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Prediction of Soot Emissions in Gas-Turbine Combustors

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From a large number of experimental data, a formulation was developed for predicting the smoke number (SN) as measured in gas-turbine exhausts according to the well-established Society of Automotive Engineers standard. Three different scales of the same combustor were used with inlet temperature and pressure ranging from 300 to 600 K and from 0.1 to 0.9 MPa, respectively. The formulation is based on the residence time that is calculated from the mass flow rate, density, and the volumes of the primary and secondary zones of the combustor. The reaction rate has an Arrhenius form with the equivalence ratio to take into consideration the air and fuel flow rates. All of the required 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 the hydrogen mass fraction. With this wide range of fuels burned in the experiments, giving a SN variation from 0 to 100, the accuracy of the prediction (standard deviation of 40% on the relative error to experimental values for each scale and 60% when all scales are combined) is acceptable for most purposes. Measured SN values already have a 20% error because of the commonly accepted variability of the technique. The formulation should be particularly useful in assessing the efficiency of new systems for smoke reduction or in calculating the SN from older experimental data where it was not measured.

Nomenclature

A = pre-exponential constant
B = pre-exponential constant
C = soot concentration, mg/L
E_d = activation energy for soot destruction (oxidation)
E_f = activation energy for soot formation
e = exponential function
h = fuel hydrogen mass fraction
K = pre-exponential constant
p = combustor inlet pressure, Pa
p_a = atmospheric pressure, Pa
R = universal constant for perfect gas
T_d = destruction or secondary zone temperature, K
T_f = formation or primary zone temperature, K
α = empirical exponent for pressure
β = empirical exponent for pressure
τ = time, s
τ_{pz} = residence in primary zone, s
τ_{sz} = residence in secondary zone, s
ϕ = equivalence ratio

Subscripts
d = soot oxidation (destruction) process
f = soot formation process
pz = primary zone
sz = secondary zone

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 have a significant 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 Society of Automotive Engineers (SAE) standard,[1] a reasonable estimate of soot present in the exhaust can be measured in terms of the smoke number (SN). This number represents the amount of soot collected on a white paper filter of a given size and contained in a known volume of exhaust gases circulated through the filter. By shining a light on this stained paper, the reflected light intensity can be compared to a clean paper. The result of this comparison graduated from 0 to 100 is the SN. This is a value regularly and easily measured while doing experimental tests. Even if the measuring technique is not perfect, it is widely used in the aeroengine industry[2] for soot measurements and large amounts of experimental data have been cumulated over the years.

The factors controlling soot formation and subsequent oxidation are numerous and not all well understood. But a general consensus does exist from experimental tests that the most critical factors are fuel properties, equivalence ratio, liner pressure drop for suitable mixing, inlet pressure, and temperature.

A literature survey revealed a number of predicting functions, but they all require some peculiar parameters usually not available from standard experimental data.[3–7] The need readily appeared to extend this work to actually predict a SN, which is a more meaningful value to the practicing engineer to quickly assess the soot content of the exhaust. Therefore, from a large bank of experimental data with some 19 different types of fuel and with consistent SN measurements, a semiempirical correlation was produced with success. The experimental values were obtained from three different scales of a conventional can-type combustor. The appellations one-third and one-half represent the geometrical scale relative to the so-called full-

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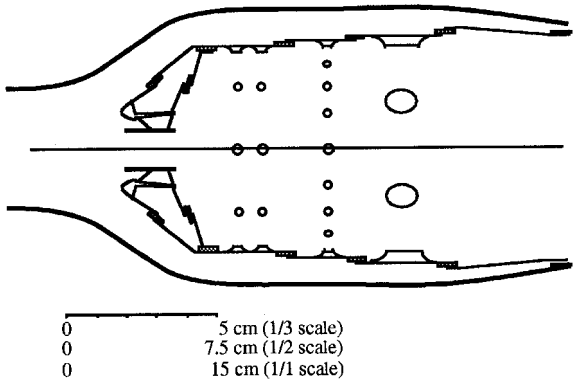

Fig. 1 Schematic of the experimental combustor.

scale combustor (286 mm diam) (Fig. 1). This paper deals with a new correlation to account for new results acquired recently with the full-scale combustor. It includes a volume effect to account for the reactor residence time. One important consideration was to formulate a correlation with usual engine performance parameters. The correlation is based on some analytical concepts, but because of 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% for each scale and 60% when the three scales are combined. To come up with these percentages, the normalized error was calculated first by taking the difference between the measured and the predicted values, then this difference was divided by the measured value and the standard deviation was calculated from these normalized errors. The inlet temperatures and pressures vary, respectively, from 315 to 600 K and from 0.2 to 0.9 MPa with three geometrical scales of the same combustor. For the variation in equivalence ratio, the global value was changed from 0.10 to 0.38 for all scales, giving a variation in local equivalence ratio in the primary zone from 0.29 to 1.38.

