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400 COMMONWEALTH DRIVE, WARRENDALE, PA 15096

**AEROSPACE
INFORMATION
REPORT**
AIR 1533

Issued 4-30-82

Revised

**PROCEDURE FOR THE CALCULATION OF BASIC EMISSION
PARAMETERS FOR AIRCRAFT TURBINE ENGINES**
E R R A T A S H E E T

Page 21: The last term in the numerator of Equation (56) should be:

$$(2 + h) \left(\frac{y}{2x} - \frac{\alpha}{2} \right) \left(\left[\text{HC} \right]_w \right)$$

Page 28: The last term in Equation (A19) should be:

$$\left(\frac{M_C + \alpha M_H}{M_{\text{AIR}}} \right)$$

Page 36: The combustion efficiency should be 97.78% instead of 97.78Δ.

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PROCEDURE FOR THE CALCULATION OF BASIC EMISSION PARAMETERS FOR AIRCRAFT TURBINE ENGINES

PURPOSE: This is a procedure for calculation of basic emission parameters, specifically, fuel-air ratio, emission index and combustion efficiency for aircraft turbine engines based on the measurement of carbon monoxide, carbon dioxide, total hydrocarbons and oxides of nitrogen.

The following effects are included:

1. Humidity and CO₂ content of inlet air
2. Interferences in the measurement of CO and oxides of nitrogen
3. Oxygen pressure broadening effect on CO₂
4. NO_x converter efficiency
5. Measurement of CO, CO₂ and NO_x on a dry, rather than a wet basis

The procedure for measurement of aircraft turbine engine emissions is given in Reference 1.

SECTIONS: The procedure is divided into the following sections:

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The technical portion of this report is divided into three main groups. The first group (Sections 4 through 11) provides the information for calculating the emissions parameters using the matrix method (which normally is accomplished with the aid of a computer). The second group (Section 12) provides the equations for hand calculating the results in the event that a computer is not available. The third group (Appendix A) contains the derivation of the equations given in the two previous groups. For this reason a certain amount of duplication will be found among the three groups.

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1. DEFINITION OF TERMS:

- 1.1 Aircraft Gas Turbine Engine: Any gas turbine engine used for aircraft propulsion or power generation, including those commonly called turbojet, turbofan, turboprop or turboshaft type engines, and afterburning engines in the nonafterburning mode of operation.
- 1.2 Combustion Efficiency: The percentage ratio of the energy actually released by the combustion process to the energy which would be realized if all the carbon in the fuel were oxidized to CO₂ and the hydrogen to water vapor.
- 1.3 Concentration: The volume fraction of the component of interest in the gas mixture -- expressed as volume percentage or as parts per million.
- 1.4 Emission Index: The mass of emissions of a given constituent per unit mass of fuel, multiplied by 1000.
- 1.5 Fuel-Air Ratio: The mass rate of fuel flow to the engine divided by the mass rate of dry air flow through the engine.
- 1.6 Gaseous Emissions: Substances emitted in the form of gas downstream of the combustion chamber and limited to carbon monoxide, carbon dioxide, nitric oxide, nitrogen dioxide and hydrocarbons.
- 1.7 Interference: Instrument response due to presence of components other than the gas (or vapor) that is to be measured.
- 1.8 Mole Fraction: The volume concentration of a gas per unit volume of the gas mixture of which it is a part. In the context of the measurements discussed in this procedure, "volume concentration (or volume fraction)" and "molar concentration (or mole fraction)" are synonymous.
- 1.9 Net Heat of Combustion: The energy released per unit mass of fuel due to its complete oxidation at constant pressure as measured by cooling the products to the initial temperature without condensation of the water vapor formed in the reaction.
- 1.10 NO_x: Oxides of nitrogen, specifically, the sum of nitric oxide (NO) and nitrogen dioxide (NO₂).
- 1.11 Nondispersive Infrared Analyzer (NDIR): An instrument that by absorption of infrared energy selectively measures specific components.
- 1.12 Parts Per Million (ppm): The unit volume concentration of a gas per million unit volumes of the gas mixture of which it is a part. (Also applicable to weight measurements but only volume relationships are referred to in these procedures.)



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1.13 Parts Per Million Carbon (ppmC): The mole fraction of hydrocarbon multiplied by 10^6 measured on a (C_1H_n) equivalence basis. Thus, 1 ppm of methane is indicated as 1 ppmC. To convert ppm concentration of any hydrocarbon to an equivalent ppmC value, multiply ppm concentration by the number of carbon atoms per molecule of the gas. For example, 1 ppm propane translates as 3 ppmC hydrocarbon; 1 ppm hexane as 6 ppmC hydrocarbon.

