THE CAPABILITY OF DIFFERENT SEMIANALYTICAL EQUATIONS FOR ESTIMATION OF NOx EMISSIONS OF GAS TURBINES

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ABSTRACT

The NOx emissions of gas turbines are depending on different influences. On the one side there are the effects fixed by the gas turbine design and on the other side the ambient effects, the fuel properties and the operational conditions.

Because the NOx emissions are difficult to calculate by chemical reactions and flow calculations, some investigators developed semianalytical equations, which in their opinion contained the most important influencing factors together with some tuning factors for the actual gas turbine design and application.

This paper shows the capability of those procedures, including a new one. It compares the calculated NOx emission with measured data. The comparisons were made for one gas turbine fired with different fuels (natural gas, propane, butane, coke oven gas), as well as for different combustor inlet conditions in case of simple and regenerative cycle operation. Reference is made also for some other gas turbine models. Also full and part load operation as well as the steam injection effects are included.

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>A</td>
<td>Air flow</td>
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<tr>
<td>AFR</td>
<td>Air/fuel ratio</td>
</tr>
<tr>
<td>cp</td>
<td>Specific heat capacity of a component</td>
</tr>
<tr>
<td>EINOx</td>
<td>Emission index for NOx, mass NOx/mass fuel ratio (according to Tuchton [11])</td>
</tr>
<tr>
<td>F</td>
<td>Fuel flow</td>
</tr>
<tr>
<td>FAR</td>
<td>Fuel/air ratio</td>
</tr>
<tr>
<td>LHV</td>
<td>Lower heating value</td>
</tr>
<tr>
<td>NOx</td>
<td>NOx emission in mg / Nm³, dry</td>
</tr>
<tr>
<td>m</td>
<td>Mass flow of a component</td>
</tr>
<tr>
<td>p</td>
<td>Combustion air pressure</td>
</tr>
<tr>
<td>R</td>
<td>Gas constant</td>
</tr>
<tr>
<td>S</td>
<td>Steam injected</td>
</tr>
<tr>
<td>sNOx</td>
<td>Specific NOx emission index, mass NOx/mass fuel ratio</td>
</tr>
<tr>
<td>T</td>
<td>Temperature of a component</td>
</tr>
<tr>
<td>t_r</td>
<td>Residence time</td>
</tr>
<tr>
<td>V</td>
<td>Volume flow of a component</td>
</tr>
<tr>
<td>X</td>
<td>Absolute humidity</td>
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<tr>
<td>φ</td>
<td>Equivalence ratio (AFR stoichiometric/AFR actual)</td>
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</table>

Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tr>
<td>Cl</td>
<td>Combustor inlet</td>
</tr>
<tr>
<td>eff</td>
<td>Effective</td>
</tr>
<tr>
<td>fl</td>
<td>Full load</td>
</tr>
<tr>
<td>Fl,ad.</td>
<td>Adiabatic flame temperature</td>
</tr>
<tr>
<td>Fir</td>
<td>Firing Temperature</td>
</tr>
<tr>
<td>HUM</td>
<td>Humidity</td>
</tr>
<tr>
<td>ISO</td>
<td>Values at ISO conditions</td>
</tr>
<tr>
<td>M</td>
<td>Steam</td>
</tr>
<tr>
<td>pl</td>
<td>Part load</td>
</tr>
<tr>
<td>R</td>
<td>Reactor (flame zone of the combustor)</td>
</tr>
<tr>
<td>air</td>
<td>Primary zone air flow</td>
</tr>
<tr>
<td>steam</td>
<td>Steam mass flow primary zone</td>
</tr>
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INTRODUCTION

The NOx emissions of a gas turbine are in general...
depend mainly on the flame temperature and the residence time of the combustion products in the high temperature zone. The flame temperature is determined by the combustion air conditions at the combustor inlet, the air/fuel ratio, type of the fuel and the NOx reduction measures, like steam or water injection. For the given combustor geometry of a gas turbine the residence time is fixed by the flame temperature and the temperature at the first stage nozzle of the gas turbine, the firing temperature as well as the combustion air flow.

