THE CONTROL OF OXIDES AND NITROGEN EMISSIONS FROM AIRCRAFT GAS TURBINE ENGINES

Volume 3: The Flow Model

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**Abstract**

The objective of this study was to develop criteria for use in the design of aircraft gas turbine combustion chambers to minimize nitrogen oxide emissions. The approach adopted involved the development of a mathematical model of NOX emission from aircraft engine combustors; a parametric analysis, using the model, to determine the sensitivity of NOX emissions to variations of model parameters and engine design variables; evaluation of critical model parameters by means of experimental measurements; and the incorporation of the model into combustor design methods to provide guidelines for minimizing NOX emission while maintaining other performance and emission characteristics. The results of the study and the NOX emission control criteria are described in Volume 1 (FAA-RD-71-111-1). Volume 2 (FAA-RD-71-111-2) describes the nitric oxide formation process and a computer program (NOXRAT) for calculating thermodynamic data. The program is based upon a six-reaction model of NO formation. Volume 3 (FAA-RD-71-111-3) describes combustion and flow processes in gas turbine combustors and a computer program (GASNOX) for calculating gas properties and NO concentrations throughout a combustor. This program is based upon a three-zone, heterogeneous model of gas turbine combustor operation. Program GASNOX is used with input data from Program NOXRAT to calculate NO emission rates.

**Key Words**

- Air Pollution
- Gas Turbine
- Nitrogen Oxides
- Theoretical Model
- Nitric Oxide
- Experimental Measurement
- Aircraft
- Design Criteria

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<table>
<thead>
<tr>
<th>Appendix</th>
<th>Subroutine</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appendix XI</td>
<td>Subroutine RUNKUT</td>
<td>137</td>
</tr>
<tr>
<td>Appendix XII</td>
<td>Subroutine DERIV</td>
<td>141</td>
</tr>
<tr>
<td>Appendix XIV</td>
<td>Subroutine ZMASS</td>
<td>146</td>
</tr>
<tr>
<td>Appendix XV</td>
<td>Subroutine PRINTS</td>
<td>160</td>
</tr>
<tr>
<td>Appendix XVI</td>
<td>Method of Calculation of Air</td>
<td>165</td>
</tr>
<tr>
<td></td>
<td>Distribution Characteristics</td>
<td></td>
</tr>
</tbody>
</table>
LIST OF FIGURES

1. ASSUMED FLOW AND DISTRIBUTION PATTERNS THROUGHOUT COMBUSTOR LINER ............ 45
2. PRIMARY ZONE COMBUSTION EFFICIENCY CORRELATION ........................................ 46
3. SCHEMATIC REPRESENTATION OF INPUT STRUCTURE ............................................ 47
4. MODULAR TREE DIAGRAM ................................................................................. 48
1. INTRODUCTION

Volume I of this report carries a full description of the complete program but omits mathematical details of the model developed to predict the nitric oxide (NOx) emissions from aircraft gas turbine combustors and also the details of two computer programs developed as part of the study for obtaining predictions from the model. It is the purpose of Volumes 2 and 3 of the report to present full descriptions of both the model and the computer programs.

It is convenient to consider the model in two parts, one part being concerned with the NOx formation process and the other with modeling the flow behavior within gas turbine combustors. The convenience arises not only due to the basic difference in the studies of these two parts, but also due to the fact that a separate computer program has been developed for each part. This approach has been adopted in the interests of economy of computation as calculation of the necessary data for the determination of the NOx formation process requires appreciable computer time but the data once collected can, of course, be applied to any combustion calculation with the same reference conditions (in this case, combustor inlet conditions) of pressure and temperature. The computer program developed for this task has the name NOXRAT, and its function is to compute the rate terms of the NOx formation process and all relevant thermodynamic data for a series of fuel-to-air ratios with a common reference state.

Volume 2 of this report is solely concerned with the nitric oxide formation process. It presents a mathematical description of the program NOXRAT and also includes a section which is essentially a user's manual for the program. Volume 3 produces the same details for the flow model developed to describe the flow conditions in a gas turbine combustor. The corresponding computer program is named GASNOX and it is so arranged that the rate terms and all relevant thermodynamic data computed in NOXRAT are punched onto a deck of computer cards which serves as input data to the main program GASNOX.

The objective of this volume of the report, therefore, is to present the theory behind the flow model and details of the computer program developed for its application.
2. THE FLOW MODEL

Calculations based upon the reaction scheme described in Volume 2 clearly show that for significant concentrations of nitric oxide to be formed during the short time it takes the gases to pass through an aircraft gas turbine engine, the temperature must exceed 2000 deg K. Such high temperatures only exist within the combustor, and only for a limited time, so clearly, nitric oxide concentrations in the exhausts of aircraft engines are solely dependent upon the flow behavior and the chemical processes occurring within the combustion chamber and it is these features that must be adequately represented in the model.

The first task, therefore, is to select a method of modeling the flow processes in the gas turbine combustor. Such combustors are conventionally divided into three zones as shown in Figure 1a. The distinction between these zones is discussed qualitatively in Volume 1, Section 3, but in the next section these distinctions are quantified. Firstly, the basic conservation equations are derived for the generalized case of an inhomogeneous, reacting gas mixture of the type that occurs in a gas turbine combustor. These equations are then reduced to conditions applicable to the three combustor zones, the primary, intermediate and dilution zones, which are of interest to this study, and finally, they are used to demonstrate how the nitric oxide levels may be calculated for each zone.

2.1 THE GENERALIZED CONSERVATION EQUATIONS

A control volume will be considered to contain products of constant fuel-to-total mass ratio, $F$, which will be termed the mixture ratio. (The constancy of $F$ is taken as it has particular utility in this study insofar as it minimizes the number of calculations for the equilibrium conditions necessary to determine local nitric oxide reaction rates.) The volume is as shown below:
where, \( S_m \) = mass flow in interval \( SF \) about \( F \)
\( [NO] \) = mass fraction of nitric oxide
\( \varepsilon \) = \( m_{fu}/m \), fractional mass flow of unburned fuel
\( \dot{S}_m' \) = mass flow per unit length of fuel ratio \( F' \), with mass fraction of \( NO = [NO] \)
which enters the volume due to mixing
\( \dot{S}_m'' \) = mass flow per unit length, with mass fraction of \( NO = [NO]'' \)
which leaves the volume due to mixing
\( SA \) = cross sectional area of element
\( \dot{r} \) = rate of formation of \( NO \) per unit volume by chemical reaction

The conservation equations become,

for \( NO \),
\[
\frac{d}{dx} (S_m [NO]) = \varepsilon SA + \dot{S}_m' [NO] - \dot{S}_m'' [NO]''
\]

for mass,
\[
\frac{d}{dx} (S_m) = \dot{S}_m' - \dot{S}_m'' - \frac{d}{dx} (\varepsilon S_m)
\]

for burned fuel,
\[
F \frac{d}{dx} (S_m) = \dot{S}_m' F' - \dot{S}_m'' F'' - \frac{d}{dx} (\varepsilon S_m)
\]

for unburned fuel,
\[
\frac{d}{dx} (\varepsilon S_m) = \dot{r}
\]
- specified

In the limit as \( dx \) tends to zero, these equations take the form,

\[
\frac{d}{dF} ([NO] \frac{dm}{dF}) = \dot{r} \frac{dA}{dF} + [NO]' \frac{d\dot{m}'}{dF} - [NO]'' \frac{d\dot{m}''}{dF}
\]

\[
\frac{d}{dF} (\frac{dm}{dF}) = \frac{d\dot{m}'}{dF} - \frac{d\dot{m}''}{dF} - \frac{d}{dx} (\varepsilon \frac{dm}{dF})
\]
The control volume considered above is only concerned with an element of mass $\delta m$ with a mixture ratio $\delta F$ about $F$. It was proposed to represent the distribution of mass about mixture ratio by a normal distribution function of the form,

$$
\frac{\delta m}{\delta F} = C \exp \left\{ -\frac{1}{2} \left( \frac{F - \bar{F}}{\sigma} \right)^2 \right\} \quad A-5
$$

The parameter $\sigma$, in statistical terms, is called the standard deviation and represents the degree of distribution of $F$ about the mean value $\bar{F}$. $C$ is termed the normalizing factor and for the purpose of this study is defined by the expression that,

$$
\int_{0}^{2\bar{F}} \frac{\delta m}{\delta F} \, dF = \dot{m}(1 - \epsilon) \quad A-6
$$

The value of $\bar{F}$ is the ratio of the total fuel burned to the total mass flow. Clearly both $C$ and $\bar{F}$ will be a function of the axial position in the combustor as they are computed from Equations A-2 and A-3.

A normal distribution has been selected as it is known to fit the spray characteristics of the type of fuel injectors used in gas turbine combustors and it provides a convenient way of describing the mixing process, by specification of the relationship $\sigma = \sigma(x)$. The value of $\delta m$, the mass flow in interval $\delta F$ about $F_i$ can also be evaluated functionally by the equation $f \, \delta m$,

$$
\delta m = \int_{F_i - \delta F/2}^{F_i + \delta F/2} \delta m \delta F \, dF \quad A-7
$$
and so the whole flow field can be readily represented by a series of discrete elements of constant, but different, mixture ratios.