1.14 Total Hydrocarbons: The total of hydrocarbon compounds of all classes and molecular weights.

2. NOMENCLATURE AND SUGGESTED VALUES:

$[CO]$	= mole fraction concentration of CO in exhaust
$[CO_2]$	= mole fraction concentration of CO_2 in exhaust
$[HC]$	= mole fraction concentration of hydrocarbon in exhaust expressed as (C_1H_n) equivalent = $ppmC/10^6$
$[H_2O]$	= mole fraction concentration of H_2O in exhaust
$[NO]$	= mole fraction concentration of NO in exhaust
$[NO_2]$	= mole fraction concentration of NO_2 in exhaust
$[NO_x]$	= mole fraction concentration of NO_x in exhaust
$[O_2]$	= mole fraction concentration of O_2 in exhaust
$[z]$	= mole fraction concentration of constituent z in exhaust
EI_z	= Emission Index of constituent z, g/kg fuel (lb/1000 lb fuel)
F	= mass rate of fuel usage, kg/h (lb/hr)
F/A	= fuel-air ratio
H_c	= net heat of combustion of fuel
h	= humidity of inlet air, moles of water vapor per mole of dry inlet air
h_{sd}	= humidity of exhaust sample leaving optional CO/CO_2 or NO_x dryer, moles of water vapor per mole of dry sample gas
J	= pressure broadening coefficient for effect of O_2 on CO_2
K	= ratio of wet concentration to completely dry concentration
K_{sd}	= ratio of completely dry concentration to semi-dry concentration (after optional CO/CO_2 or NO_x dryer)
L	= interference coefficient for effect of CO_2 on CO
L'	= interference coefficient for effect of CO_2 on NO/NO_x
M	= interference coefficient for effect of H_2O on CO

2. NOMENCLATURE AND SUGGESTED VALUES (Continued):

M'	= interference coefficient for effect of H_2O on NO/NO_x
m, n	= molecular constants for fuel, $C_m H_n$
M_{AIR}	= molecular weight of dry air = 28.965
M_C	= atomic weight of carbon = 12.011
M_H	= atomic weight of hydrogen = 1.008
M_N	= atomic weight of nitrogen = 14.0067
M_O	= atomic weight of oxygen = 15.9994
M_Z	= molecular weight of constituent z
N'_2	= sum of nitrogen (N_2) and argon (A) in inlet air
P_T	= total moles of exhaust products (Equations 1 and 12)
P_Z	= moles of exhaust constituent z per mole of fuel (Equation 1)
R	= mole fraction of O_2 in dry inlet air = 0.20948
S	= mole fraction of nitrogen plus argon in dry inlet air = 0.79020
T	= mole fraction of carbon dioxide in dry inlet air = 0.00032
W_Z	= mass emission rate of constituent z, kg/h (lb/hr)
x, y	= molecular constants for exhaust hydrocarbons, $C_x H_y$
X	= moles of dry air/mole of fuel
Z	= parameter defined in Equation 59
α	= (atomic) hydrogen-carbon ratio of fuel = n/m
η	= NO_x converter efficiency
η_b	= combustion efficiency, %

Subscripts:

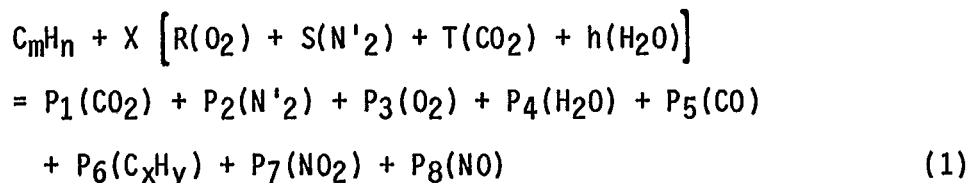
c	= corrected value
d	= completely dry basis
ms	= measured value
sd	= semi-dry basis
w	= wet basis
z	= constituent z
N	= NO_x dryer

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3. INTRODUCTION: The three basic parameters used in turbine engine gaseous emission studies are the emission index (EI), fuel-air ratio (F/A) and combustion efficiency (η_b). Other parameters have been defined but they usually can be easily derived from the above values.

By making certain assumptions, the emission index, fuel-air ratio and combustion efficiency can be calculated from the measurements of carbon monoxide (CO), carbon dioxide (CO₂), total hydrocarbons (HC), and oxides of nitrogen (NO_x) in the exhaust. The procedure involves the solution of a set of simultaneous equations based on the combustion chemical equation. A matrix solution suitable for computer use is described in this report. Algebraic equations are also presented in case a computer is not readily available.

