new combustor configuration with desired operation conditions, it is difficult to make NOx emission level prediction with sufficient accuracy. Therefore, full-pressure combustion tests need to be performed to obtain information regarding NOx emission characteristics.

In the present work is proposed a simplified NOx prediction model which could predict the NOx characteristics over the whole operating range of a dry low NOx combustor, in which both the diffusion and premixed combustion flames are used together. Additionally, results of comparison between predicted NOx emission level using the present model and the experimental data of full pressure tests are presented.

![Figure 1. Combustion liner cooling air ratio as a function of $\phi_{ex}$ and $\phi_p$.](image)

**NOx Prediction Model**

It is reported by Rizk et al. (1993), Nicol et al. (1993), Rokke et al. (1993) and Sano(1993) that the generation mechanism of thermal NOx from combustion follows the extended Zeldovich mechanism, nitrous oxide mechanism involving $N_2O$ and prompt NO etc. and that the dominant generation mechanism differs depending on the combustion conditions.

The operating conditions and features of DLNC, to which the applicability of the present model is tested are as follows. Natural gas is used as the fuel, diffusion flame and multiple premixed flames (premix equivalence ratio < 0.6) are used in parallel, the residence time is shorter in the diffusion combustion area, whereas that in multiple premixed combustion areas is longer.

Taking into consideration of the above mentioned features, following hypothesis has been made.
1) NOx generation mechanism follows the extended Zeldovich mechanism.

2) Regarding the NOx generation from diffusion combustion, adequate diffusion combustion ratio $\beta$ and equivalence ratio of diffusion combustion $\phi_d$ are assumed. That means, $\beta G_{f1}$ fraction of diffusion fuel having flow rate $G_{f1}$ is burnt at equivalence ratio $\phi_d$ and remaining fraction of $(1-\beta)G_{f1}$ is burnt in reactor 2 or in succeeding reactors including reactor 3.

3) Well stirred reactor (WSR) model is applied to each combustion area which consists of one diffusion combustion zone and several premix combustion zones. And each combustion area (WSR) activate independent combustion reaction and finally mixed with each other in the downstream.

For reactor 2, amount of fuel to be burnt, air required for combustion, and combustion gas and equivalence ratio represented by $G_{fp}$, $G_{ap}$, $G_{g2}$, and $\phi_2$, respectively are calculated as follows:

$$G_{fp} = (1-\beta)G_{f1} + G_{f2}$$

$$G_{ap} = (G_{a1} - \beta G_{f1} / \alpha_{th} \times \phi_d) + G_{a2}$$

$$G_{g2} = G_{fp} + G_{ap}$$

$$\phi_2 = \frac{G_{fp}}{G_{ap}}$$

$\alpha_{th}$ is theoretical fuel-air ratio.

Following this way, combustion occurs in reactor 1 at diffusion combustion equivalence ratio $\phi_d$ and in reactor 2, at $\phi_2$.

Based on these equivalence ratios, the combustion gas temperatures in respective reactors, $T_{f1}$ and $T_{f2}$, are obtained.

NOx concentration was obtained on the basis of expanded Zeldovich mechanism as follows:

$$O + N_2 \rightarrow NO + N$$

$$N + O_2 \rightarrow NO + O$$

$$N + OH \rightarrow NO + H$$

and 41 radical equations concerning the dissolution of hydrocarbon. Various forms of expression can be chosen depending on the degree of simplification. In the present work, however, from the view point of accuracy and practical applicability, NOx concentration vs. temperatures of combustion flame is expressed using the residence time (5, 10, and 20 ms) as a parameter as shown in Figure 3. The residence time of 5 ms corresponds to the pilot flame (i.e. diffusion flame) and 10 to 20 ms are assumed for premixed combustion flames. 5ms and 10ms are common value to combustor A, B, C and 3 staged combustor (Fig. 6), because the residence time of diffusion combustion zone and premix combustion zone of each combustors is approximately same value. These residence time are estimated from mean combustion gas velocity of each reactors.

Pressure 1.23 MPa in Fig. 3 is selected for decreasing extrapolating range of pressure effect on NOx, because 1.23 MPa is approximately mean operating pressure level of real combustor.
Experimental Apparatus and Test Conditions

A schematic view of the experimental set up is shown in Figure 4. The experimental apparatus consists of combustion test rig, combustion air system, fuel system, exhaust system and cooling water system. Natural gas supplied through the gas compressor is used as fuel, combustion air is supplied from the compressor, and temperatures are controlled by the air cooler. The test rig includes the test combustor, transition piece, thermocouple rakes and exhaust gas sampling probes etc. Probe system enables continuous sampling of combustor outlet gas (contain NOx, THC, CO, O2, CO2).