2.3 APPLICATION TO THE PRIMARY ZONE

The model of the flow behavior described previously assumes that no mixing takes place in the primary zone after the specified distribution of mass mixtures ratios is attained. Thus, referring to the control volume above,

\[ \delta m' = \delta m'' = 0 \]

and further, it is also assumed that only a certain fraction \( \beta \) of the total fuel entering the zone is burned and that this fraction burns instantaneously.

\[ \frac{d}{dx} (\delta m) = 0 \]

so equation (A-1) reduces to,

\[ \frac{d}{dx} (\delta m [No]) = \rho \delta A \]  

A-8

or,

\[ [No] = \int_0^x \frac{\delta A}{\delta m} \, dx \]  

A-9

or alternatively.

\[ [No] = \frac{1}{\rho} \int_0^x \frac{\delta A}{\delta m} \, dx \]  

A-10

where \( \rho \) is the density of the element and \( t \) is the time it takes to pass through the primary zone. It is taken that \( \rho = \bar{\rho} \), the mean density in the primary zone where,

\[ \bar{\rho} = \frac{1}{m} \int_0^\infty \rho \delta m \, dF \]  

A-11

* The nature of the normal distribution function is that \( f(F)dF \) only tends to zero as \( F \) tends to \( \pm \infty \). Negative \( F \)'s have no physical significance so a constraint is imposed upon the function that \( 0 < F < 2F \) thus preserving the useful feature of symmetry about \( F \). In fact, if \( \sigma \) is less than \( \bar{F}/3 \), this constraint modifies the function to only a very small extent as it can be shown that the integral is greater than 99.7 percent of what over the range \( \pm \infty \). Practically, a range of \( \sigma \) from 0 to \( \bar{F}/3 \) will represent a wide range in distribution characteristics. It should also be noted that \( C \) and \( m \) are simply related by the equation \( C = \bar{\rho} \delta m \), if the limits are expressed from \( \pm \infty \).
but the value of \( \tau \) cannot be so simply expressed for the case of a completely-stirred reactor. Theoretical considerations dictate (see Ref 1) that various fractions of the mass flow \( \dot{m} \) have different residence times according to the function,

\[
F(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right)
\]

where \( \tau \) is the mean residence time and is equal to the ratio of \( \left( V_p \bar{V} / \dot{m} \right) \) and where \( V_p \) is the volume of the primary zone. The relationship,

\[
\tilde{f}(t) = \frac{t_{\text{res}}}{\tau} \int_0^{t_{\text{res}}} \exp\left(-t/\tau\right) dt
\]

then defines a fraction \( \tilde{f}_e \) of \( \dot{m} \) which has a residence time within the range \( dt \) about \( \tau \). It is therefore necessary to solve Equations A-10 and A-13 to compute a series of \( \tilde{f}_e \) values corresponding to the [NO]_e concentrations over the range of \( t \) from zero to infinity. The mean nitric oxide concentration at the exit of the zone for an element of mixture ratio \( F \), \( [\text{NO}]_F \), is then calculated from,

\[
[\text{NO}]_F = \sum_{r=0}^{\infty} \tilde{f}_e \times [\text{NO}]_e
\]

and the process repeated for all elements over the mixture range of interest.

Finally, an over-all mass mean average nitric oxide concentration for all products leaving the primary zone can then be computed by summing all products \( [\text{NO}]_F \times \dot{m} \) and dividing by the total mass flow rate through the primary zone.

2.4 APPLICATION TO THE INTERMEDIATE ZONE

In the intermediate zone, mixing is assumed to occur over the length of the zone \( L \), such that at the exit it is uniformly mixed. We postulate that mixing is characterized by the expression,
where $c_0$ is the prescribed deviation for the primary zone, $A_1$ is a model constant and $x_1$ is the axial distance from the primary zone exit. The distribution of the mixture ratio $F$ is therefore known at every point, i.e., $S_m = f(F, x) \, \delta x$ is prescribed by Equations A-5, A-6, and A-15. The problem therefore reduces to determining $S_{m'}$, $S_{m''}$, and $F'$ from Equations A-2 and A-4 and to making certain assumptions about the mixing process, as $[\text{NO}]'$ and $[\text{NO}]''$ must be determined in order that Equation A-1 can be solved for $[\text{NO}]$ as a function of $F$ and $x$.

We will postulate that all mixing occurs at conditions corresponding to entry conditions into the control volume so,

$$\frac{[\text{NO}]}{[\text{NO}]} = \frac{[\text{NO}]}{[\text{NO}]}$$

and also that,

$$S_{m''} = K S_m$$

A-16

which is to say that the flow out of the elemental control volume, due to mixing, is proportional to the amount flowing into the control volume. Clearly $K$ must have units of $1/\text{length}$ and the physical interpretation of $K$ can best be thought of in terms of the ratio, $C_N$, of the mass flow rate leaving the element over the length of the intermediate zone to the mass flow rate within the element. If this latter mass flow rate is constant, then clearly

$$S_{m''} = C_N S_m$$

or,

$$K = C_N / x_L$$

A-17

It will be assumed that the value of $K$ is known. Equation A-2 then yields,

$$S_{m'} = \frac{d}{dx} (S_m) + \dot{R} + K S_m$$

where it is to be noted that the restrictions,
\[ K > 0 \]
\[ K > \left\{ \frac{1}{\delta \dot{m}} \left( \frac{d}{dx} (\delta m) + \dot{R} \right) \right\}_{\text{max}} \]

must be satisfied for the model to be valid.

The gases flowing into the control volume as a result of mixing, \( \delta \dot{m} \), will originate from two sources: firstly, from the mixing of gases already within the combustor liner, which we will denote as \( \delta \dot{m}_1 \), and secondly by the mixing action of the diluent air with previously mixed gases, which we will call \( \delta \dot{m}_2 \). Clearly,

\[ \delta \dot{m}' = \delta \dot{m}_1 + \delta \dot{m}_2 \]  

A-19

and we will postulate that,

\[ \delta \dot{m}_2 = \frac{\delta \dot{m}}{m} \dot{m}_2 \]  

A-20

that is, that the amount of diluent air entering the control volume is in proportion to the total mass flow rate in the volume. The problem is then defined in terms of \( \delta \dot{m}' \), \( \delta \dot{m}'' \), and \( F' \) as,

\[ \delta \dot{m}_m = \frac{d}{dx} (\delta m) + K \delta m - \frac{\delta m}{m} \dot{m}_2 + \dot{R} \]  

A-21

from Equations A-17, A-19, and A-20, and also as a consequence of Equation A-3.

\[ F' = \frac{F}{\delta \dot{m}'} \left( \delta \dot{m}'' + \frac{d}{dx} (\delta m) \right) + \frac{\dot{R}}{\delta \dot{m}'} \]  

A-22

The value of \([\text{NO}] \) must now be calculated. Clearly, the total nitric oxide mass which leaves all the elements by mixing must also return via the mixing process to preserve conservation of the specie. The following relationship is assumed to apply, therefore, that

\[ [\text{NO}] = \frac{2}{5} \left( \frac{\delta \dot{m}''}{\delta \dot{m}'} \times [\text{NO}]'' \right) \]  

A-23

The value of \( \dot{R} \), the rate of burning of the unburned fuel which leaves the primary zone (see Equation A-4), is now all that is necessary to calculate NO concentrations throughout the intermediate zone.
It is postulated that this rate of burning is controlled by the mixing process, so in keeping with the Equation A-15, the following is assumed,

$$
\varepsilon = \varepsilon_0 \left(1 - A_3 \left(x_1/L\right)^{A_4}\right)
$$

where $A_2$ and $A_3$ are model constants, $\varepsilon_0$ is the fractional mass of unburned fuel entering the intermediate zone and is given by

$$
\varepsilon_0 = (1 - R) \frac{m_f}{m}
$$

$R$ may therefore be computed, as by definition (see Equation A-4), it is equal to $\frac{d}{dx} \left(\varepsilon S_m\right)$. Thus the problem is defined as,

- $S_m'$ is known from Equations A-19 and A-21
- $S_m''$ is known from Equation A-16
- $[NO]'$ is known from Equation A-23
- $[NO]''$ is equal to $[NO]'_x$
- and $S_m = \mathcal{F}(F,X)S_F$, is given by the specified distribution function.

If these values are substituted into the conservation equation for nitric oxide (Equation A-2) then it can be shown that,

$$
[NO]'_x dx - [NO]_x = \int_x^{x+dx} \frac{C}{V} dx + \int_x^{x+dx} [\Delta NO] K dx
$$

$$
= \frac{S_m + dS_m}{S_m} + \int_x^{x+dx} [\Delta NO] dx + \int_x^{x+dx} [NO]_0 dx
$$

where $V$ is the velocity and

$$
[\Delta NO] = \left(\frac{[NO]'}{[NO]_x} - [NO]''_x\right)
$$

This equation has to be evaluated in a stepwise manner in order to calculate the relationship $[NO] = \mathcal{F}(F,X)S_X$ in the intermediate zone. It is then a simple matter to compute an over-all mass average nitric oxide concentration at each axial station from,

*Another way to express these relationships is as:

$$
m_{\text{fu}} = (1 - R) m_f
$$

$$
m_{\text{fu}} = m_{\text{fu}} \left(1 - A_3 \left(x_1/L\right)^{A_4}\right)
$$
and so complete the computation.

2.5 APPLICATION TO THE DILUTION ZONE

In the dilution zone all gases are assumed to perfectly mix to a mean mixture ratio. All fuel is assumed to have been burned previously in the combustor and only diluent air enters the zone. For this case therefore, one cannot consider a control volume of constant mixture ratio $F$, as was done at the introduction to this section, as $F$ must change with axial distance due to the added air flow. For the special case of the assumptions made above, this change may be accounted for by modifying only Equation A-3 of the conservation equations so that this dependency of $F$ with $X$ is properly accounted for.

The conservation Equations A-1 through A-4, can be shown to be given by,

$$
\frac{d}{dx} (S_m [NO]) = \dot{X} S_A
$$

$$
\frac{d}{dx} (S_m) = \dot{\bar{S}} m_a
$$

$$
\frac{d}{dx} (S_m F) = 0
$$

$$
\frac{d}{dx} (\bar{S} S_m) = 0
$$

as the above assumptions imply that,

$$
\bar{S} m'' = S_m a
$$

and,

$$
\bar{NO} = F' = \bar{R} = S_m'' = 0
$$

The conservation equation for nitric oxide can be reduced to the form,

$$
[NOC]_{x+dx} - [NOC]_x = \left( \frac{\dot{\bar{X}}}{\bar{Q} V} \right) dx + \int_{F}^{F+dF} \frac{\bar{NO}}{F} dF
$$

which predicts directly, the mean average nitric oxide concentration at the new axial position. This process can be repeated in a step-wise manner to the end of the combustion chamber and hence the nitric oxide concentration at the exit plane may be predicted.
2.6 COMPUTATIONAL PROCEDURE

A summary is presented below of the computational procedure necessary to combine the flow model and the chemical reaction scheme presented in Volume 2 in order to predict nitric oxide emissions from aircraft turbine engines.

2.6.1 Required Input

The following input is required in order for the computation to proceed:

a. Chemical Reaction Scheme

1. A means of evaluating the adiabatic flame temperature, density and composition of the equilibrium products for the combustion of hydrocarbons in air. Program NOXRAT described in Volume 2 serves the purpose.