4. COMBUSTION CHEMICAL EQUATION: The chemical equation for the combustion of hydrocarbon fuel and air is:



where P_1 through P_8 are the number of moles of CO₂, N'₂, O₂, H₂O, CO, C_xH_y, NO₂ and NO, respectively.

The following assumptions are made:

- (1) Hydrogen (H₂) is not present in the exhaust
- (2) Free carbon (C) is not present in the exhaust
- (3) Unburnt or partially burnt hydrocarbons can be characterized by C_xH_y
- (4) Any oxides of nitrogen present are in the form of NO or NO₂

In the equation it is assumed that dry air consists of O₂, N'₂ and CO₂, and

$$R + S + T = 1 \quad (2)$$

Suggested values for R, S and T (based on Reference 2) are:

$$\begin{aligned} R &= .20948 \\ S &= .79020 \\ T &= .00032 \end{aligned}$$

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4. COMBUSTION CHEMICAL EQUATION (Continued):

The value for S includes the sum of nitrogen and argon. This may be broken down into .78084 moles of nitrogen plus .00936 moles of argon. During the chemical reaction, the number of moles of argon remains unchanged.

The suggested value for the molecular weight of dry air, M_{AIR} , is 28.965.

Since the composition of the hydrocarbons in the exhaust, (C_xH_y), is not usually known, it should be assumed that $x = m$ and $y = n$ for the final calculations. However, most of the equations which follow are the result of the generalized solution. Whenever the above assumption is made, it is so indicated.

Suggested values for the carbon number of the fuel, m , are as follows:

Jet B and JP-4	9.5
Jet A and JP-8	12.5
JP-5	13.0

It should be assumed that $x = m$. The calculations are very insensitive to the value of x so that the use of an approximate value is justified.

The characteristic hydrogen-carbon ratio of the exhaust hydrocarbon, y/x , also appears in the calculations and does have a significant effect on the results. If it is assumed that $x = m$ and $y = n$, then $(y/x) = (n/m) = \alpha$. The hydrogen-carbon ratio of the fuel, α , should be determined by actual analysis.

The humidity of the inlet air, h , is expressed as moles of water vapor per mole of dry air. It is equal to the specific humidity (mass of water vapor per mass of dry inlet air) multiplied by $(28.965/18.016)$.

5. BASIC MATRIX SOLUTION: A set of ten simultaneous equations may be written based on the combustion equation:

C balance:

$$m + TX = P_1 + P_5 + xP_6 \quad (3)$$

H balance:

$$n + 2hX = 2P_4 + yP_6 \quad (4)$$

O balance:

$$(2R + 2T + h)X = 2P_1 + 2P_3 + P_4 + P_5 + 2P_7 + P_8 \quad (5)$$



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5. BASIC MATRIX SOLUTION (Continued):

N balance:

$$2SX = 2P_2 + P_7 + P_8 \quad (6)$$

$$[CO_2]_w \cdot P_T = P_1 \quad (7)$$

$$[CO]_w \cdot P_T = P_5 \quad (8)$$

$$[HC]_w \cdot P_T = xP_6 \quad (9)$$

$$[NO_x]_w \cdot P_T = P_7 + P_8 \quad (10)$$

$$[NO]_w \cdot P_T = P_8 \quad (11)$$

$$P_T = P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7 + P_8 \quad (12)$$

The recommended method is to solve these equations by computer using one of the standard determinant or matrix methods for the solution of simultaneous linear equations (Reference 3). A typical computer program is given in Appendix C. The solution provides the value for X, the moles of dry air/mole of fuel, and the several P values.

The data are entered in matrix form in the computer routine. Table 1 is the matrix for Equations (3) through (12).

In the above equations (7) through (11), the concentrations are all on the wet basis. In some instances measurements are made on a dry or semi-dry basis. Other effects which may need to be included are instrument interferences, oxygen pressure broadening, and NO_x converter efficiency. These items will now be discussed individually.

6. INTERFERENCES: Carbon dioxide and water vapor in the exhaust produce interference effects on CO measured with a nondispersive infrared gas analyzer, and on NO and NO_x measured with a chemiluminescence analyzer. Other interferences may be present but are considered to be negligible.