Correlation Development

The concept was formulated from a well-stirred reactor including the primary zone and the secondary zone. 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 the soot is oxidized. With the usual quenching in the dilution zone, it is assumed that the soot concentration leaving the secondary zone remains the same through the dilution zone to the exhaust plane where SN measurements are usually taken.

Mathematical Modeling

A simple mathematical formulation is possible to represent the soot formation and oxidation in a given reactor. This takes the form of a first-order differential equation also used by Najjar[3]:

$$C' + bC = a \tag{1}$$

C results from combustion and C' will be the first time derivative. The a and b parameters are Arrhenius-type exponential reaction rate functions for the formation and oxidation processes and dependent on pressure and temperature:

$$a = AP^{\alpha}e^{(-E_f/RT_f)} \tag{2}$$

$$b = BP^{\beta}e^{(-E_d/RT_d)} \tag{3}$$

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 C, giving that formation depends only on the time derivative $C' = a$, or simply put, the rate of formation. But since oxidation is possible only after some soot has been formed, the rate of oxidation is proportional to C, giving that $C' = -bC$, with the final result that $C' = a - bC$. A, B, a, and b are constants, E is the activation energy for formation/destruction, 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 solution of this first-order nonhomogeneous differential equation will be obtained from integration and will have the following form:

$$C(\tau) = (a/b) + ce^{-b\tau} \tag{4}$$

where the constant of integration c can be evaluated by stating that no soot is formed ($C = 0$) at a time of zero ($t = 0$). Then c will be

$$c = -(a/b) \tag{5}$$

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

$$C(\tau) = (a/b)(1 - e^{-b\tau}) \tag{6}$$

The amount of soot leaving the secondary zone will not be burned subsequently by assuming frozen state in the dilution zone, and that is what is measured in the exhaust plane of the combustor.

The residence times τ_{pz} and τ_{sz} are calculated from the combustor volume and the airflow rate in each zone. Therefore, what is formed and later oxidized in the reactor, leaves the secondary zone with a concentration that is dependent on the total time spent in the reactor, which is represented by the sum of residence time in the primary and secondary zones:

$$C_{sz} \xrightarrow{at} \tau = \tau_{pz} + \tau_{sz}$$

then

$$C_{sz} = (a/b)\{1 - \exp[-b(\tau_{pz} + \tau_{sz})]\} \tag{7}$$

The final equation used to correlate the experimental data becomes:

$$C_{sz} = \frac{A}{B}\left(\frac{P}{P}\right)^{\alpha-\beta} e^{\left(\frac{E_d}{RT_d} - \frac{E_f}{RT_f}\right)} \times \{1 - \exp[-B(\tau_{pz} + \tau_{sz})]P^{\beta}e^{-E_d/RT_d}\} \tag{8}$$

Although the pressure terms canceled each other, the term left in the exponential did not seem to account for all of the effect, therefore, an expression normalized to atmospheric pressure, was kept at the pre-exponential level. The constants have been simplified such that

$$K = A/B$$

Using a least-square solution technique for an overdetermined set of equations, the constants were calculated as follows:

$$C_{sz} = 12.22863V^{-0.188154}Ma^{0.6}\frac{(1 + 3.4h)^{-12.7}}{(1 - \phi)^{1.5}}\left(\frac{P}{P_a}\right)^{-0.75} \times e\left(\frac{11{,}000}{T_d} - \frac{11{,}000}{T_f}\right)\left\{1 - \exp[-10^5(\tau_{pz} + \tau_{sz})] \times \left(\frac{P}{P_a}\right)^{0.5} e^{-11{,}000/T_d}\right\} \quad (9)$$

Knowing the influence of the fuel concentration, but with a strong desire to keep the formulation simple, the global equivalence ratio and the incipient soot formation equivalence ratio, $(1 + 3.4h)$, were introduced in the relationship. The formulation $(1 + 3.4h)$ is valid only for a premixed flame, and in our case we deal strictly with data from diffusion flames. This was used as a starting point and it seemed to work well enough in the correlation development to keep it. Also, the Mach number M and the volume of the reactor V, to include the primary and secondary zones, seemed to allow a better fit of all the data.