2. Values of the rate constants $k_i$ to $k_r$. Fuel properties in terms of $C_i:H_j$ ratio.

b. Combustor Dimensions

These should be expressed in such a way as to allow calculation of:

1. Volume of the primary zone.
2. Area of the intermediate and dilution zones as a function of distance $X$.

c. Combustor Operating Conditions

The following should be expressed as a function of aircraft operating mode,

1. Combustor inlet temperature and pressure.

2. Total fuel flow rate.

3. Air-flow conditions in terms of the fraction entering the primary zone and the rate of addition at the walls as it varies with axial position along the combustor.

d. Other Inputs to be Specified

1. The functions, $\sigma = \sigma(X)$ (see Equation A-15) and $\varepsilon = \varepsilon(X)$ (see Equation A-24)
2. The value of $K$, or $C_N$, which defines the fraction of gases that leave an element of constant mixture ratio $F$ due to mixing (see Equation A-16)

2.6.2 Preliminary Calculations

Two preliminary calculations must be performed before the computation of NO concentration levels can be undertaken. These involve,

a. The determination of a value for $B$, the fraction of total fuel entering the primary zone that is burned in the zone.

b. A consideration of the mixing characteristics of the cooling air that enters the combustor liner from the walls of the intermediate and dilution zones. The bulk of such flow normally enters perpendicular to the direction of the mainstream product flow and has then to be deflected and entrained before it can enter the fully developed mixing processes. This action must require a finite time (i.e., distance) to occur, and its effect upon the nitric oxide formation process has to be considered.

Combustion Efficiency

A correlation does exist to relate primary zone combustor efficiency to the fuel loading parameter $m_f/V_p^2$. The correlation is given in Reference 2 and is reproduced in Figure 2. There is significant scatter in the data points used to obtain the correlation and the values of the primary zone efficiency determined using the correlation can be expected to have error limits of approximately $\pm 20$ per cent of the indicated value.

Air Distribution Characteristics

In the calculation of the rate of diluent air addition to the intermediate and dilution zones, some provision must be made for the time (hence distance) necessary for the dilution gases to mix into the mainstream flow. This mixing lag could conceivably affect NO
emissions significantly under certain circumstances as it controls the rate of temperature change at positions downstream of the primary zone exit. A simple method was developed to take some account of this effect and is described fully in Appendix XVI. The method is consistent with the mixing assumptions used to develop the model for the intermediate zone of the combustor and at the same time, it determines the fraction of the air that enters the primary zone.

2.6.3 Prediction Procedure

In the interests of economy of use of Program NOXRAT which determines the flame temperatures and concentrations of the C-H-O-N species at equilibrium conditions, hence the NO formation rates, the distribution function of mixture ratio \( F \), versus mass fraction (Equation A-5), is considered as a series of elements of differing \( SF \). The first task in each step is to calculate the mass fraction in each element from the equation,

\[
\frac{\mathrm{d}m}{F} = \int \frac{S_m}{SF} \, dF
\]

for the prescribed conditions and thus relate \( S_m \) to \( F \).

The \( SF \) increments are selected, then the adiabatic flame temperatures \( T \), the density \( \rho \) and the corresponding equilibrium concentrations of the species \( N, N_2O, NO, C_2, 0, OH, \) and \( NO \) are determined from Program NOXRAT for each \( F \). These specie concentrations are then used to determine the values of \( R_1, R_6, K_1, \) and \( K_2 \) (for each \( F \)) which are needed to compute the rate of nitric oxide formed by chemical reaction and the calculation then proceeds as follows.

**Primary Zone**

a. The specified value of \( \varphi \), the fraction of fuel burned in the primary zone, is used to compute \( \bar{F} \). \( S_m \) can then be determined for all \( F \) values over the range of interest \((0 < F < \bar{F})\).
b. The value of the mean residence time $\bar{\tau}$ is determined from Equation A-12.

c. Nitric oxide concentrations at the primary zone exit can then be computed for each $F$ and for the prescribed residence time distribution by solving in an iterative manner the relationship,

$$[\text{NO}]_F = \sum_{t=0}^{\infty} [\text{NO} ]_t \times F_t$$

d. Finally the mass average nitric oxide concentration is computed for all gases leaving the primary zone from the relationship,

$$[\bar{\text{NO}}]_F = \sum_{t=0}^{F=2F} [\text{NO}]_F \times S_{t=0}$$

Intermediate Zone

The calculation procedure for this zone, for each incremental step in the axial direction, is essentially identical to that for the primary, except for the necessity to compute a change in NO concentration due to the mixing process. The procedure is as follows:

a. For $X<X+AX$, new values of $\bar{\tau}$ are computed at each $F$ from Equation A-5.

b. The value of $[\text{NO}]_F$, the concentration of nitric oxide in the gases entering the control volume by mixing over the step is computed according to Equation A-23.

c. The nitric oxide concentration at position $X+\Delta X$ is then computed for each mixture ratio $F$ by integration of Equation A-26.

d. Finally the new mass average nitric oxide concentration is computed as for Step d above.

These steps are repeated to the end of the intermediate zone.

Dilution Zone

The results of the intermediate zone calculation serve as input to the dilution zone. At this stage all elements in the combustor are
of equal composition and temperature, and dilution proceeds by the addition of pure air and so can use the relationship (see Equation A-29) that,

\[
[\text{NO}]_{x+d} - [\text{NO}]_x = \int_x^1 \frac{d}{V} \ dx + \int_F^d \frac{[\text{NO}]}{F} \ dF
\]

This can be integrated in a stepwise manner with respect to \( x \) by interpolation of the nitric oxide rate data at each step to determine the nitric oxide concentration conditions at the corresponding \( F \) value.

The nitric oxide formation rate quickly reduces in this zone as the temperature decreases rapidly.
3. PROGRAM GASNOX

3.1 INTRODUCTION

3.1.1 Program Function and Capabilities

Program GASNOX is a digital computer program written in Fortran IV language for use with the CDC 6600 computing system. The program has been developed for the purpose of predicting the nitric oxide emission level from an aircraft gas turbine combustor. Based on a given set of combustor dimensions, operating conditions, kinetic rate constants, thermodynamic properties, equilibrium compositions, and a primary zone mixing parameter, the program will compute nitric oxide concentrations as a function of axial position in annular and canannular combustors.

The analytical procedures on which the computer program is based have been discussed in Section 2 of this volume and in Reference 3. Briefly, the model considers a combustor to consist of three zones: primary, intermediate, and dilution. The primary zone is modeled as a partially stirred reactor with the variation of gas composition, temperature, and residence time occurring within the zone taken into account statistically. The program predicts only the gross features of the flow at the zone exit. The intermediate zone represents a transition between the primary and dilution zones. Here mixing occurs between the heterogeneous products from the primary zone and the entering cooling air. The program predicts the gross features of the flow as a function of axial position in this zone. In the dilution zone, the flow is uni-dimensional with the gases uniformly mixed across each cross section. Only the mean mixture ratio is considered, and this only changes as the remaining compressor air is mixed into the combustor. The procedures incorporated into the program have been found to be quite acceptable in terms of accuracy and calculation efficiency.
3.1.7 Report Arrangement

The main body of the report begins with a section in which the input data necessary for the solution of any case are described in detail; this includes instructions for preparing and supplying these data to the program and a sample case in the appropriate format. The next section contains a discussion of the various types of output data obtained from the program and also of the output data from the sample case. A description of the error messages printed by the program is also included. Following that is a section containing miscellaneous information regarding the operation of the program with the CDC 6600 computing system.

The first appendix consists of a general discussion of the overall logic structure of the program. The next appendix gives the Fortran nomenclature for the variables in the COMMON blocks of the program. The remaining appendices except the last provide detailed descriptions of the various components (main routine and subroutines) which make up the over-all program, one appendix for each component. The appendix for each new subroutine contains a presentation of the input and output variables, an internal Fortran nomenclature, a description of the step-by-step calculation procedure, and a Fortran listing of the subroutine. The last appendix contains a discussion of the method of calculation of the air distribution characteristics.

3.2 INPUT DATA

3.2.1 General Description

Program GASNOX requires the following input data in order to determine the nitric oxide emission level from an aircraft gas turbine engine.

a. Combustor Dimensions
   1. \( V_P \) - Volume of the primary zone
   2. \( X_L \) - Length of the intermediate zone (from the exit of the primary)
3. \( X_{\text{END}} \) - Distance from the primary zone exit to the exit from the combustor liner

4. \( R_X \) - Radius of liner at position \( X \) for canannular configuration

5. \( R_X^1, R_X^0 \) - Inner and outer radii of liner at position \( X \) for annular configuration

b. Combustor Operating Conditions

1. \( T \) - Inlet temperature

2. \( P \) - Operating pressure

3. \( \phi_p \) - Mass mean equivalence ratio in the primary zone (before fuel burns)

4. \( \phi \) - Fraction of fuel entering the primary zone which burns in the zone

5. \( E_{\text{rat}} \) - Variable for altering \( p \) parametrically yet maintaining constant the over-all air-to-fuel ratio in the combustor

6. \( (M_{\alpha X})_{\%} \) - Total mass per cent of air mixed with the product stream at position \( X \) in the liner

7. \( M_A \) - Total mass of air fed into the combustor liner

8. \( \bar{\omega}_p \) - Mean primary zone residence time (applies only if \( V_p \) is set equal to zero)

c. Mixing Parameter for the Primary Zone

1. \( S_o \) - Degree of mixedness in the primary zone (where \( \omega_o \) in the distribution function is given by \( \omega_o = S_o \cdot \phi_p \))

d. Kinetic Constants for each Mixture Ratio Element

1. \( R_1 \) - Forward reaction rate constant for the first reaction (see Section 2, Volume 2 or Ref 3)

2. \( R_6 \) - Forward reaction rate constant for the sixth reaction (see Section 2, Volume 2 or Ref 3)
3. $K_1$ - Ratio of forward reaction rate constants
   (see Section 2, Volume 2 or Ref 3)
4. $K_2$ - Ratio of forward reaction rate constants
   (see Section 2, Volume 2 or Ref 3)

e. Thermodynamic Properties for each Mixture Ratio Element
1. $\rho$ - Density of the combustion products
2. $T_f$ - Adiabatic flame temperature of the combustion products.

f. Equilibrium Compositions for each Mixture Ratio Element
1. $(\text{NO})_e$ - Nitric oxide equilibrium mole fraction
2. $(\text{CO})_e$ - Carbon monoxide equilibrium mole fraction
3. $(\text{C}(s))_e$ - Solid carbon equilibrium mole fraction
4. $(\text{CH}_2)_e$ - Unburned hydrocarbons (exclusive of CO and $\text{C}(s)$) equilibrium mole fraction.