Because the calculations of the NOx emissions are very difficult to perform and their results are uncertain, many investigators have developed different semianalytical equations in the past, which of course are different because of the wide range of gas turbine applications they investigated. The constants for these equations were determined using measured data for a specific case, therefore they are applicable only to the similar cases.

For heavy duty gas turbines some of the existing correlations were examined and sets of constants or tuning factors for the parameters which influence the NOx emission were varied. It can be seen that nearly all of the proposed correlations include only some parameters which should be incorporated. These are mainly the ambient conditions, the combustor inlet conditions (temperature and pressure), the composition of the burned fuel, the gas turbine load and the reduction methods, like steam or water injection, or lean premixed combustion respectively.

One investigated correlation is that proposed by G.L. Touchton [1]

\[ \text{EINOX} = A \cdot \frac{\text{t}}{R_\text{H}} \cdot e^{-C (\text{R}_\text{H} - \text{T}_\text{C})^2} \cdot \text{R}_\text{H} \cdot R_\text{STIM} \]  

(1)

which takes into account the residence time, combustion air pressure and temperature, air humidity and the equivalence ratio, which is defined as the ratio of the air to fuel ratios for stoichiometric and the actual combustion.

The system is not easy to handle because the constants A, C and D have to be determined by experiments. The equation (1) fits very well as long as CH₄ or natural gas is burned, but does not fit if other fuels are burned or NOx emissions for different gas turbines have to be calculated. The system can be used also for the calculation of NOx emissions in case of steam or water injection for NOx reduction. The applicability of the system for the prediction of NOx emissions was demonstrated in [5]. Figure 1, which is taken from [5], shows a typical result.

Becker et al. [2] published the correlation

\[ \text{NOx}_{\text{gen}} = 5.73 \times 10^{-4} + e^{0.0083 \text{R}_\text{G}^2 \cdot p_\text{G}} \]  

(2)

with combustion air pressure and flame temperature as parameters. The fitting is made with two coefficients, which therefore must include the effect of the residence time and the temperature level in the combustor. If one compares the NOx emissions of combustors of the similar design at base load the correlation could be well used. For part load operation the residence time may differ to much, and hence other coefficients have to be used.

There is another correlation suggested by Perkavec in [3]

\[ \text{NOx} = 8.28 \cdot p_\text{G}^{1.4} \cdot \text{FAR}^{1.4} \cdot m^{2.2} \cdot e^{200} \cdot e^{-65 \cdot (X, X_2)} \]  

(3)

which considers the combustion air pressure and temperature, the absolute humidity of the combustion air including injected water or steam as well as the air and fuel flows as the influencing parameters.

Finally, there is also a correlation published by Odgers and Kretchmer [4]

\[ \text{NOx}_{\text{ODG}} = 29 \cdot e^{-(21.67 \cdot \text{T}_\text{C}} - 250 \cdot \text{R}_\text{H}^{0.9} \cdot [1 - e^{-250 \cdot R_\text{H}}] \]  

(4)

with combustor pressure, flame temperature and residence time as influencing parameters.

Restrictions mentioned with respect to equ. (2) are valid also for constants used in equ. (3) and (4). In general, it can be stated that the correlations are giving good results for gas turbines for which the correlations were developed and sets of constants defined, and as long as changes of the operating conditions are in small scope.

It can be clearly seen, that for all above mentioned correlations the set of the coefficients used in the particular correlation is crucial. That means, that for calculating NOx emissions of different gas turbines under different operating conditions and for different fuels all given correlations and sets of constants have to be redefined using additional measurements on the gas turbine in scope and under similar conditions.

Therefore a new semianalytical equation for calculating the NOx emissions was developed, which takes into account all mentioned influencing factors and contains
a minimum of constants accompanying them. The need for redetermining these constants should be minimized.

