SMOKE NUMBER PREDICTION IN GAS TURBINE EXHAUST

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ABSTRACT

From a large number of experimental data, an equation was developed for prediction of the smoke number as measured in gas turbine exhaust according to the well established SAE standard. Two different scales of combustors were used with inlet temperatures and pressures ranging from 300 to 600 K and from 0,1 to 0,9 MPa respectively. The formulation is based on the residence time which is calculated from the mass flow rate, density and volume of the primary and secondary zones of the combustor. The reaction rate has an Arrhenius form with the global equivalence ratio to account for the air and fuel flow rates. All these parameters can be evaluated from desired operating conditions. Nineteen different types of fuel were used varying from a paraffinic mixture to a pure aromatic compound. The fuel is characterized by its calorific value and hydrogen mass fraction.

With the wide range of fuels burned in the experiment giving a smoke number variation from 0 to 100, the accuracy of the equation (Standard Deviation of 40%) is acceptable for most purposes. The formulation should be particularly useful in assessing the efficiency of new systems for smoke reduction or in calculating the smoke number from older experimental data where it was not measured.

NOMENCLATURE

- A: pre-exponential constant
- B: pre-exponential constant (function of hydrogen fuel mass fraction)
- $E_1$: activation energy for soot formation
- $E_2$: activation energy for soot oxidation
- e: exponential function
- F: pre-exponential constant (function of hydrogen fuel mass fraction)
- G: pre-exponential constant (function of hydrogen fuel mass fraction)
- h: hydrogen fuel mass fraction
- P: combustor inlet pressure - MPa
- $P_a$: atmospheric pressure - MPa
- R: universal constant for perfect gas
- SN: Smoke Number
- $T_{pz}$: primary zone temperature - K
- $T_{sz}$: secondary zone temperature - K
- Y: soot concentration - mg / L
- $\alpha$: empirical exponent for pressure
- $\beta$: empirical exponent for pressure
- $\delta$: empirical exponent for pressure
- $\gamma$: empirical exponent for pressure
- $\lambda$: empirical exponent for equivalence ratio
- $\kappa$: empirical exponent for equivalence ratio
- $\Phi$: equivalence ratio
- $\tau$: time - s
- $\tau_{pz}$: residence in primary zone - s
- $\tau_{sz}$: residence in secondary zone - s

Subscripts

- pz: primary zone
- sz: secondary zone
- 1: soot formation process
- 2: soot oxidation process

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INTRODUCTION

Soot prediction is always a concern for aircraft gas turbine users for its high visibility in the exhaust plume and the pollution side effects of these particles in suspension in the atmosphere. Also higher concentrations of soot inside the different zones of the combustor will significantly impact on the durability of the liner. Even if visibility is not a problem for tactical reasons, infrared detectors would trigger more readily to even low amounts of soot particles in the hot exhaust gases. For the combustion engineer to predict the amount of soot inside the chamber or leaving the exhaust of a new or modified engine is not an easy task. From the well established SAE standard [1], a reasonable estimate of soot present in the exhaust can be measured in terms of the Smoke Number. This number represents the amount of soot collected on a white paper filter of a given size placed in exhaust gases. By shining a light on this paper, left collecting soot for a specific period of time, the reflected light intensity can be compared to a clean paper. The result of this comparison graduated from 0 to 100 is the Smoke Number (SN). So this is a value regularly and easily measured while doing experimental tests. Repeatability will be a problem if you do not follow the standard very closely. Even if the measuring technique is not perfect, at the moment nothing better exists for soot measurements and large amounts of experimental data have been cumulated over the years because it is an easily measurable and meaningful value.

The factors controlling the soot formation and subsequent oxidation are numerous and not all well understood. But a general concensus does exist from experimental tests that the most critical factors are fuel properties, fuel/air ratio, combustor pressure, inlet pressure and temperature.