The input data is read in three categories: 1) the kinetic, thermodynamic, and equilibrium data and the combustor inlet temperature and pressure; 2) the combustor airflow distribution and radius versus axial position; and 3) the remaining combustor dimensions, operating conditions, and the primary zone mixing parameter. With this structure there may be several sets of data in a given computer run. Figure 3 is a schematic representation of the data input structure.

3.2.2 Detailed Description of Input Data

The information required to prepare the input data for a case is furnished in the table given below. This information contains a description of each input item as well as a description of the form in which these items are written on input data sheets. The descriptions of the input items refer frequently to several points, relevant to the selection of input values, which are discussed in the following subsection. The discussions of these points provide additional detailed information useful in preparing the input data for any case.

The first input item read by Program GASNOX is the integer variable $\text{IDATA}$ which identifies the number of sets of data in category 1. This input is then followed by the first set of category 1 data (see point a).
<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Input Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-6</td>
<td>Int</td>
<td>IDATA</td>
<td></td>
<td>Number of sets of data in category 1</td>
</tr>
<tr>
<td>2</td>
<td>1-72</td>
<td>A</td>
<td>SET(1)</td>
<td></td>
<td>Descriptive data identifying atomic composition of fuel and the turbine inlet temperature</td>
</tr>
<tr>
<td>3</td>
<td>1-14</td>
<td>A</td>
<td>SET(1)</td>
<td></td>
<td>Descriptive data of units of combustor inlet pressure</td>
</tr>
<tr>
<td>3</td>
<td>15-29</td>
<td>P</td>
<td>FP</td>
<td>PPP</td>
<td>Combustor inlet pressure (atm)</td>
</tr>
<tr>
<td>3</td>
<td>30-51</td>
<td>A</td>
<td>SET(1)</td>
<td></td>
<td>Descriptive data of set of kinetic constants used in calculation (see Volume 1, Table 2; descriptive data of $k_s$)</td>
</tr>
<tr>
<td>3</td>
<td>52-66</td>
<td>$k_s$</td>
<td>FP</td>
<td>EKS</td>
<td>Fuel-to-air mass ratio at stoichiometric conditions</td>
</tr>
<tr>
<td>4</td>
<td>1-12</td>
<td>F_i</td>
<td>FP</td>
<td>FF(1)</td>
<td>Mixture ratio of an element</td>
</tr>
<tr>
<td>4</td>
<td>13-24</td>
<td>$\phi_i$</td>
<td>FP</td>
<td>PHI(1)</td>
<td>Equivalence ratio of an element</td>
</tr>
<tr>
<td>4</td>
<td>25-36</td>
<td>$\rho_i$</td>
<td>FP</td>
<td>RHO(1)</td>
<td>Density of combustion products for an element (gm/cm$^3$)</td>
</tr>
<tr>
<td>4</td>
<td>37-48</td>
<td>$T_i$</td>
<td>FP</td>
<td>ATT(1)</td>
<td>Adiabatic flame temperature for an element (deg K)</td>
</tr>
<tr>
<td>4</td>
<td>49-60</td>
<td>$(\text{NO}_i)_e$</td>
<td>FP</td>
<td>BCON6(i)</td>
<td>Equilibrium mole fraction of NO for an element</td>
</tr>
<tr>
<td>4</td>
<td>61-72</td>
<td>$(\text{CO}_i)_e$</td>
<td>FP</td>
<td>BCON2(i)</td>
<td>Equilibrium mole fraction of CO for an element</td>
</tr>
<tr>
<td>5</td>
<td>1-12</td>
<td>$(\text{C}(s)_i)_e$</td>
<td>FP</td>
<td>BCON1(i)</td>
<td>Equilibrium mole fraction of C$(s)$ for an element</td>
</tr>
<tr>
<td>5</td>
<td>13-24</td>
<td>$(\text{CH}_2)_i_e$</td>
<td>FP</td>
<td>CH2(i)</td>
<td>Equilibrium mole fraction of unburned hydrocarbons exclusive of C$(s)$ and CO for an element</td>
</tr>
<tr>
<td>5</td>
<td>25-36</td>
<td>$(r_i)_1$</td>
<td>FP</td>
<td>R1(1)</td>
<td>Forward reaction rate for the first kinetic reaction (see Section 2, Volume 2 or Ref 3) (gm-mole/cm$^3$-sec) for an element</td>
</tr>
<tr>
<td>Line</td>
<td>Location</td>
<td>Input Item</td>
<td>Type of Number</td>
<td>Fortran Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
<td>------------</td>
<td>----------------</td>
<td>----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>5</td>
<td>37-48</td>
<td>(R_b)_i</td>
<td>FP R6(1)</td>
<td></td>
<td>Forward reaction rate for the sixth kinetic reaction (see Section 2, Volume 2 or Ref 3) (gm-mole/cm³-sec) for an element</td>
</tr>
<tr>
<td>5</td>
<td>49-60</td>
<td>(K_1)_i</td>
<td>FP EK1(1)</td>
<td></td>
<td>Ratio of forward reaction rate constants (see Section 2, Volume 2 or Ref 3) for an element</td>
</tr>
<tr>
<td>5</td>
<td>61-72</td>
<td>(R_2)_i</td>
<td>FP EK2(1)</td>
<td></td>
<td>Ratio of forward reaction rate constants (see Section 2, Volume 2 or Ref 3) for an element</td>
</tr>
</tbody>
</table>

Lines 4-5 are repeated for each of the 35 discrete mixture ratio elements specified in the distribution function. At the conclusion of this data, the integer variable KASE is read. KASE identifies the number of sets of data in category 2 that follow for the given set of data in category 1.

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Input Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>74</td>
<td>1-6</td>
<td>Int KASE</td>
<td>FP</td>
<td></td>
<td>Number of sets of data in category 2</td>
</tr>
<tr>
<td>75</td>
<td>1-12</td>
<td>X</td>
<td>FP AXX(J)</td>
<td></td>
<td>Axial position in the combustor (in)</td>
</tr>
<tr>
<td>75</td>
<td>13-24</td>
<td>(M_a_x)</td>
<td>FP APR(J)</td>
<td></td>
<td>Per cent of total mass of airflow in combustor liner at position X (cumulative)</td>
</tr>
<tr>
<td>75</td>
<td>25-36</td>
<td>R_x</td>
<td>FP ARR(J)</td>
<td></td>
<td>Radius of liner at position X; applies only for canannular configuration (in) (see point b)</td>
</tr>
<tr>
<td>75</td>
<td>37-48</td>
<td>R_x1</td>
<td>FP ANR(J)</td>
<td></td>
<td>Inner radius of liner at position X; applies only for annular configuration (in) (see point b)</td>
</tr>
<tr>
<td>75</td>
<td>49-60</td>
<td>R_x0</td>
<td>FP ANNR(J)</td>
<td></td>
<td>Outer radius of liner at position X; applies only for annular configuration (in) (see point b)</td>
</tr>
</tbody>
</table>
Line 75 is repeated for each of 11 axial positions in the combustor. The first axial position must be taken as \( X = 0 \); that is, at the exit of the combustor primary zone.

There may be as many sets of data in category 3 for each set of data in category 2 as the user desires. The number of these data sets is read as the variable IN, on line 86.

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Input Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>86</td>
<td>1-6</td>
<td>Int IN</td>
<td></td>
<td></td>
<td>Number of sets of data in category 3</td>
</tr>
</tbody>
</table>

Following the data on line 86 is the data of category 3.

<table>
<thead>
<tr>
<th>Line</th>
<th>Location</th>
<th>Input Item</th>
<th>Type of Number</th>
<th>Fortran Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>87</td>
<td>1-12</td>
<td>VP ( V_p )</td>
<td>FP</td>
<td>VP</td>
<td>Volume of primary zone ( (\text{in}^3) ) (see point c)</td>
</tr>
<tr>
<td>87</td>
<td>13-24</td>
<td>XL ( X_L )</td>
<td>FP</td>
<td>XL</td>
<td>Length of intermediate zone ( \text{(in)} )</td>
</tr>
<tr>
<td>87</td>
<td>25-36</td>
<td>X(_{\text{END}})</td>
<td>FP</td>
<td>XEND</td>
<td>Length of intermediate zone and dilution zone ( \text{(combined)} ) ( \text{(in)} )</td>
</tr>
<tr>
<td>87</td>
<td>37-48</td>
<td>( \phi_p )</td>
<td>FP</td>
<td>EQUIV</td>
<td>Mass mean equivalence ratio in the primary zone ( \text{(before fuel burns)} )</td>
</tr>
<tr>
<td>87</td>
<td>49-60</td>
<td>( \rho )</td>
<td>FP</td>
<td>BETA</td>
<td>Combustion efficiency in the primary zone</td>
</tr>
<tr>
<td>87</td>
<td>61-72</td>
<td>( M_A )</td>
<td>FP</td>
<td>TOTAiR</td>
<td>Total mass of air fed into the combustor liner ( \text{(lb/sec)} )</td>
</tr>
<tr>
<td>88</td>
<td>1-12</td>
<td>S ( S_0 )</td>
<td>FP</td>
<td>S</td>
<td>Degree of mixedness in the primary zone</td>
</tr>
<tr>
<td>88</td>
<td>13-24</td>
<td>( \varepsilon_{\text{rat}} )</td>
<td>FP</td>
<td>ERAT</td>
<td>Variable for varying ( \varepsilon_{\text{rat}} ) parametrically yet maintaining constant air-to-fuel ratio in the combustor</td>
</tr>
<tr>
<td>88</td>
<td>25-36</td>
<td>( \overline{\varepsilon_{\text{rat}}^P} )</td>
<td>FP</td>
<td>TAUBAR</td>
<td>Mean primary zone residence time ( \text{(applies only if } V_p \text{ is set equal to zero) (see point c) } )</td>
</tr>
</tbody>
</table>
Lines 87-88 are repeated for each set of data in category 3 that the user wishes to specify.