Validation

To evaluate the prediction of the correlation against experimental values, an expression developed by Odgers and Magnan[8] was slightly modified to better relate SN with soot concentration as

$$C_{sz} = \frac{0.177\text{SN}}{(100 - \text{SN})^{0.472}} \quad (10)$$

Then using Eq. (10) with Eq. (9) will give a predicted SN that can be compared to measured values. Figures 2 and 3 show a comparison of these predicted and measured results for the full- and the half-scale combustors tested at atmospheric pressure. Figure 4 also compares a predicted SN against a measured SN, but for the one-third scale over a pressure range of 0.1–0.9 MPa. The standard deviation is 40% for each combustor with some 430 data points from 19 different types of fuel. For the one-third scale, a good portion of the experimental data results from low soot producing fuels. Considering the inherent errors with the SN measurement technique of some ±10% and the number of data points, the correlation has

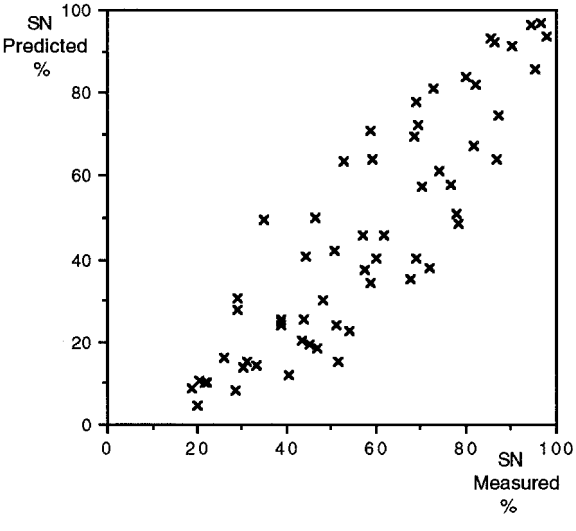

Fig. 2 Experimental SN values against predicted SN values, full-scale combustor, five types of fuels, 60 data points, and atmospheric pressure.

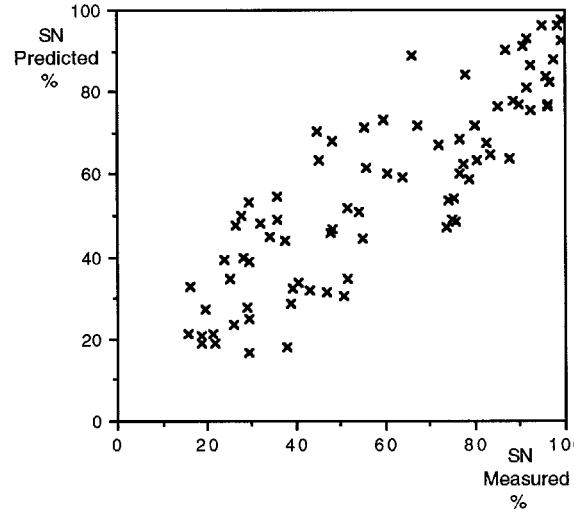

Fig. 3 Experimental SN values against predicted SN values, half-scale combustor, five types of fuels, 80 data points, and atmospheric pressure.

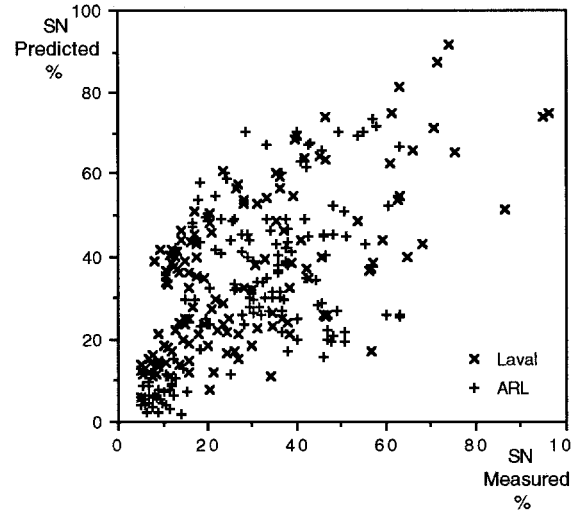

Fig. 4 Experimental SN values against predicted SN values, one-third-scale combustor, 19 types of fuels, 290 data points, and pressure from atmospheric to 0.9 MPa.