In the case of reactor 1, for example, $T_r$ is obtained from diffusion combustion equivalence ratio $\phi_d$ and $(NOx)_1$ represent the NOx at 1.23 MPa is obtained on basis of $T_r$ and residence time. Also, $(NOx)_1$ defined as the NOx generated from reactor 1 is calculated on the basis of pressure $P$ under the prediction condition as follows. Pressure dependence on NOx is assumed to have the following power law effect.

$$(NOx)_1 = (\frac{P}{1.23})^{x}(NOx)_{}^{*1}$$

The power law effect of pressure on NOx is reported by Touchton et al. (1976), Lewis (1981).

Here, the power index $x$ varies depending on the diffusion combustion condition and equivalence ratio (or flame temperature) of premixed combustion etc., therefore it need to be chosen from the experimental data or separate assumption.

Based on $(NOx)_1$ and $(NOx)_2$ in each reactor as obtained by the above mentioned method, $(NOx)_x^*$, which represent the NOx emission level at combustor exit, is obtained from the following expression in the form of weighted average as follows:

$$(NOx)_x^* = \frac{G_{e1}(NOx)_1 + G_{e2}(NOx)_2}{G_{e1} + G_{e2}}$$

In Figure 5 is shown the exhaust gas sampling system. The individual component of exhaust gas is measured by the following method:

- O2 - Horiba Model MPA-21 Paramagnetic Oxygen Analyzer
- CO - Horiba NDIR Analyzer Model AIA-23
- HC - Horiba Model FIA-22-2 Total Hydrocarbon Analyzer(Heated Oven Flame-Ionization Detector)
- CO2 - Horiba NDIR Analyzer Model AIA-23
- NO, NO2 - Horiba Chemiluminescence Analyzer (with NO2 to NO converter) Model CLA-53M

In Figure 6 is presented the air distribution and the concept of three fuel-stage preliminary test combustor for evaluating flame interaction effect on NOx emission level.

Combustion air $G_{e1}$ and diffusion combustion fuel $G_{r1}$ are fed to the first stage upstream region and in this region pilot flame is generated by diffusion combustion for stabilization. Amount of combustion air and premixed combustion fuel, represented by $G_{e2}$, $G_{r2}$ and $G_{e3}$, respectively, are fed to the second and third
stages, where premixed combustion takes place after being completely and uniformly premixed, and finally flowed into the combustor in turn.

Specifications of these combustors (A, B, C) are presented in Table 1. Combustor A is a multi-can type diffusion combustor with a swirler to serve as the flame stabilizer. The swirler comprises of 12 rectangular air ducts having swirl angle of 30° and 12 fuel nozzle ports. The specifications of the swirler and fuel nozzle are presented in Figure 7. In Figure 8 is shown the configuration of Combustor B. This is a 2 fuel-stage premixed combustor with a swirler same as that used in the diffusion combustion section of combustor A. In this combustor, fuel and air are mixed in eight premixing ducts which are mounted around the combustion liner, and this mixed fluid is injected into the combustor for premixed combustion. Combustor C has nearly the same configuration as that of B, having a diameter half to that of Combustor B. In Table 2 are presented the test conditions. Natural gas is used as the fuel in both the cases.

<table>
<thead>
<tr>
<th>Table 1. Specifications of combustor A, B, C.</th>
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<tbody>
<tr>
<td>A combustor</td>
</tr>
<tr>
<td>Diameter : 360 mm</td>
</tr>
<tr>
<td>Length : 900 mm</td>
</tr>
<tr>
<td>Fuel : NG (Diffusion)</td>
</tr>
<tr>
<td>B combustor</td>
</tr>
<tr>
<td>Diameter : 360 mm</td>
</tr>
<tr>
<td>Length : 930 mm</td>
</tr>
<tr>
<td>Fuel : NG (Diffusion &amp; Premixed)</td>
</tr>
<tr>
<td>C combustor</td>
</tr>
<tr>
<td>Diameter : 180 mm</td>
</tr>
<tr>
<td>Length : 530 mm</td>
</tr>
<tr>
<td>Fuel : NG (Diffusion &amp; Premixed)</td>
</tr>
</tbody>
</table>

**Figure 5. Gas sampling system.**

**Figure 6. Dimensions and air splits of 3 fuel staged combustor for preliminary testing.**

**Figure 7. Fuel nozzle and swirler.**

**Figure 8. Combustor B. (Low NOx combustor liner)**
Table 2. Test conditions.

<table>
<thead>
<tr>
<th>Fuel: NG</th>
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<tbody>
<tr>
<td>Inlet Air Pressure: ~ 1.27 MPa</td>
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<tr>
<td>Inlet Air Flow: ~ 26 kg/s</td>
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<tr>
<td>Inlet Air Temp.: ~ 350 °C</td>
</tr>
<tr>
<td>Exit Gas Temp.: ~ 1200 °C</td>
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Comparisons of the Test Results with the Predictions