3.2.3 Discussion of Input Data

Some important aspects to be considered in appropriately specifying the input data are discussed below. Reference to these discussions has been made in the preceding subsection in which the input format was described. The points referred to are as follows:

a. Data in category 1 (lines 2-73) are generated by Program NOXRAT described in Volume 2.

b. If a canannular configuration is tested, the variables $R_x$ and $R_y$ are set equal to zero. If an annular configuration is tested, the variable $R_x$ is set equal to zero.

c. If the user chooses to specify the volume of the primary zone, $V_p$, then the mean primary zone residence time ($\bar{\tau}_p$) is set equal to zero in the input. $\bar{\tau}_p$ is then calculated by the program. If, on the other hand, the user chooses to specify $\bar{\tau}_p$, he must set $V_p$ equal to zero in the input.

3.2.4 Description of Sample Case Input

Completed input data sheets are shown on pages 32 and 33. In this table lines 1-73 comprise the data and controls for category 1 (note: lines 6-73 are omitted for brevity); lines 74-85 comprise the data and controls for category 2; and lines 86-88 comprise the data and controls for category 3.

In this case, the fictitious combustor examined has an inlet temperature of 700 deg K and an operating pressure of 5.78 atm. The combustor is 10 inches in length from the exit of the primary zone, has a primary zone volume of 55 in$^3$, and is being operated with a mean primary zone equivalence ratio (before the fuel burns) of 0.9. The over-all air-to-fuel ratio is 92.

3.3 OUTPUT DATA

The output of Program GASNOX consists entirely of printed data. The printed data falls into two main categories: normal output, and
error messages with additional output. The normal output which is illustrated by the sample case included in the report, will be described first.

3.3.1 Normal Output

The information included in the normal output can be divided into the following categories:

1. General input data and miscellaneous calculated input data.
2. Elemental primary zone exit conditions from the converged solution.
3. Over-all primary zone exit conditions from the converged solution.
4. Over-all intermediate zone conditions at various axial positions in the zone from the converged solution.
5. Over-all dilution zone conditions at various axial positions in the zone from the converged solution.

A description of the items in each category is given below.

The normal output of a typical case begins with the items in category 1—general input data and miscellaneous calculated input data. This data consists of:

a. Axial position in the combustor (where the origin is taken as the primary zone exit) (in).
b. Total mass per cent of air mixed with the product stream at position X.
c. Radius of liner at position X for can annular configuration or inner and outer radii of liner at position X for annular configuration (in).
d. The case number; this number corresponds to the set of combustor dimensions, operating conditions, and the primary zone mixing parameter for the given combustor airflow characteristics.
e. The cumulative normal distribution data.
f. The atomic formula of the fuel.
g. The combustor air inlet temperature (deg K).
h. The combustor operating pressure (atm).
i. A code number identifying the set of kinetic constants employed in the reaction scheme.

j. The value of the fuel-to-air mass ratio at stoichiometric conditions.

k. For each element in the distribution function: the mixture ratio (mass fuel to mass fuel and air); the equivalence ratio; the density of the combustion products in gm/cm$^3$; the adiabatic flame temperature of the combustion products in deg K; the equilibrium mole fraction of NO, CO, C(s), and CH$_2$ (unburned hydrocarbons); and the kinetic parameters $R_1$, $R_6$ (in gm-moles/cm$^3$-sec), $K_1$ and $K_2$ (dimensionless) defined in Section 2 of Volume 2.

l. The volume of the primary zone (in$^3$).

m. The length of the intermediate zone (in).

n. The length of the intermediate and dilution zone (combined) (in).

o. The mean primary zone equivalence ratio (before the fuel burns).

p. The combustion efficiency in the primary zone.

q. The total mass of air fed into the combustor liner (lb/sec).

r. The degree of mixedness in the primary zone.

s. The variable used for altering the mean primary zone equivalence ratio parametrically without changing the over-all air-to-fuel ratio in the combustor.

t. The total mass of fuel fed into the combustor (lb/hr).

u. The over-all air-to-fuel ratio in the combustor.

The normal output of a typical case continues with the items in category 2--elemental primary zone conditions for the converged solution. These items, which begin after a statement describing them, consist of:

a. The mass fraction in the element.

b. The NO concentration in the element (ppm) (vol).

c. The cumulative sum of the NO formed up to and including the element (lb/sec).

d. The element number.
Only those elements with a finite rate of formation of NO are included in this output table.

The normal output of a typical case continues, after a statement describing the data, with the items in category 3—over-all primary zone exit conditions from the converged solution. This data consists of:

a. The axial position in the combustor (in).
b. The mass mean primary zone equivalence ratio, accounting for the inefficiency of the primary zone combustion.
c. The mass mean exit temperature of the primary zone (deg F).
d. The mass mean density of the primary zone combustion products (lb/ft^3).
e. The mass mean primary zone residence time (msec).
f. The mass mean concentration of NO in the primary zone (ppm) (vol).
g. The mass mean concentration of NO in the primary zone, expressed as NC_2 (lb/1000 lb fuel burned).
h. The mass mean equilibrium concentration of C(s) in the primary zone (ppm) (vol).
i. The mass mean equilibrium concentration of C(s) in the primary zone (lb/1000 lb fuel burned).
j. The mass mean equilibrium concentration of CO in the primary zone (ppm) (vol).
k. The mass mean equilibrium concentration of CO in the primary zone (lb/1000 lb fuel burned).
l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C(s)) in the primary zone (ppm) (vol).
m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C(s)) in the primary zone (lb/1000 lb fuel burned).
n. The fuel loading (lb/sec-ft^3-atm^2).

The normal output of a typical case continues, after a statement describing the data, with the items in category 4—over-all intermediate zone conditions at axial positions in the zone corresponding to the converged solution. This data consists of:
a. The axial position in the combustor (in).
b. The mass mean equivalence ratio, at the given axial station in the intermediate zone, accounting for the inefficiency of the primary zone combustion.
c. The mass mean exit temperature at the given axial station in the intermediate zone, (deg F).
d. The mass mean density of the combustion products at the given axial station in the intermediate zone (lb/ft^3).
e. The mass mean residence time of the combustion products from the combustor entrance to the given axial station in the intermediate zone (msec).
f. The mass mean concentration of NO at the given axial station in the intermediate zone (ppm) (vol).
g. The mass mean concentration of NO, expressed as NO_2, at the given axial station in the intermediate zone (lb/1000 lb fuel burned).
h. The mass mean equilibrium concentration of C(s) at the given axial station in the intermediate zone (ppm) (vol).
i. The mass mean equilibrium concentration of C(s) at the given axial station in the intermediate zone (lb/1000 lb fuel burned).
j. The mass mean equilibrium concentration of CO at the given axial station in the intermediate zone (ppm) (vol).
k. The mass mean equilibrium concentration of CO at the given axial station in the intermediate zone (lb/1000 lb fuel burned).
l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C(s)) at the given axial station in the intermediate zone (ppm) (vol).
m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C(s)) at the given axial station in the intermediate zone (lb/1000 lb fuel burned).

If the chemical rate of production of NO is frozen at any axial station in the intermediate zone, the program prints a message to that effect and proceeds with the dilution zone calculations and output.

The normal output of a typical case concludes, after a statement describing the data, with the items in category 5-- over-all dilution
zone conditions at axial positions in the zone corresponding to the converged solution. If the chemical rate of formation of NO was frozen at any axial station in the intermediate zone, only the dilution zone exit conditions are printed. The data in this category consists of:

a. The axial position in the combustor (in).

b. The mass mean equivalence ratio, at the given axial station in the dilution zone, accounting for the inefficiency of the primary zone combustion.

c. The mass mean exit temperature at the given axial station in the dilution zone (deg F).

d. The mass mean density of the combustion products at the given axial station in the dilution zone (lb/ft$^3$).

e. The mass mean residence time of the combustion products from the combustor entrance to the given axial station in the dilution zone (msec).

f. The mass mean concentration of NO at the given axial station in the dilution zone (ppm) (vol).

gh. The mass mean concentration of NO, expressed as NO$_2$ at the given axial station in the dilution zone (lb/1000 lb fuel burned).

i. The mass mean equilibrium concentration of C$_(s)$ at the given axial station in the dilution zone (ppm) (vol).

j. The mass mean equilibrium concentration of C$_(s)$ at the given axial station in the dilution zone (lb/1000 lb fuel burned).

k. The mass mean equilibrium concentration of CO at the given axial station in the dilution zone (lb/1000 lb fuel burned).

l. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C$_(s)$) at the given axial station in the dilution zone (ppm) (vol).

m. The mass mean equilibrium concentration of unburned hydrocarbons (exclusive of CO and C$_(s)$) at the given axial station in the dilution zone (lb/1000 lb fuel burned).

If the chemical rate of prediction of NO is frozen at any axial station in the dilution zone, the program prints a message to that
effect after completing the dilution zone calculations and printing
the output at the axial position that corresponds to the combustor exit.