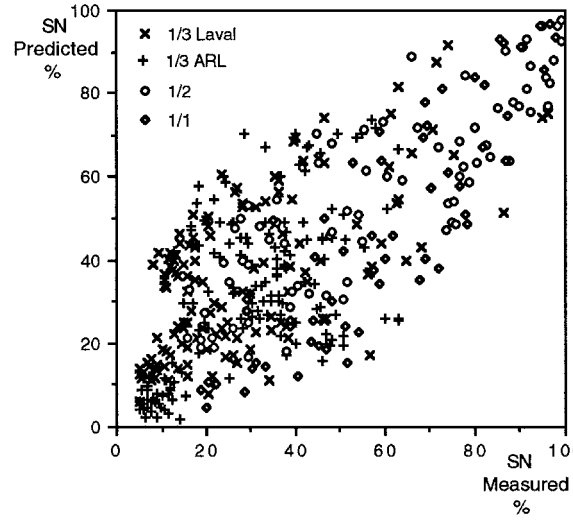

Fig. 5 Experimental SN values against predicted SN values, three scales of the same combustor, 19 types of fuels, 428 data points, and pressure from atmospheric to 0.9 MPa.

an acceptable standard deviation. The predicted values for all geometries, except for the one-third-scale Laval data set, showed the same accuracy and demonstrated that the scale and pressure effects were correlated well in Eq. (9). A correlation with the one-third and one-half scale data was discussed in a previous paper,[9] but when the results for the three scales were put together (Fig. 5), the correlation could not account adequately for the volume effect. In this new expression, the volume change would translate into a longer residence time for a larger geometry. Although the residence time is explicitly calculated and used as a parameter in the last exponential of Eq. (9), it could not totally account for the variation. The added term $V^{-0.188}$ will produce a reduction in soot with the added residence time to allow a more complete burnout. The Mach number also has some influence on the residence time, but it is believed to be partially in terms of rate of mixing, where a higher M would produce more intense mixing in some situations. Again, its inclusion in the final expression demonstrates its strong influence on the residence time where a rising M would notably reduce the residence time to cause an increased soot level in the exhaust as shown in Fig. 6. The strongest influence comes from h; as we depart significantly from paraffin-type fuels, this parameter will decrease in value as we go towards heavier fuels. These aromatic fuels are much more difficult to burn completely, therefore, with a decreased h value more soot is collected in the exhaust. This phenomena is well demonstrated in Fig. 7 for the full scale where sufficient data points were completed. Figure 8 shows more explicitly the change of predicted and measured SN against the hydrogen mass fraction. The SN values are overpredicted, but nevertheless, the correlation is able to consider the fuel type effect reasonably well. Figure 9 also includes the predicted values against ϕ to show an interesting phenomena with a change from a lean to a rich primary zone. The increase in the equivalence ratio will normally contribute to higher combustion temperatures and with the consequence that the larger amount of soot produced in the primary zone will be oxidized in the hotter secondary zone. For fuels with h values of 7.74 and 10.5%, Figures 7 and 9 reveal the opposite, the measured SN values increase with equivalence ratio. This occurs when the primary zone becomes too rich, that is when the local ϕ is much greater than 1 or the global ϕ exceeds a value of about 0.28. The correlation will satisfactorily predict a rich condition in the primary zone as long as it does not exceed an equivalence ratio of 1.15, beyond this value the accuracy will deteriorate appreciably. For pressure P, no consensus exists, and so it seems to account for the unknown chemistry that is difficult to otherwise adequately quantify. Finally, E for formation and oxidation seems to be in line with what is published in the literature. Reference 3 reports a value of $-13{,}000$ to $-21{,}000$ K for the formation activation energy and -160 to $-39{,}000$