After a review of the literature to survey available correlations to predict Smoke Number in the exhaust of a gas turbine combustor, it was realized that many efforts had been spent on modeling the soot formation/destruction process, giving some insight on soot concentration profiles inside the combustor [2, 3, 4, 5, 6]. The need readily appeared to extend this work to actually predict a Smoke Number, which is a more meaningful value to the practicing engineer to quickly assess the soot content of the exhaust for conditions other than those tested. Therefore from a large bank of experimental data with some 19 different types of fuel and with consistent SN measurements, a semi-empirical correlation was produced with success. The experimental values were obtained from two different scales of a conventional can type combustor. The appellations 1/3 and 1/2 represent the geometrical scale relative to a so-called full scale combustor (286 mm diam) yet to be tested (Figure 1). One important consideration kept in mind was to use as much as possible easy to get parameters. So the correlation is based on some analytical concepts, but due to the great complexity of the process, some empirical constants had to be incorporated to close the gap. The developed equation gives results with a standard deviation of 40%. The inlet temperatures and pressures vary respectively from 315 to 600 K and from 0.2 to 0.9 MPa with two scales of combustors.

Figure 1 Schematic of the experimental combustor

CORRELATION DEVELOPMENT

A series of two well-stirred reactors is the conceptual idea of soot formation and oxidation simultaneously occurring in both the primary and secondary zones. Modeling of the process would flow sequentially from the first reactor, where soot formation occurs, to the second reactor where soot is burned (oxidation). The net result of this operation for the two reactors in the primary zone of the combustor would be an excess of soot produced over what is burned. From the well known fact that fuel rich burning will produce soot, it is then very plausible that the primary zone will be a net producer of soot. This net produced quantity flows down to the secondary zone where two more reactors contribute to soot formation/oxidation again. With the usual quenching in the dilution zone, it is assumed that the soot leaving the secondary zone is the same coming out of the dilution zone or exhaust. Figure 2 is a schematic representation of the concept.

MATHEMATICAL MODELING

A simple mathematical formulation is possible to represent the soot formation and oxidation in each reactor. This takes the form of a first order differential equation also used by Najjar [2]:

\[ Y' = a - b \times Y \]  

(1)
Y is the soot concentration (mg/L) resulting from combustion and Y’ will be the first time derivative. The a and b parameters are Arrhenius type exponential reaction rate functions for each reactor in each zone and dependant on pressure and temperature:

\[
a_{pz} = A_{pz} \times P^a \times e^{-E_{1,pz} / (R \times T_{1,pz})} \\
b_{pz} = B_{pz} \times P^b \times e^{-E_{2,pz} / (R \times T_{2,pz})}
\] (2a)

\[
a_{sz} = A_{sz} \times P^a \times e^{-E_{1,sz} / (R \times T_{1,sz})} \\
b_{sz} = B_{sz} \times P^b \times e^{-E_{2,sz} / (R \times T_{2,sz})}
\] (2b)

The parameter a characterizes the soot formation process and the parameter b is for the oxidation process. In the physical interpretation of the differential equation, it is assumed that formation is independent of soot concentration (Y), giving that formation depends only on the time derivative (Y’ = a). But since oxidation is possible only after some soot has been formed, the rate of oxidation is proportional to Y, giving that Y’ = -bY, with the final result that Y’ = a - bY.

The Parameters A, B, a, b and y are constants, E is a constant activation energy for each type of reactor and T is the equilibrium temperature calculated from an enthalpy balance by providing inlet temperature, inlet pressure, fuel calorific value, fuel hydrogen mass fraction, an equivalence ratio of unity in the primary zone and the local equivalence ratio for the secondary zone. The subscript (1) refers to the formation process and (2) is for oxidation, and the other subscripts are for primary (pz) and secondary (sz) zones. The solution of this first order non-homogeneous differential equation will be obtained from integration and will have the following form:

\[Y(T) = \frac{a_{pz}}{b_{pz}} \times (1 - e^{-b_{pz}T_{pz}}) + c \times e^{-b_{sz}T_{sz}}
\] (3)

where the constant of integration c can be evaluated by stating that no soot is formed (Y = 0) at a time of zero (T = 0). The other limit of integration is the zonal residence time to yield the soot concentration leaving the zone. Then c will be:

\[c_{pz} = -\frac{a_{pz}}{b_{pz}}
\] (4)