3.3.2 Error Messages and Additional Output

In addition to the normal output, various messages may appear in
the output of a case. These messages either indicate that difficulty
has been encountered during execution of the case or that the user
has specified the printing of intermediate output to examine progress
in the iterations. The messages are considered below in the order of
their appearance in the program.

a. If intermediate output is requested by the user, the program
will print the value of the total mass contained in each
mixture ratio element and the value of the parameters that
define the range of the mass distribution function. These
values are printed in Subroutine ZMASS; they are printed
for each converged axial position in the combustor.

b. If, in calculating the values of \((\alpha_T)_i\), the number of
iterations on a given element equal ten, the program prints
the number of iterations and the last value of \((\alpha_T)_i\).
This is a nonfatal error as the program assumes the value
of \((\alpha_T)_i\) to be the last value calculated. The error
message is printed in Subroutine PRCALC. This error is
caused by limiting the number of iterations to ten; it
can be relieved by increasing the limit.

c. Potential error due to lack of convergence, SUMTNO(1) =
+X.XXXXXXXXXXX+XX prior value of SUMTNO(1) = +X.XXXXXXXXXXX+XX
1 = XXX

This message is printed in Subroutine PRCALC for a primary
zone element that fails to satisfy convergence criteria after
five iterations. This is a nonfatal error as the program
assumes that the value of SUMTNO(1) is the last value cal-
culated. The error is caused by limiting the number of
iterations to five; it can be remedied by increasing the
limit.
d. If intermediate output is requested by the user, the program will print the value of the nitric oxide content of each mixture ratio element for each converged axial position in the combustor. These values are printed in Subroutine PRINTS.

e. If the number of iterations attempting to satisfy the mixing criteria equal 40 for any mixture ratio element at any axial station in the intermediate zone, Subroutine ZINTER will print the most recent value of $E_i$ and the number of iterations. This is a fatal condition to the program causing immediate termination of the calculations. This procedure is a safety control to keep the program from continuing into an indefinite loop; it is likely caused by some trouble in the calculation of element masses and can only be remedied by detailed examination of the flow rates into and out of each mass element.

f. $X(\text{CM}) = +X.XXXXXXJ +XX$
   \[ \text{AVE. RHO(GM/CC)} = +X.XXXXXX +XX \]
   \[ \text{AVE. NO(GM/GM)} = +X.XXXXXX -XX \]

This message is printed from Subroutine ZINTER at the end of each iteration loop in the intermediate zone if intermediate output is requested by the user. The meaning of the message is quite clear; both the density and nitric oxide concentrations are mass averages. $J$ is the number of iterations.

g. RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED LIMIT, $\text{DIFNO} = +X.XXXXXX +XX$ $N = XXXX$ $X = CMS$

This nonfatal message is printed by Subroutine ZINTER at each axial position in the intermediate zone where convergence criteria on the NO iterations are not satisfied. $N$ here is the number of steps each major step is divided into for the last iteration; $\text{DIFNO}$ identifies the difference in the calculated nitric oxide levels at the end of the major step down the combustor to position $X$. There are two possible reasons for the appearance of the message:

1. The number of steps allowed in the Runge-Kutta integration are inadequate.
2. The convergence limit is too narrow.
Relaxation of either of these control criteria will eliminate the iteration difficulty.

h. \( X(Chi) = \frac{+X.XXXXXX+XX}{GM/MM} = +X.XXXXXX+XX = \text{AVE.RHO} \)
\( \text{AVE.NO} = +X.XXXXXX+XX \)

This message is printed from Subroutine DILUTE at the end of each iteration in the dilution zone if intermediate output is requested by the user. The meaning of the message is quite clear except for the last two variables printed; these variables are rate of change of nitric oxide mass fraction with position due to chemical reaction and dilution, respectively. Both the density and nitric oxide concentrations are mass averages. \( J \) is the number of iterations.

i. If intermediate output is requested by the user, Subroutine DILUTE prints the difference between the calculated nitric oxide levels for the last two iterations at the end of each major step down the combustor. In addition, DILUTE also prints the number of integration steps each major step is divided into for the last iteration.

j. RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED LIMIT.
\( \text{DIFNO} = +X.XXXXXX+XX \quad \text{N} = XXXX \quad X = +X.XXXXXX+XX \)

This nonfatal message is printed by Subroutine DILUTE at each axial position in the dilution zone where convergence criteria on the NO iterations are not satisfied. \( N \) here is the number of steps each major step is divided into for the last iteration; \( \text{DIFNO} \) identifies the difference in the calculated nitric oxide levels at the end of the major step down the combustor to position \( X \). There are two possible reasons for the appearance of the message:

1. The number of steps allowed in the Runge-Kutta integration are inadequate.
2. The convergence limit is too narrow.

Relaxation of either of these control criteria will eliminate the iteration difficulty.
3.3.3 Description of Sample Case Output

The output from the fictitious sample case described on pages 33 and 34 is presented on pages 35-42. The data on pages 35-38 represents the input data for this fictitious case while calculated results are shown on pages 39-42. From the data it is seen that the mean primary zone residence time for the combustor is 2 msec; and, in that time, a mass average concentration of 300 ppm (vol) of nitric oxide has been formed. Within a distance of 1.5 inches down the combustor intermediate zone, the chemical rate of formation of nitric oxide is negligible in comparison with the amount of nitric oxide previously formed. Consequently, only the dilution of the total nitric oxide formed to that point is important to the final emission figure of 73 ppm (vol).

3.4 MISCELLANEOUS OPERATIONAL INFORMATION

Program GASNOX occupies approximately 20,000 core locations during loading and approximately 12,000 core locations during execution on the CDC 6600 computer. Actual program length is approximately 7100 core locations. Hence, the total storage requirement for this program is comfortably within the CDC 6600 core capacity of 131,000 locations.

The execution time for Program GASNOX depends upon the characteristics of the particular combustor being analyzed. It has been found, however, that a typical case will require approximately 10 to 15 seconds of central processor time on the CDC 6600 with another 1 to 2 systems seconds necessary to satisfy input/output requirements. Approximately 12 systems seconds are required to load and compile the program.

There are no known sources of convergence difficulties in the program save the limits imposed on the number and accuracy of the Runge-Kutta integrations. These requirements are adequate for most applications of the program; they are neither too restrictive to cause convergence difficulties nor too loose to permit an abundance of iterations and excessive computer costs.
### LOCATION

| Line  | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Line 1| 1   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 2|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 3|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 4|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 5|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 6|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 7|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 8|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 9|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 10|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 11|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 12|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 13|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 14|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 15|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 16|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 17|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 18|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 19|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| Line 20|    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
3.5 DATA INPUT SHEET

ENGINEER: RDS  PROJECT: Turbine Combustors  PROJECT NO: 1152

TITLE: Sample to Illustrate the Use of Program GASNOX  SHEET: 2 OF 2

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### 3.6 SAMPLE CASE OUTPUT

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**CASE NO. = 1**

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**CUMULATIVE NORMAL DISTRIBUTION DATA**

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### ELEVANT

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THE REST OF THE INPUT VARIABLES

THE VOLUME OF THE PRIMARY ZONE IS 5.50000e+01 CU. IN.

THE LENGTH OF THE INTERMEDIATE ZONE IS 7.00000E+00 IN.

THE LENGTH OF THE INTERMEDIATE ZONE AND DILUTION ZONE (COMBINED) IS 1.00000E+01 IN.

THE MEAN PRIMARY ZONE EQUIVALENCE RATIO IS 8.00000E+01

THE COMBUSTION EFFICIENCY IN THE PRIMARY ZONE IS 9.00000E+01

THE TOTAL MASS OF AIR FED INTO THE COMBUSTOR IS 5.00000E+00 LR./SEC.

THE DEGREE OF MIXEDNESS IS 6.00000E+01

ERAT = 1.00000E+00

THE MEAN PRIMARY ZONE RESIDENCE TIME (ONLY APPLIES IF THE VOLUME OF THE PRIMARY ZONE IS ZERO IN INPUT) IS 0.0 SEC.

THE COMPUTED TOTAL MASS OF FUEL FED INTO THE COMBUSTOR IS 1.95703402 LR./HR.

THE COMPUTED OVERALL AIR-TO-FUEL RATIO IS 9.19763E+01
### Primary Zone Exit Conditions

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This is the main printout for the primary zone.

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<th>NO</th>
<th>NOX</th>
<th>C(5)</th>
<th>C(5)</th>
<th>CO</th>
<th>CO</th>
<th>CH2</th>
<th>CH2</th>
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<tr>
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This is the fuel loading 5.11234E+02 I.E./SEC=CU/FT=AMO=AMO.

---
This is the main printout for the intermediate zone.

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<th>C(S)</th>
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***Nitric Oxide reaction frozen at this point***
This is the main printout for the dilution zone.

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<td>LBS PER</td>
<td>LBS PER</td>
<td>LBS PER</td>
<td>LBS PER</td>
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4. REFERENCES


5. FIGURES
Figure 1  ASSUMED FLOW AND DISTRIBUTION PATTERNS THROUGHOUT COMBUSTOR LINER
Figure 2 PRIMARY ZONE COMBUSTION EFFICIENCY CORRELATION

FUEL LOAD FACTOR

\( M_f / V_p \) \( P^2 - lb/sec ft^3 \) \( Atm^2 \)

REPRODUCED FROM REFERENCE 2
FIGURE 3 - SCHEMATIC REPRESENTATION OF INPUT STRUCTURE
FIGURE 4 - MODULAR TREE DIAGRAM
### 6. NOMENCLATURE

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<td>Model constant in equation A-15</td>
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<tr>
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<td>( )&quot;</td>
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<td>( )⁻</td>
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7. APPENDICES
APPENDIX I - OVER-ALL PROGRAM LOGIC

Program GASNOX consists of a main routine and twelve subroutines. The subroutines are PRIMRY, ZINTER, DILUTE, PRCALC, PRRAT, CHECKK, CALCBC, RUNKUT, DERIV, MINT, ZMASS, and PRINTS. Information is transmitted within the computer program through blocks of COMMON and as arguments of certain subroutines. The over-all control of the programmed calculation procedure is maintained by the main routine.

The logic flow begins at the start of the main routine where the input data is read and then printed. Subroutine PRIMRY, which controls the combustor primary zone calculations, is then called.

The primary zone is modeled as a partially stirred reactor, with the variations in gas composition, temperature, and residence time taken into account statistically. Thus, PRIMRY first calls Subroutine ZMASS to calculate element masses. ZMASS, in turn, calls Subroutines MINT and CALCBC. MINT provides interpolated values of tabulated functions of one variable assuming a linear relationship between the adjacent tabular entries. CALCBC calculates values of the mass flow coefficient at each axial station of the combustor primary and intermediate zones. CALCBC also calls Subroutine MINT. After calling ZMASS, Subroutine PRIMRY calls Subroutines PRCALC and PRINTS. PRCALC controls and calculates the average nitric oxide level in the primary zone for each specified mixture ratio element in the mass distribution function. PRCALC calls Subroutines PRRAT and MINT to conduct its calculations; PRRAT solves the analytical expression relating the elemental nitric oxide concentration to the elapsed time in the primary zone. PRINTS provides the written output of the calculated results of the program.