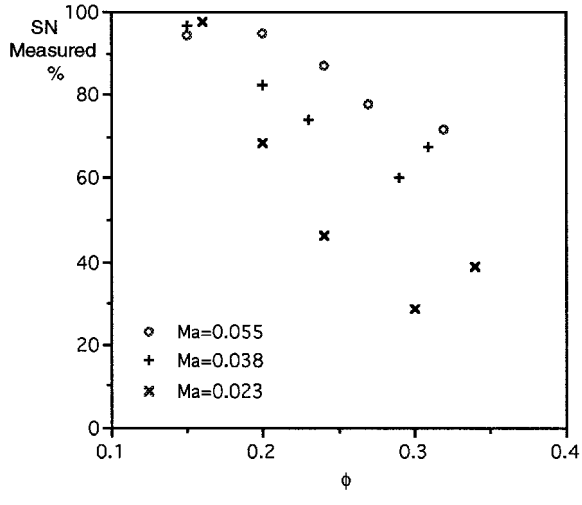

Fig. 6 Equivalence ratio against measured SN values, full-scale combustor, fuel 23, benzene at three different Mach numbers.

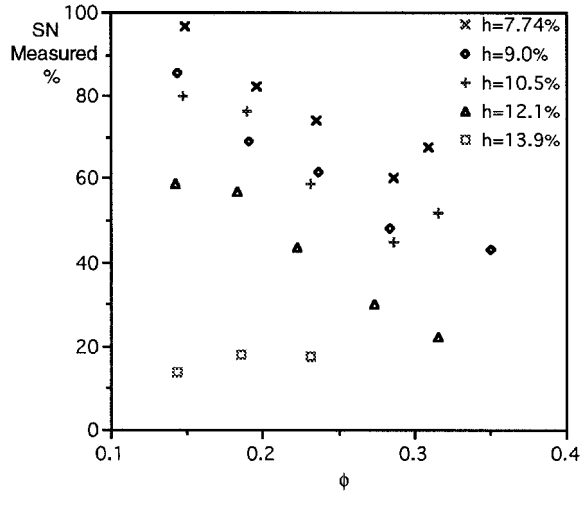

Fig. 7 Equivalence ratio against measured SN values, full-scale combustor, five different types of fuels for the same Mach number.

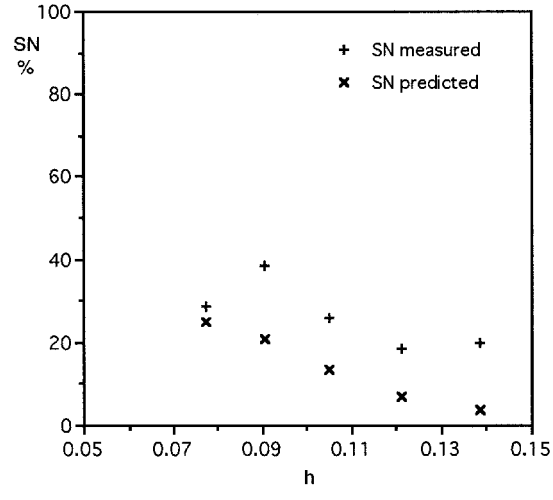

Fig. 8 Fuel hydrogen mass fraction against predicted and measured SN values for five different types of fuels, full-scale combustor with the same inlet atmospheric conditions, and a Mach number of 0.024.

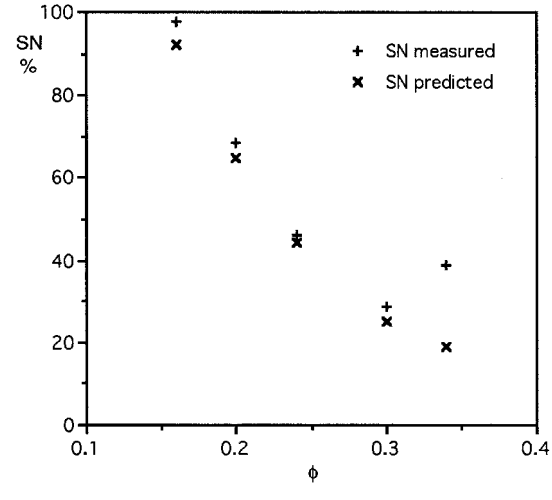

Fig. 9 Equivalence ratio against predicted and measured SN values, full-scale combustor with same inlet atmospheric conditions, a Mach number of 0.024, and fuel 23 (benzene).