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TABLE 1

BASIC MATRIX FOR SOLUTION OF COMBUSTION EQUATIONS (3) THROUGH (12)

P_T	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	X	CONST.
0	1	0	0	0	1	x	0	0	-T	m
0	0	0	0	2	0	y	0	0	-2h	n
0	2	0	2	1	1	0	2	1	$\begin{matrix} -2R \\ -2T - h \end{matrix}$	0
0	0	2	0	0	0	0	1	1	-2S	0
$[CO_2]_w$	-1	0	0	0	0	0	0	0	0	0
$[CO]_w$	0	0	0	0	-1	0	0	0	0	0
$[HC]_w$	0	0	0	0	0	-x	0	0	0	0
$[NO_x]_w$	0	0	0	0	0	0	-1	-1	0	0
$[NO]_w$	0	0	0	0	0	0	0	-1	0	0
-1	1	1	1	1	1	1	1	1	0	0

Note: the elements of the matrix are the coefficients, in the determinant Equations (3) to (12), of the unknown quantities as listed at the top. Thus, top line reads as $P_1 + P_5 + xP_6 - TX = m$ which is (3), bottom line reads as $-P_T + P_1 + P_2 + P_3 + P_4 + P_5 + P_6 + P_7 + P_8 = 0$ which is (12).

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6. INTERFERENCES (Continued):

For CO, the interference has a "zero shift" effect:

$$[CO]_c = [CO]_{ms} + L [CO_2] + M [H_2O] \quad (13)$$

For NO and NO_x, the interference has a "concentration factor" effect:

$$[NO_x]_c = [NO_x]_{ms} \left(1 + L' [CO_2] + M' [H_2O] \right) \quad (14)$$

where L, L', M and M' are interference coefficients to be determined by experiment or from the vendor. Typical values are: $L = -1.3 \times 10^{-4}$; $M = -4.5 \times 10^{-4}$; $L' = 0.14$; $M' = 0.28$.

If the CO sample is dried before analysis, the interference from water vapor usually becomes negligible.

The interference effects may be included in the matrix solution, by recalling that

$$[CO_2] P_T = P_1 \text{ and } [H_2O] P_T = P_4.$$

For CO, equation (8) becomes:

$$[CO]_{ms} P_T + L P_1 + M P_4 - P_5 = 0 \quad (15)$$

For NO_x, equation (10) becomes:

$$[NO_x]_{ms} P_T + L' [NO_x]_{ms} P_1 + M' [NO_x]_{ms} P_4 - P_7 - P_8 = 0 \quad (16)$$

For NO, equation (11) becomes:

$$[NO]_{ms} P_T + L' [NO]_{ms} P_1 + M' [NO]_{ms} P_4 - P_8 = 0 \quad (17)$$

7. OXYGEN PRESSURE BROADENING: Recently it has been found that the oxygen content in the sample gas has an effect on the CO₂ level measured using NDIR instruments. This is referred to as the oxygen pressure broadening effect, resulting from the broadening of the absorption bands as a function of the oxygen concentration even though the oxygen itself does not absorb infrared energy at these wave lengths.

This effect may be compensated for by using the following equation:

$$[CO_2]_c = [CO_2]_{ms} \left(1 + J [O_2] \right) \quad (18)$$

7. OXYGEN PRESSURE BROADENING (Continued):

where J = pressure broadening coefficient.

Since $[O_2]_{P_T = P_3}$, Equation (7) may be written:

$$[CO_2]_{ms} P_T + J [CO_2]_{ms} P_3 = P_1 \quad (19)$$

These equations assume that the CO_2 instrument was calibrated using CO_2 calibration gases having N_2 as the diluent.

The pressure broadening effect is not included in Reference 1, but it is treated here since it may be included later as more information on this subject becomes available.

8. NO_x CONVERTER EFFICIENCY: The NO_x converter, whose function is to convert any NO_2 present in the sample into NO , has an efficiency, η , which is somewhat less than 100%. The procedure for determining this efficiency is specified in Reference 1. Although there are slight performance differences between thermal type and reduction type converters, the two are treated the same in this report.

Two values are obtained from the NO_x analyzer, namely $[NO_x]_{ms}$ when the sample flows through the converter, and $[NO]_{ms}$ when the converter is bypassed. Ignoring interference effects, the measured NO value is correct, but from the definition of converter efficiency,

$$[NO_2]_c = \frac{1}{\eta} [NO_2]_{ms} \quad (20)$$

The corrected value for NO_x is then:

$$[NO_x]_c = \frac{1}{\eta} [NO_2]_{ms} + [NO]_{ms} \quad (21)$$

The measured value of NO_x is used in the matrix solution:

$$\begin{aligned} [NO_x]_{ms} &= [NO_2]_{ms} + [NO]_{ms} \\ &= \eta [NO_2]_c + [NO]_c \end{aligned} \quad (22)$$

Since $[NO_2]_c P_T = P_7$ and $[NO]_c P_T = P_8$,

$$[NO_x]_{ms} P_T = \eta P_7 + P_8 \quad (23)$$

Hence the converter efficiency effect is accommodated simply by multiplying the P_7 term by the coefficient, η .