Having completed the primary zone calculations, GASNOX calls Subroutine ZINTER to perform and control the intermediate zone analysis if the primary zone mixing parameter is other than zero. If the mixing parameter is set at zero, GASNOX skips over the intermediate zone calculations and proceeds with dilution zone calculations via Subroutine DILUTE.
The intermediate zone of the combustor is divided into a series of finite length axial elements in which the heterogeneous products from the primary zone mix with one another and with the entering cooling air. By the end of the zone the distribution is collapsed to a uni-dimensional profile. To accomplish this mixing process ZINTER calls on Subroutines ZMASS, CHECKK, RUNKUT, MINT, and PRINTS. The function of Subroutines ZMASS and MINT are as before; PRINTS writes the calculated mass mean conditions at the end of each finite length axial combustor segment. Subroutine CHECKK calculates the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it at a given axial position in the combustor. RUNKUT is employed to obtain the solution to the first order ordinary differential equation between nitric oxide concentration and axial position in the combustors by the Gill variation of the Runge-Kutta numerical integration scheme. In doing so, RUNKUT calls Subroutine DERIV which calculates the rate of nitric oxide formation with respect to axial distance in the combustor intermediate or dilution zone.

In the dilution zone, the flow is uni-dimensional with the gases uniformly mixed across each cross section. To perform and control these calculations GASNOX calls on Subroutine DILUTE. DILUTE in turn calls on Subroutines ZMASS, MINT, RUNKUT, and PRINTS for calculations and printout at specified axial stations in the zone. The only deviation of these subroutines from their previously described functions occurs in ZMASS: since the mixture ratio distribution is collapsed to a flat profile, it omits reference to Subroutine CALCBC.

This concludes the description of the over-all logic structure of Program GASNOX. A modular diagram of GASNOX is provided as Figure 4.
APPENDIX II - COMMON FORTRAN NOMENCLATURE

The following tables contain the COMMON Fortran nomenclature for Program GASNOX. COMMON consists of seven labeled blocks; the nomenclature is arranged in alphabetic order for each block. Singly subscripted arrays are indicated by their respective indices.

I - Element index
J - Incremental station index for the X direction
K - Distribution index

Nomenclature for COMMON/DATA1/

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR(J)</td>
<td>M_{A</td>
<td>x}</td>
<td>Combustor airflow at axial station X</td>
</tr>
<tr>
<td>ATT(I)</td>
<td>T_i</td>
<td>Adiabatic flame temperature for an element i</td>
<td>deg K</td>
</tr>
<tr>
<td>A1</td>
<td>A_1</td>
<td>Exponent in relationship governing collapse of mixture ratio distribution function</td>
<td></td>
</tr>
<tr>
<td>A2</td>
<td>A_2</td>
<td>Factor in relationship defining the rate at which unburned fuel is burned in the intermediate zone</td>
<td></td>
</tr>
<tr>
<td>A3</td>
<td>A_3</td>
<td>Exponent in relationship defining the rate at which unburned fuel is burned in the intermediate zone</td>
<td></td>
</tr>
<tr>
<td>BCON1(I)</td>
<td>(C_{s i})_e</td>
<td>Equilibrium mole fraction of carbon for an element i</td>
<td></td>
</tr>
<tr>
<td>BCON2(I)</td>
<td>(CO_i)_e</td>
<td>Equilibrium mole fraction of carbon monoxide for an element i</td>
<td></td>
</tr>
<tr>
<td>BCON6(I)</td>
<td>(NO_i)_e</td>
<td>Equilibrium mole fraction of nitric oxide for an element i</td>
<td></td>
</tr>
<tr>
<td>BETA</td>
<td></td>
<td>Combustion efficiency in the primary zone</td>
<td></td>
</tr>
<tr>
<td>CH2(I)</td>
<td>(CH_2_i)_e</td>
<td>Equilibrium mole fraction of unburned hydrocarbons exclusive of C(s) and CO for an element i</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------------------------------------------------------------------------------------------</td>
<td>------------</td>
</tr>
<tr>
<td>CK</td>
<td>CN</td>
<td>Mixing characteristic</td>
<td></td>
</tr>
<tr>
<td>CUMDIS(K)</td>
<td></td>
<td>Value of cumulative normal distribution</td>
<td></td>
</tr>
<tr>
<td>EnS</td>
<td>k_s</td>
<td>Fuel-to-air mass ratio at stoichiometric conditions</td>
<td></td>
</tr>
<tr>
<td>EK1(I)</td>
<td>(k_1)</td>
<td>Ratio of forward reaction rate constants (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EK2(I)</td>
<td>(k_2)</td>
<td>Ratio of forward reaction rate constants (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>FF(I)</td>
<td>F_i</td>
<td>Mixture ratio</td>
<td></td>
</tr>
<tr>
<td>FNOXP</td>
<td>(NO_o)</td>
<td>NO formed in the flame front</td>
<td>ppm</td>
</tr>
<tr>
<td>PHIP</td>
<td>(\bar{\phi}_p)</td>
<td>Mean primary zone equivalence ratio accounting for the inefficiency of the primary zone combustion</td>
<td></td>
</tr>
<tr>
<td>PPP</td>
<td>P</td>
<td>Operating pressure</td>
<td>atm</td>
</tr>
<tr>
<td>RHO</td>
<td>(\rho_i)</td>
<td>Density of combustion products for an element</td>
<td>gm/cm^3</td>
</tr>
<tr>
<td>RR(J)</td>
<td>R_x</td>
<td>Radius of combustor liner if canannular configuration; equivalent radius of combustor liner if annular configuration</td>
<td>in; cm</td>
</tr>
<tr>
<td>RI(I)</td>
<td>(R_1)</td>
<td>Forward reaction rate for the first kinetic reaction (see Volume 2, Section 2 or Ref 3)</td>
<td>gm-mole/cm^3 -sec</td>
</tr>
<tr>
<td>R6(I)</td>
<td>(R_6)</td>
<td>Forward reaction rate for the sixth kinetic reaction (see Volume 2, Section 2 or Ref 3)</td>
<td>gm-mole/cm^3 -sec</td>
</tr>
<tr>
<td>S</td>
<td>(S_o)</td>
<td>Degree of mixedness in the primary zone</td>
<td></td>
</tr>
<tr>
<td>VP</td>
<td>(V_p)</td>
<td>Volume of the primary zone</td>
<td>in^3; cm^3</td>
</tr>
<tr>
<td>XEND</td>
<td>X_END</td>
<td>Length of intermediate zone and dilute zone (combined)</td>
<td>in; cm</td>
</tr>
<tr>
<td>XL</td>
<td>(X_L)</td>
<td>Length of intermediate zone</td>
<td>in; cm</td>
</tr>
<tr>
<td>XX(J)</td>
<td>X</td>
<td>Axial position in the combustor</td>
<td>in; cm</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>---------</td>
<td>-----------------------------------------------------------------------------</td>
<td>------------------------</td>
</tr>
<tr>
<td>ZP(K)</td>
<td>z_p</td>
<td>Limit of integration of cumulative normal distribution</td>
<td></td>
</tr>
</tbody>
</table>

**Nomenclature for COMMON/OUT1/**

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVCH2D</td>
<td>$[\text{CH}_2]_e$</td>
<td>Average equilibrium concentration of unburned hydrocarbons exclusive of $C(s)$ and CO at a given axial station in the combustor</td>
<td>gm/cc</td>
</tr>
<tr>
<td>AVCH2F</td>
<td>$[\text{CH}_2]_e$</td>
<td>Average equilibrium concentration of unburned hydrocarbons exclusive of $C(s)$ and CO at a given axial station in the combustor</td>
<td>gm/1000 gm fuel burned</td>
</tr>
<tr>
<td>AVCH2G</td>
<td>$[\text{CH}_2]_e$</td>
<td>Average equilibrium concentration of unburned hydrocarbons exclusive of $C(s)$ and CO at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>AVCH2P</td>
<td>$[\text{CH}_2]_e$</td>
<td>Average equilibrium concentration of unburned hydrocarbons exclusive of $C(s)$ and CO at a given axial station in the combustor</td>
<td>ppm(vol)</td>
</tr>
<tr>
<td>AVECOD</td>
<td>$[\text{CO}]_e$</td>
<td>Average equilibrium concentration of CO at a given axial station in the combustor</td>
<td>gm/cc</td>
</tr>
<tr>
<td>AVECOF</td>
<td>$[\text{CO}]_e$</td>
<td>Average equilibrium concentration of CO at a given axial station in the combustor</td>
<td>gm/1000 gm fuel burned</td>
</tr>
<tr>
<td>AVECOG</td>
<td>$[\text{CO}]_e$</td>
<td>Average equilibrium concentration of CO at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>AVECOP</td>
<td>$[\text{CO}]_e$</td>
<td>Average equilibrium concentration of CO at a given axial station in the combustor</td>
<td>ppm(vol)</td>
</tr>
<tr>
<td>AVECSD</td>
<td>$[\text{C}_s]_e$</td>
<td>Average equilibrium concentration of $C(s)$ at a given axial station in the combustor</td>
<td>gm/cc</td>
</tr>
<tr>
<td>AVECSF</td>
<td>$[\text{C}_s]_e$</td>
<td>Average equilibrium concentration of $C(s)$ at a given axial station in the combustor</td>
<td>gm/1000 gm fuel burned</td>
</tr>
<tr>
<td>AVECSG</td>
<td>$[\text{C}_s]_e$</td>
<td>Average equilibrium concentration of $C(s)$ at a given axial station in the combustor</td>
<td></td>
</tr>
</tbody>
</table>
### Fortran\ Symbol | Symbol | Description | Units
--- | --- | --- | ---
AVECSP | $T_{\text{eq}}$ | Average equilibrium concentration of $C_s$ at a given axial station in the combustor | ppm(vol)

### Nomenclature for COMMON/OUT2/

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVENFU</td>
<td>$\bar{\text{NO}}_{\text{up}}$</td>
<td>Average nitric oxide concentration at prior axial station in the combustor</td>
<td>g/1000 gm fuel burned</td>
</tr>
<tr>
<td>AVENOD</td>
<td>$\bar{\text{NO}}$</td>
<td>Average nitric oxide concentration at a given axial station in the combustor</td>
<td>g/cc</td>
</tr>
<tr>
<td>AVENOF</td>
<td>$\bar{\text{NO}}$</td>
<td>Average nitric oxide concentration at a given axial station in the combustor</td>
<td>g/1000 gm fuel burned</td>
</tr>
<tr>
<td>AVENOOG</td>
<td>$\bar{\text{NO}}$</td>
<td>Average nitric oxide concentration at a given axial station in the combustor</td>
<td>ppm(vol)</td>
</tr>
<tr>
<td>ILAST</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$ILAST = 0$ if the nitric oxide chemical reaction is not frozen at a given axial position in the combustor</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$ILAST = 1$ if the nitric oxide chemical reaction is frozen at a given axial position in the combustor</td>
<td></td>
</tr>
<tr>
<td>RRO</td>
<td>$(\rho)^r$</td>
<td>Mean density of combustion products at a given axial station in the combustor</td>
<td>g/cc</td>
</tr>
</tbody>
</table>