K for soot oxidation, a value of −11,000 K does not appear too badly out of range.

The following text discusses the accuracy of SN measurements used to explain the scatter in the prediction in Fig. 4. Table 1 reports the possible errors with the SN technique on a mass basis of eventual soot collected on a white paper filter with a filtration capacity of 1.3 μm used in our laboratory, as opposed to a Whatman No. 4 at 25 μm recommended in the SAE standard.[1] To improve on these possible errors with a subsequent better repeatability in the measurements, the following steps were taken in our laboratory at Laval University:

1) Use a much smaller filter retention capability, as stated earlier (1.3 μm instead of 25 μm).

2) Ensure a constant alignment of the filter in the holder for reflectance readings before and after soot collection.

3) Collect the sample gas with a very short unbent line.

4) Vary the sampling rate with correction to a standard SN value.

Since the errors in Table 1 are reported on a mass basis, they have to be translated to an error in SN value to compare the accuracy of SN measurements between the three different data sets used in this article to make up the correlation. Using Eq. (10), it was possible to calculate the error in SN value by assuming the mass of soot collected was altered, from a standard mass of sample gas through the filter, to account for possible errors up to ±30%. Figure 10 shows the translation of the mass error in SN values. With a maximum mass error of 30%, the SN value will be affected from 0% for a measured SN of 0 or 100 to a maximum of ±12.5 in SN variation for a measured SN value of 50. The experimental SN results from the full- and the half-scale combustors on Figs. 2 and 3 do include these extra steps to ensure accurate measurements of −15 to +10% on a mass basis, corresponding to a ±7 in SN variation. But for the one-third scale results with inadequate corrective measures such as steps 2 and 3, the scatter on the data set is much greater, proving much more difficult to correlate properly as shown in Fig. 4, and therefore, corresponding more to the large errors related in column 1 of Table 1. The maximum error in Fig. 4 is about +30 in SN values for measured values in the range 10–30, which would correspond to a mass error of about −60%. This is beyond the errors stated in Table 1 to indicate another possible source of error with a required corrective measure as in step 4.

Table 1 List of possible errors on a mass basis with SN measurements as reported

	Related errors (mass basis), %	
Problems	Refs. 2, 4, and 9	Laval
Batch variation/reading/ alignment errors	±10	±5
Line mass losses	±25	±5
Filtration losses	−20	−5
Total errors	−45 to +35	−15 to +10

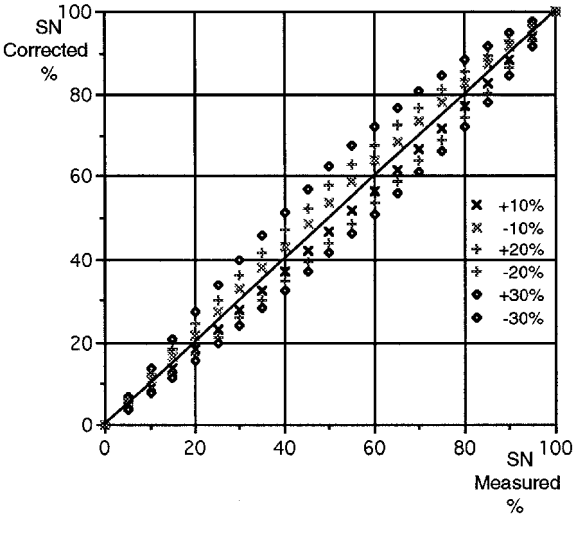

Fig. 10 Measured SN values against corrected SN values for errors in soot collection on the paper filter as reported in Table 1.