DESCRIPTION OF THE CORRELATION

The idea of the correlation is, that the NOx emission in general depends mainly on flame temperature. It is well known, that because of different flame temperatures for different fuels the NOx emission of a gas turbine burning pure carbon monoxide or pure hydrogen is much higher than for natural gas, whereas a low btu gas with a high content of inert gas may cause lower NOx emission.

The flame temperature for the evaluation of the resulting NOx emission can be calculated for the adiabatic, nonequilibrium combustion without dissociation using a heat balance consideration for the combustor. The eqn. (5) is valid for gas operation and steam injection only. In the case of water injection the heat for vaporization has also to be considered. The thermodynamic data needed for the calculation is from [8], [9] and [10].

\[
T_{\text{Flame}} = \frac{\dot{m}_{\text{Air}} \cdot C_{P_{\text{Air}}} \cdot T_{\text{Air}} + \dot{m}_{\text{Fuel}} \cdot (C_{P_{\text{Fuel}}} \cdot T_{\text{Fuel}} + LHV) + \dot{m}_{\text{Steam}} \cdot C_{P_{\text{Steam}}} \cdot T_{\text{Steam}}}{\dot{m}_{\text{Air}} \cdot C_{P_{\text{Air}}} - \dot{m}_{\text{Air}} \cdot C_{P_{\text{Air}}}}
\]

(5)

The real flame temperature is lower, of course, but the calculated one by the heat balance for the combustion chamber is for the developed NOx correlation sufficiently exact. The obtained dependence of the NOx emission from the flame temperature is given in figure 2. The curve can be approximated by an exponential function. This leads to the following expression

\[
\text{NOx} = \text{sNOx} \cdot e^{\frac{T_{\text{Flame}} - 2208}{247.7} + \frac{\dot{m}_{\text{Air}}}{\dot{V}_{\text{Air}}}}
\]

(6)

in which both numeric values within the exponential function can be regarded as constant. First, the specific NOx emission index sNOx must be determined for a reference adiabatic flame temperature of 2208. degree C corresponding to that of a particular gas turbine burning natural gas. The adiabatic flame temperature must be then calculated for the actual conditions using equ. (5). Then applying equ. (6) the actual sNOx can be evaluated. However, all investigated heavy duty gas turbines have nearly the same sNOx because of similar combustor design according to the same design philosophy. In order to get the NOx emission in mg/Nm3, dry the last term of equ. (6) has to be added. In this case, the total dry exhaust flow has to be taken.

If NOx emissions of gas turbines with different pressure ratios are compared or if different loads for a gas turbine are in scope, the dependence of pressures of the flame temperature must be considered. There is similar information for this function in [6] and [7]. The change of flame temperature with changing pressure of combustion air can be approximated by an exponent of 0.6 (see figure 3). Therefore the deviation of flame temperature is:

\[
f_{\text{Flame}} = \left(1 + \frac{P_{\text{Air}}}{100.}\right)^{0.6}
\]

(7)

It must be remarked, that the approximation for the influence of the combustion air pressure (see figure 3) with the exponent 0.6 is sufficiently exact only in the range of pressures between 5 and 12 bar.

After some conversions and inserting equ.(7) into equ. (6) the following equation can be obtained

\[
\text{NOx} = \text{sNOx} \cdot e^{\frac{T_{\text{Flame}} - 2208}{247.7} + \frac{\dot{m}_{\text{Air}}}{\dot{V}_{\text{Air}}}}
\]

(8)

The above equation can safely be used if no significant changes of residence time will happen and the temperature level in the combustor stays nearly the same. That means for part load operation, where the combustion air temperature changes as well as the firing temperature is lower and also the velocity through the combustor changes because of reduced air flow through the compressor, the equation must be supplemented.