The equation to relate the soot formation/oxidation with the soot leaving the primary zone, according to the model, can be established:

\[Y_{pz} = \frac{a_{pz}}{b_{pz}} \left(1 - e^{-b_{pz}T_{pz}}\right)
\] (5)

From the initial equation (1), it can be stated that the amount of soot coming into the reactor of the secondary zone is the amount produced in the primary zone, Y_{pz}. Hence for a time of zero at the entrance of the second zone where there is no new soot, the constant of integration c_{sz} can also be evaluated from the expression of the secondary zone:

\[Y_{sz} = Y_{pz} + D Y_{sz} = \frac{a_{sz}}{b_{sz}} + c_{sz} \times e^{-b_{sz}T_{sz}}
\] (6)

\[c_{sz} = Y_{pz} - \frac{a_{sz}}{b_{sz}}
\] (7)

With proper substitution of c_{sz} in equation (6):

\[Y_{az} = \frac{a_{sz}}{b_{sz}} + \left(\frac{Y_{pz} - a_{sz}}{b_{sz}}\right) \times e^{-b_{sz}T_{sz}}
\] (8)

By replacing Y_{sz} from equation (5) into (8), the final expression for Y_{sz} will be:

\[Y_{az} = \frac{a_{pz}}{b_{pz}} \left(1 - e^{-b_{pz}T_{pz}}\right) + a_{sz} \times \left(1 - e^{-b_{sz}T_{sz}}\right)
\] (9)

The first portion of the equation is the amount of soot coming into the secondary zones and subject to oxidation and the second member of the equation is the result of formation/oxidation in the secondary zone alone. Therefore with this equation, the quantity of soot in the primary zone and also in the secondary zone are known as well as the final concentration leaving the combustor. Now before the final expression can be formulated, some simplifications are possible. The temperature of formation and oxidation can be assumed the same in the primary zone and also the secondary zone:

\[T_{1,pz} = T_{2,pz} = T_{pz}
\]
\[T_{1,sz} = T_{2,sz} = T_{sz}
\] (10)

The activation energy will be assumed the same for each formation or oxidation process in each reactor:

\[E_{1,pz} = E_{1,sz} = E_1
\]
\[E_{2,pz} = E_{2,sz} = E_2
\] (11)

The expression for soot concentration at the exit of the secondary zone becomes:
The constants and exponents have been simplified after some initial attempts:

\[ A_{pz} / B_{pz} = G \]
\[ A_{sz} / B_{sz} = F \]
\[ B_{pz} = B_{sz} = 1 \]

\( F \) and \( G \) are new constants and \( \tau_{pz}, \tau_{sz} \) are residence times in the primary and secondary zones, calculated from the combustor volume and air flow rate in each zone.

Knowing the influence of the fuel concentration, but with a strong desire to keep the formulation simple, the global equivalence ratio was introduced in the relationship with pressure normalized to atmospheric pressure. After some further attempts in the development of the correlation, significant improvements were achieved by including the zonal temperature in the final correlation:

\[
Y_{sz} = \frac{A_{pz}}{B_{pz}} \times \frac{p^{\alpha}}{p^{\beta} \times e^{\frac{(E_2-E_1)/R T_{pz}}{p^{\beta} \times \tau_{pz} \times e^{-E_2 R T_{pz}}}}} \times \left[ 1 - e^{-\left( -B_{pz} \frac{p^{\beta} \times \tau_{pz} \times e^{-E_2 R T_{pz}}}{p^{\beta} \times \tau_{pz} \times e^{-E_2 R T_{pz}}} \right)} \right] 
\]

\( E_2 \) and \( E_1 \) are activation energies, and \( R \) is the gas constant.