Steps 2 and 3 were the subject of a previous paper[9] and no further comments will be added, but step 4 needs to be elaborated to clarify the procedure involved. A good portion of the low SN values for the one-third scale were not usable because of the inaccuracy of reflectivity measurements at low soot collection rate on the white paper filter. As stated,[9] a technique was developed to vary the quantity of sample gas through the filter by changing either the sampling rate or the collection time so that the mass of soot on the paper would be increased to improve the sensitivity of the technique. The principle applies as follows, for fuels or operating conditions reducing the propensity to soot emissions, the mass of collected soot was increased significantly by increasing the sample rate or the collection time, and for very sooty situations where the filter gets stained very quickly, the rate or sampling time was reduced to increase the sensitivity of the reflectivity reading. The SAE standard allows for variation of the exhaust gas sample mass, but in many circumstances the 12–21 kg/m^2 range had to be exceeded. Once the reflectivity readings are converted to an SN value with the formula (SN = 1 − R_s/R_w), a correction has to be applied to provide a standardized SN value at a filter loading of 16.2 kg of exhaust gas per m^2 of filter area as required. The technique required in the SAE standard to plot SN values against mass loading on a logarithmic abscissa to get a straight line for suitable interpolation of the standard 16.2 kg/m^2 will not produce a straight line if you are outside the 12–21 kg/m^2 that is required to improve sensitivity and avoid too many repetitive measurements. A correlation was developed to correct a measured SN value to a standardized value. The correlation had a deficiency in the fact that SN values above 100 could be calculated. The experimental data were better correlated to give Eq. (10), which is a mass of soot contained in a known volume of exhaust gas (C: concentration). If the mass of exhaust gas is changed, the concentration of soot in the exhaust sample should remain constant giving the following identity:

$$C = \frac{m_{\text{soot}/1}}{V_{\text{gas}/1}} = \frac{m_{\text{soot}/2}}{V_{\text{gas}/2}} \tag{11}$$

Equation (10) was expressed in terms of concentration, but in fact, a mass of soot was collected on the filter and then an associated SN value was calculated from reflectivity measurements. Once this is all completed, since the volume of gas sample is known, a concentration can be calculated by dividing m_{soot} by V_{gas}. In other words, Eq. (9) can be truly written as

$$m_{\text{soot}/1} = \frac{KK\ \text{SN}_1}{(100 - \text{SN}_1)^{0.472}} \quad \text{or} \quad m_{\text{soot}/2} = \frac{KK\ \text{SN}_2}{(100 - \text{SN}_2)^{0.472}} \tag{12}$$

If the expressions in Eq. (12) are substituted in Eq. (11), we get

$$\frac{[KK\ \text{SN}_1/(100 - \text{SN}_1)^{0.472}]}{V_{\text{gas}/1}} = \frac{[KK\ \text{SN}_2/(100 - \text{SN}_2)^{0.472}]}{V_{\text{gas}/2}} \tag{13}$$

The density of an exhaust gas sample for a given fuel at a particular operating condition will be fairly constant, then Eq. (13) can be related to different sampled masses of exhaust gas the following way:

$$\left[\frac{\text{SN}_1}{(100 - \text{SN}_1)^{0.472}}\right] = \frac{m_{\text{gas}/1}}{m_{\text{gas}/2}}\left[\frac{\text{SN}_2}{(100 - \text{SN}_2)^{0.472}}\right] \tag{14}$$

Condition 2 would relate to any SN measurement that is not at the standard mass loading and condition 1 would correspond to a standard mass loading of 16.2 kg/m^2. All of the data for the full and half scales were corrected according to this formulation. As a matter of fact, these SN values seem to correlate much better and more consistently. The continuation of our data acquisition program will definitely assist to better clarify the global picture, especially redoing measurements for one-third scale to assist in improving the correlation so that it could be more consistent with the physical interpretation of the soot formation/oxidation process.

Summary and Conclusions

The initial intent of using as many of the inlet parameters to correlate with the SN was successful, giving a standard deviation of 40% for each of three scales of a typical combustor. 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_{pz} and T_{sz}) of each zone. Since a first attempt of using multiple reactors was unsuccessful, the analytical approach using one reactor with soot formation and destruction considered globally demonstrated a way to consider most of the significant parameters in a simpler model. It is obvious that an Arrhenius-type formulation used cannot explain all of the phenomena occurring in the combustor. It is extremely difficult with a more complex model to do much better until the influence from each parameter can be more adequately known, 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.

The application of this semi-empirical correlation was not validated against other combustors although this will be attempted in the near future. There is no reason for its applicability to other combustors except for the constants; however, it is unlikely they would apply because of the sensitivity of an exponential formulation. This is what has to be tested with some guidelines to assist the practitioner.

As stated, because of the extreme sensitivity of smoke emissions to even minor changes in the combustor, it seems very unlikely that there will ever be a model that 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 three combustors of different sizes.

Acknowledgments

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