In the literature, [1] and [6], nearly the same calculation for the residence time at ISO conditions and base load, it will lead to the following relation

\[
f_{\text{residence}} = \frac{\rho_{\text{Air}} \cdot V_{R}}{\dot{m}_{\text{Air}} \cdot R \cdot T_{R}}
\]

(9)

If one relates the residence time to a reference value at ISO conditions and base load, it will lead to the following relation

\[
\frac{f_{\text{residence}}}{f_{\text{residence,ISO}}} = \frac{m_{\text{Rig}} \cdot P_{\text{Rig}} \cdot T_{\text{Rig}}}{\dot{m}_{\text{Air}} \cdot P_{\text{Air}} \cdot T_{\text{Air}}}
\]

(10)

Also the temperature level in the combustor changes from full to part load operation. That means, that on the one side the flame temperature or the temperature in the primary zone stays nearly the same, but the firing temperature on the other side is lower. The distance from the end of the primary zone to the first stage nozzle, where such a high temperature for NOx generation occurs, becomes smaller. The influence of changing temperature level in the combustor can be explained by
the geometrical relationship as follows

\[ f_{\text{zr}} = \frac{L_1}{L_2} \left( \frac{T_{\text{fl,ad}} - T_{\text{fl,d}}} {T_{\text{fl,ad}} - T_{\text{fl,d}}} \right) \]

(11)

Also, it can be found that in the case of steam injection the decrease of the adiabatic flame temperature calculated with the heat balance is not sufficient. This means, that the specific NOx emission index \( s_{\text{NOx}} \) or the adiabatic flame temperature has to be additionally corrected. In this case the specific NOx emission index is corrected in dependence of steam/fuel ratio to

\[ s_{\text{NOx}}^* = s_{\text{NOx}} \times (1 - 0.3571 \times \frac{S}{F}) \]

(12)

Adding these effects on the residence time and specific NOx emission index and including them in equation (8) will bring the final semianalytical equation for the NOx emission in mg/Nm³, dry

\[ \frac{m_{\text{NOx}}}{V_{\text{in,d}}} = \frac{m_{\text{NOx}}}{V_{\text{in,d}}} \times \frac{f_{\text{zr}}}{f_{\text{zr}}^*} \times \frac{T_{\text{fl,d}}}{T_{\text{fl,d}}} \]

(13)

It should be mentioned that the only coefficients in this correlation are those used for the calculation of the effects of the flame temperature and which are nearly constant for all investigated cases. The only real variable is the value of \( s_{\text{NOx}} \) which is a characteristic value for every combustor design. It can be shown that even this variable becomes constant for a family of gas turbines designed following a similar design philosophy. The influence of steam injection on \( s_{\text{NOx}} \) given by equation (12) can also be regarded as constant for all investigated cases.

### COMPARISON OF DIFFERENT CORRELATIONS WITH MEASURED DATA

The above mentioned and discussed correlations were used for the prediction of emissions of some General Electric gas turbines (see table 1) burning different gaseous fuels (see table 2) and operating under different conditions. Also steam injection for NOx reduction was considered. The predicted emissions were compared with corresponding measured data.

It can be found, that the above discussed correlations (equ. (2) to (4)) with coefficients as published, are not predicting the NOx emissions well for every measured case. In order to get better results the optimization of the sets of coefficients for each correlation was performed using the measured data for the particular gas turbine. The variation of the resulting sets of coefficients is shown in table 3. With these sets of coefficients, it is possible to predict the NOx emissions quite well.

Significant deviations of the predicted emissions from the measured data happen if a gas turbine is burning an alternative fuel gas, like propane or butane. Therefore, the optimization of the set of coefficients was performed also for different fuel gases. The multiple figures 4 to 10 give the impression how the above mentioned correlations can fit the measured NOx emissions.

Finally the proposed new system was applied and figures 11 to 19 show the comparison of the predicted data compared with the measured data. In general most of the needed thermodynamic data for the calculation using equ.(13), like the combustion air temperature and pressure, the air and fuel flows etc., were measured. However some of them were not available from measurements, so a cycle calculation was performed for the actual conditions and the missing data were taken from these calculations.