The following relationships were developed for the constants \( F, G \) and \( B \):

\[
F = -77.07 \times 10^{18} + 9.4362 \times 10^{21} \times h - 27.686 \times 10^{21} \times h^2
\]

\[
G = \left( 0.84819 + 0.9852 \times \frac{h}{h^2} \right)
\]

\[
B = \left( 24.149 - 126.34 \times h + 125.92 \times h^2 \right)
\]

They are best-fit functions with respective accuracy of 99%, 96% and 97%. The parameter \( h \) is the hydrogen mass fraction of the fuel. The best fit values for \( E_1/R, E_2/R, \beta, \gamma, \lambda \) and \( \kappa \) have been respectively set at 14 000, 6 500, 0.5, 1.0, -2.5 and -3.6. Some initial guidance for the activation energy was used from [2] where values for kerosene were 12 100 and 7 800. Similarly for the equivalence ratio, where Khan [4] suggests an exponent value of -3. The literature did not reveal any exponent for the pressure term since all reported correlations used the partial pressure of the reactants rather than inlet pressure. However since partial pressure is function of inlet pressure and equivalence ratio, its effect is reflected in the exponent of these two variables, as given in the proposed model.

**VALIDATION**

To evaluate the results of the correlation against experimental values, an expression developed by Odgers & Magnan [7] was slightly modified to relate better the SN with soot concentration as:

\[
Y_{sz} = \frac{0.177 \times SN}{(100 - SN)^{0.472}}
\]

Then using equation (18) with equation (14) will give a predicted Smoke Number which can be compared to measured values. Figure 3 shows a comparison of these predicted and measured results for the 1/2 scale combustor at atmospheric pressure. Figure 4 also compares a predicted SN against a measured SN but for the 1/3 scale for a pressure range of 0.1 to 0.9 MPa. The standard deviation is 40% with some 300 data points from 19 different types of fuel. A good portion of the experimental data result from low soot producing fuels. Considering the inherent errors with the SN measurement technique and the number of data points, the correlation has a reasonable standard deviation. The predicted values for both geometries showed the same accuracy and demonstrated that the scale and pressure effects were correlated well in equation (14). The inherent errors with the SN measurement technique are displayed more evidently on Figure 3 with an underprediction of the SN between 10 and 60. As explained at reference [7], two significant errors are due to non homogeneous paper and improper alignment of the sampling paper for reflectivity measurements. These relative errors are even more significant for low SN values.
SUMMARY AND CONCLUSIONS

The initial intent of using as many of the inlet parameters as possible to correlate with the Smoke Number was successful, giving a reasonable standard deviation of 40%. The inlet conditions considered were equivalence ratio, type of fuel, inlet pressure and geometry scale through residence time. The inlet temperature did not have an influence on the predicted results, which shows its effect is well accounted for in the calculated equilibrium temperatures \( T_{pe}, T_{sz} \) of each zone.

Since a first attempt at using a single reactor was unsuccessful, the analytical approach using two reactors in series, with soot formation and destruction simultaneously taking place in both, demonstrated a way to consider most of the significant parameters. It is obvious that the Arrhenius type equation used cannot explain all the phenomena occurring in the combustor. It is very doubtful if a more complex model could do much better, but, nonetheless, further refinements to this mathematical formulation are still underway. Also with a continuation of the experimental program, more tests will further extend the range of the correlation, especially for fuels at higher Smoke Numbers.

The application of this semi-empirical correlation was not validated against other combustors because of the difficulty to evaluate zonal residence times from the available data. Otherwise there is no reason against its applicability to other combustors except for the constants; it is unlikely that they would apply because of the high sensitivity of an exponential formulation to even minor modifications.

As stated above, due to the extreme sensitivity of smoke emissions to even minor changes in the combustor, it seems very unlikely that there will ever be a model which can be transported from one combustor to another. This will hold true even for complex analytical models since even these are restricted in spatial resolution. The use of a descriptive correlation is mainly for the prediction of conditions other than those tested. Although it might be noted that the correlation works for two combustors of different sizes.

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REFERENCES

1. Aircraft Gas Turbine Smoke Measurement, SAE ARP 1179A.