In Figure 9 is plotted the measured and predicted variation of NOx emission level with combustor exit temperature in the case of three-stage combustor test. This test is performed by keeping air flow rate, air temperature, and air pressure constant, and varying fuel flow rate only. The symbol * and the line indicated by AA represent the measured and calculated NOx concentration, respectively, at the combustor outlet for the case of increasing the fuel fed to the second stage (premixed fuel), while keeping the first stage diffusion fuel flow rate constant. The symbol I and the line indicated by BB represent the measured and calculated NOx concentration, respectively, for the case of increasing the fuel fed to the third stage (premixed fuel), while keeping the first (diffusion fuel) and the second stage (premixed fuel) fuel flow rate constant. In the calculations are used the equivalence ratio of diffusion combustion \(\phi_d\) as 1.0, because in case of diffusion flame, most of NOx is formed in the stoichiometric region. And diffusion combustion ratio \(\beta\) is chosen as 0.125 which is the same as \(\beta\) of combustor A. \(\beta\) of combustor A was already evaluated by comparing with measured NOx emissions and predicted NOx. \(\beta\) of 3 staged combustor, combustor A, B, and C are approximately same value, because the hardware of these combustors like as swirler etc. is same or similar configuration. Residence time in reactor 1 (WSR-1) as 5 ms, that in reactor 2 (WSR-2) and 3 (WSR-3) as 10 ms were calculated from one dimensional conditions. And the power index \(x\) as 0.5 is often assumed in diffusion flames, like as Touchton et al. (1976). In this study, \(x\) as 0.5 used in calculations, because NOx emissions from DLNC which has diffusion flame and premix flames (premix equivalence ratio < 0.6) mainly depend on diffusion flame. In Figure 9, results of calculation for both the cases indicated by AA and BB showed a good agreement with the measured values.

Next the results regarding the application of this model to three combustors (A, B, C) are presented.

In Figure 10 is plotted the variation of measured and predicted relative NOx concentration with the combustor outlet gas temperature for test combustor A. Line represents the predicted value, whereas open circle represents the test results. In the calculations are
assumed the diffusion combustion equivalence ratio $\phi_d$ as 1.0, residence times in reactor 1 and 2 as 5 ms and 10 ms, respectively, and the power index $x$ in the NOx pressure relation as 0.5. The varying parameter i.e. diffusion combustion ratio $\beta$ is defined as the ratio of the fuel burnt at equivalence ratio $\phi_d = 1.0$ to the fuel entered to reactor 1. Test combustor A is only for diffusion combustion. It can be seen from this figure that for this type of combustor with swirler, a good agreement between measured and predicted values could be achieved if $\beta$ is assumed to be 0.125.

In Figure 11 is plotted the variation of measured and predicted relative NOx concentration with the combustor exit gas temperature for test combustor B. In both the experiment and calculation, the premixed fuel ratio of combustor is used as the varying parameter. In the case of predicting NOx emission in test combustor B, $\beta$ is chosen as 0.125 which is same as that used in the case of combustor A, since the swirler used in the combustor B has the same configuration as that used in combustor A. Also, in this calculations are assumed the diffusion combustion equivalence ratio $\phi_d$ as 1.0, residence time in reactor 1 and reactor 2 as 5 and 10 ms, respectively, and the power index in the NOx pressure relation as 0.5. Although there occurred some discrepancies between experiment and prediction in the case of premixing fuel ration of 0% (diffusion fuel ratio of 100%), a relatively good agreement between experiment and prediction could be observed, including the 100% gas turbine load region, which has a high combustion temperature.

In Figure 12, are plotted the results for test combustor C. In this case the size is 1/2 to that of other test combustors, whereas the configurations is nearly the same as others, and the residence times in the combustion zone are designed to have almost the same value. For these test conditions also, calculations are carried out using the same values of model parameters as that used in combustor A and B. Although there occurred some discrepancies between predicted and measured values of NOx for 100% diffusion combustion, as was observed in the case of combustor B too, a very good agreement between measured and predicted values could be observed in the region where the combustion gas temperature is high.

**Summary**

In present work, has been proposed a simple semi-experimental NOx prediction model for Dry Low NOx Combustor which used diffusion flame and multiple lean premixed flames.

Based on this model NOx prediction showed a good agreement with the experimental data under full pressure combustion conditions for test combustor. In the calculations the equivalence ratio of premixed flames are known, while the diffusion combustion ratio $\beta$ was chosen from the experimental data. The value of $\beta$, in particular, is considered to differ depending on the change in geometry and operating conditions of combustor. Therefore, depending on the combustor type, $\beta$ has some typical value.

In order to apply this model to a wider range of combustor operating conditions, it is thought that a similar type of simplified model can be formed by combining other mechanism of NOx.
References

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