For every measured case (different gas turbine and different fuel) the specific NOx emission index \( s_{\text{NOx}} \) for full load operation was determined. It can be shown, that this value is nearly constant (see table 3 for PG65-41 for different fuels). The difference in \( s_{\text{NOx}} \) for the measured G3142 emissions is mainly based on measuring uncertainties, so an average value was used for all predictions (see table 3).

That is the reason for the deviations of the calculated to measured NOx emissions for example at the full load point without steam injection (see figures 11 to 14). It is possible to bring the calculated value to coincide with the measured value by using the slightly different actual \( s_{\text{NOx}} \). The difference in \( s_{\text{NOx}} \) between the G3142's and the PG5361 is based on combustion chamber design according to different design parameters, like the fuel to air ratio. The combustion chamber with the so called P
Table 2: Composition of different gaseous fuels in mol%.

<table>
<thead>
<tr>
<th></th>
<th>G3142</th>
<th>G3142 / PG6541</th>
<th>G3142R</th>
<th>PG5361</th>
<th>PG6541</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Natural Gas</td>
<td>Propane</td>
<td>Butane</td>
<td>Coke Oven Gas</td>
<td>Natural Gas</td>
</tr>
<tr>
<td>CH4</td>
<td>96.03</td>
<td>-----</td>
<td>-----</td>
<td>22.22</td>
<td>86.82</td>
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<tr>
<td>C2H6</td>
<td>0.7</td>
<td>1.11</td>
<td>0.15</td>
<td>2.38</td>
<td>0.56</td>
</tr>
<tr>
<td>C3H8</td>
<td>0.22</td>
<td>89.85</td>
<td>6.71</td>
<td>0.17</td>
<td>0.03</td>
</tr>
<tr>
<td>C4H10</td>
<td>0.078</td>
<td>8.95</td>
<td>92.2</td>
<td>0.08</td>
<td>0.01</td>
</tr>
<tr>
<td>C5H12</td>
<td>0.018</td>
<td>0.09</td>
<td>0.94</td>
<td>0.02</td>
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<tr>
<td>C6+</td>
<td>0.014</td>
<td>-----</td>
<td>-----</td>
<td>0.09</td>
<td>-----</td>
</tr>
<tr>
<td>CO2</td>
<td>0.11</td>
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<td>-----</td>
<td>1.58</td>
<td>4.29</td>
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<tr>
<td>H2</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>57.16</td>
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<tr>
<td>O2</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>1.0</td>
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<tr>
<td>N2</td>
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<td>-----</td>
<td>9.0</td>
<td>8.29</td>
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<tr>
<td>CO</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>6.22</td>
<td>-----</td>
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</tbody>
</table>

Table 3: Summary of the sets of coefficients used in discussed correlations.
liner operating in the PG5361 burners with a little excess of air. This can be considered in the calculation method by a greater air/fuel ratio and therefore lowering the adiabatic flame temperature or, as shown, with the lower value for sNOx.

The resulting NOx emissions illustrated in fig. 11 to 14 are for the same gas turbine burning different fuels, that means the variation of the NOx emission depending mainly on the different adiabatic flame temperature implied by different fuel gases.

Figure 15 shows the influence of the combustor inlet temperature for the G3142 gas turbine operating in regenerative cycle in contrast to the simple cycle (see figure 11). The higher combustion air temperature has an influence on the adiabatic flame temperature and therefore on the NOx emission.

It can be seen that even in case of different gas turbines (G3142, PG5361 and PG6541) the prediction was good (see figure 11, 16 and 17).

The testing was performed also for cases with steam injection and the results are also acceptable. This is presented in all figures 4 to 19 with the curves for steam flow as parameter.

The calculated emissions do not form a smooth line for some applications (see figure 15) because, as already mentioned, the correlation 13 demands some thermodynamic data for the actual gas turbine, like compressor discharge pressure and fuel gas flow, which, in general, are not known in every case: if the correspondent measured data are used and the accuracy was not high, a curve like that on figure 15 will be obtained. If the measured data are accurate or the cycle calculation is necessary, the predicted emissions form a smooth line (see figure 16).

In the discussed cases the measured NOx emissions are for nearly stoichiometric combustion. The proposed new prediction method can also be used for lean premixed combustion by varying the air mass flow of the primary zone in the heat balance which is used for calculating the adiabatic flame temperature.

CONCLUSION

From the shown diagrams it can be seen that nearly all discussed correlations can be used for prediction of NOx emissions in cases, which are similar to those in scope during the determination of the sets of coefficients used in them. The proposed new correlation for the prediction of NOx emissions of heavy duty gas turbines however is well suited also for other gas turbines and different operational conditions as long as the differences considered are not too big. The new system is therefore able to cover a broader range of applications.

For applications on gas turbines with different design the coefficients for the chosen correlation must be redetermined. In this case too the proposed correlation is very useful too, because there are altogether only three slightly varying coefficients to be redetermined only in exceptional cases despite the fact that all discussed influencing factors are taken into account.

Acknowledgment

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References

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Figure 1: NOx emissions over the gas turbine load with steam injection as parameter

Figure 2: Influence of flame temperature on NOx emissions

Figure 3: Influence of combustion air pressure on flame temperature

Figure 4a: Measured and calculated NOx emissions of G 3142 J burning natural gas; calculation performed with equ. 2.
Figure 4b: Measured and calculated NOx emissions of G3142 J burning natural gas; calculation performed with equ.3.

Figure 4c: Measured and calculated NOx emissions of G3142 J burning natural gas; calculation performed with equ.4.

Figure 5: Measured and calculated NOx emissions of G3142 J burning propane; calculation performed with equ.2 (fig.5a), equ.3 (fig.5b) and equ.4 (fig.5c)
Figure 6: Measured and calculated NOx emissions of G 3142 J burning butane; calculation performed with equ.2 (fig.6a), equ.3 (fig.6b) and equ.4 (fig.6c)

Figure 7: Measured and calculated NOx emissions of G 3142 J burning coke oven gas; calculation performed with equ.2 (fig.7a), equ.3 (fig.7b) and equ.4 (fig.7c)
Figure 8: Measured and calculated NOx emissions of G 3142R J burning natural gas in regenerative cycle; calculation performed with eq.2, eq.3 and eq.4

Figure 9a: Measured and calculated NOx emissions of PG 5371 burning natural gas; calculation performed with eq.2

Figure 9b: Measured and calculated NOx emissions of PG 5371 burning natural gas; calculation performed with eq.3

Figure 9c: Measured and calculated NOx emissions of PG 5371 burning natural gas; calculation performed with eq.4
Figure 10: Measured and calculated NOx emissions of PG 6541 B burning natural gas; calculation performed with equ.2 (fig.10a), equ.3 (fig.10b) and equ.4 (fig.10c).

Figure 11: Measured and calculated NOx emissions of G 3142 J burning natural gas.

Figure 12: Measured and calculated NOx emissions of G 3142 J burning propane.

Figure 13: Measured and calculated NOx emissions of G 3142 J burning butane.
Figure 14: Measured and calculated NOx emissions of G3142 J burning coke oven gas.

Figure 15: Measured and calculated NOx emissions of G3142R J burning natural gas in regenerative cycle.

Figure 16: Measured and calculated NOx emissions of PG5371 burning natural gas.

Figure 17: Measured and calculated NOx emissions of PG6541 B burning natural gas.

Figure 18: Measured and calculated NOx emissions of PG6541 B burning propane.

Figure 19: Measured and calculated NOx emissions of PG6541 B burning butane.