### Nomenclature for COMMON/OUT3/

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVET</td>
<td>$ar{\tau}$</td>
<td>Average temperature of combustion products at a given axial station in the combustor</td>
<td>$\deg$ K</td>
</tr>
<tr>
<td>FBARD</td>
<td>$\bar{\tau}$</td>
<td>Mean mixture ratio at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>IMAX</td>
<td>$i_{\text{MAX}}$</td>
<td>Subscript of mass element with highest equivalence ratio</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>INDIC</td>
<td>I</td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>INDIC = 1 for primary zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>INDIC = 2 for intermediate zone type calculation</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>INDIC = 3 for dilution zone type calculation</td>
<td></td>
</tr>
<tr>
<td>LEN</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LEN = 0 if intermediate zone calculations end at ( X_L )</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LEN = 1 if intermediate zone calculations end at ( X_{END} )</td>
<td></td>
</tr>
<tr>
<td>NO(i)</td>
<td>( [NO_i] )</td>
<td>Nitric oxide concentration for an element ( i ) of the distribution function</td>
<td></td>
</tr>
<tr>
<td>PHIBAR</td>
<td>( \phi )</td>
<td>Mean equivalence ratio at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>RHCBAR</td>
<td>( \rho )</td>
<td>Mean density of combustion products at a given axial station in the combustor</td>
<td>( \text{g/m}^3 )</td>
</tr>
<tr>
<td>TAUBAR</td>
<td>( \tau_i )</td>
<td>Mean residence time in the combustor at a given axial station</td>
<td>( \text{sec} )</td>
</tr>
<tr>
<td>TAUDIL</td>
<td>( \tau_{dil} )</td>
<td>Mean residence time in the combustor dilution zone</td>
<td>( \text{sec} )</td>
</tr>
<tr>
<td>TAUINT</td>
<td>( \tau_{int} )</td>
<td>Mean residence time in the combustor intermediate zone</td>
<td>( \text{sec} )</td>
</tr>
<tr>
<td>VELOC</td>
<td>V</td>
<td>Velocity of combustion products at a given axial station in the combustor</td>
<td>( \text{cm/sec} )</td>
</tr>
<tr>
<td>XD</td>
<td>( X_D )</td>
<td>Axial position (downstream) in the combustor</td>
<td>( \text{cm} )</td>
</tr>
<tr>
<td>XU</td>
<td>( X_U )</td>
<td>Axial position (upstream) in the combustor</td>
<td>( \text{cm} )</td>
</tr>
</tbody>
</table>

For common output:

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIRD</td>
<td>( M_A X_D )</td>
<td>Airflow at a given axial station in the combustor</td>
<td>( \text{g/m}^3 )</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>---------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-----------</td>
</tr>
<tr>
<td>ANO</td>
<td>$\bar{\text{NO}}_{\text{AN}}$</td>
<td>Average nitric oxide concentration at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>AQQ</td>
<td>Q</td>
<td>Measure of the round-off error in the Runge-Kutta integration routine at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>AREAD</td>
<td>$A_{x_D}$</td>
<td>Cross-sectional area of combustor at a given axial station in the combustor</td>
<td>$\text{cm}^2$</td>
</tr>
<tr>
<td>ASLOPE</td>
<td>$\left(\frac{\delta M_i}{\delta x}\right)_{x_D}$</td>
<td>Rate of change of airflow rate in the combustor liner with axial position at a given axial station in the combustor</td>
<td>$\text{gm/sec-cm}$</td>
</tr>
<tr>
<td>AVEMW</td>
<td>$\bar{m}_W$</td>
<td>Average molecular weight of reaction products at a given axial station in the combustor</td>
<td>$\text{gm/gm-mole}$</td>
</tr>
<tr>
<td>CONSN0(1)</td>
<td>$\left[\text{NO}^*_{i_e}\right]$</td>
<td>Nitric oxide equilibrium concentration for an element i of the distribution function</td>
<td></td>
</tr>
<tr>
<td>DDM(1)</td>
<td>$(\delta M_i)_D$</td>
<td>Elemental mass flow rate at the downstream limit of integration</td>
<td>$\text{gm/sec}$</td>
</tr>
<tr>
<td>DELMD(1)</td>
<td>$(\Delta M_i)_D$</td>
<td>Elemental mass flow rate at the downstream limit of integration</td>
<td>$\text{gm/sec}$</td>
</tr>
<tr>
<td>DIFNO(1)</td>
<td></td>
<td>Difference in NO concentrations for successive iterations for an element i of the distribution function</td>
<td></td>
</tr>
<tr>
<td>DMDDA(1)</td>
<td>$(\delta m_A)_{i}$</td>
<td>Elemental mass flow of gases into control volume due to mixing of the dilution air with previously mixed gases</td>
<td>$\text{gm/sec-cm}$</td>
</tr>
<tr>
<td>DMDDM(1)</td>
<td>$(\delta m_M)_{i}$</td>
<td>Elemental mass flow of gases into control volume due to mixing action of gases already within the combustion liner</td>
<td>$\text{gm/sec-cm}$</td>
</tr>
<tr>
<td>DMDDP(1)</td>
<td>$(\delta m')_{i}$</td>
<td>Total elemental mass flow of gases into control volume due to mixing</td>
<td>$\text{gm/sec-cm}$</td>
</tr>
<tr>
<td>DMDDPP(1)</td>
<td>$(\delta m'')_{i}$</td>
<td>Total elemental mass flow of gases out of control volume due to mixing</td>
<td>$\text{gm/sec-cm}$</td>
</tr>
<tr>
<td>DMFFED</td>
<td>$(\bar{M}<em>f)</em>{\text{fed}}$</td>
<td>Total mass flow of fuel fed to the combustor</td>
<td>$\text{gm/sec}$</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
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<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>DMFT</td>
<td>$(M_f)_X_D$</td>
<td>Total mass flow of combusted fuel at a given axial station in the combustor</td>
<td>gm/sec</td>
</tr>
<tr>
<td>DMFUD</td>
<td>$(M_{fu})_X_D$</td>
<td>Total mass flow of unburned fuel at a given axial station in the combustor</td>
<td>gm/sec</td>
</tr>
<tr>
<td>DMFUO</td>
<td>$(M_f)_o$</td>
<td>Total mass flow of unburned fuel at the primary zone exit</td>
<td>gm/sec</td>
</tr>
<tr>
<td>E(1)</td>
<td>$E_i$</td>
<td>Proportionality factor between mass flow rate out of an element $i$ due to mixing and the total mass flowing into it</td>
<td>cm$^{-1}$</td>
</tr>
<tr>
<td>EKKD</td>
<td>$K_D$</td>
<td>Proportionality factor between mass flow rate out of an element due to mixing and the total mass flowing into it</td>
<td>cm$^{-1}$</td>
</tr>
<tr>
<td>FB(1)</td>
<td>$(F_B)_i$</td>
<td>Boundaries between which each mixture ratio value applies</td>
<td></td>
</tr>
<tr>
<td>FPRIME(1)</td>
<td>$(F')_i$</td>
<td>Mixture ratio at entrance to elemental control volume $i$</td>
<td></td>
</tr>
<tr>
<td>NOEQXD</td>
<td>$[NO]_{e,X_D}$</td>
<td>Mass average nitric oxide equilibrium concentration at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>NOP(1)</td>
<td>$[NO]_{i}$</td>
<td>Nitric oxide concentration of the mass flowing into an elemental control volume due to mixing at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>NOZERO(1)</td>
<td>Indicator</td>
<td>NOZERO = 0 if chemical rate of production of NO in an element $i$ is finite NOZERO = 1 if chemical rate of product of NO in an element is zero</td>
<td></td>
</tr>
<tr>
<td>RDOT(1)</td>
<td>$R_i$</td>
<td>Elemental rate of change of unburned fuel with axial station in the combustor</td>
<td>gm/sec-cm</td>
</tr>
<tr>
<td>RSUBX</td>
<td>$R_X_D$</td>
<td>Combustor radius at a given axial station in the combustor</td>
<td>cm</td>
</tr>
<tr>
<td>SIG</td>
<td>$\sigma$</td>
<td>Standard deviation of the distribution function at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>SIGZER</td>
<td>$\sigma_o$</td>
<td>Standard deviation of the distribution function in the primary zone of the combustor</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>----------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>SLOPE(I)</td>
<td>[\frac{\partial (\tilde{m}_i)}{\partial x}]</td>
<td>Rate of change of elemental mass flow rate with axial position at a given axial station in the combustor</td>
<td>gm/sec-cm</td>
</tr>
<tr>
<td>SUEA(I)</td>
<td></td>
<td>Difference in NO concentrations for successive iterations for an element i of the distribution function</td>
<td></td>
</tr>
<tr>
<td>TSLOPE</td>
<td>[\frac{\partial m^\ast}{\partial x}]</td>
<td>Rate of change of total mass flow rate with axial position at a given axial station in the combustor</td>
<td>gm/sec-cm</td>
</tr>
<tr>
<td>UDM(I)</td>
<td>(\tilde{m}_i)</td>
<td>Elemental mass flow rate at the upstream limit of integration</td>
<td>gm/sec</td>
</tr>
</tbody>
</table>

**Nomenclature for COMMON /OUT5/**

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>MSTARD</td>
<td>(M^\ast)</td>
<td>Total mass flow at downstream limit of integration</td>
<td>gm/sec</td>
</tr>
<tr>
<td>MSTARU</td>
<td>(M^\ast)</td>
<td>Total mass flow at upstream limit of integration</td>
<td>gm/sec</td>
</tr>
<tr>
<td>DILL</td>
<td>(\tilde{r})</td>
<td>Rate of change of NO concentration with axial position in the combustor dilution zone due to air dilution</td>
<td>cm(^{-1})</td>
</tr>
<tr>
<td>REAT</td>
<td>(\tilde{r})</td>
<td>Rate of change of elemental NO concentration with axial position in the combustor due to chemical reaction</td>
<td>cm(^{-1})</td>
</tr>
</tbody>
</table>
APPENDIX III - MAIN ROUTINE GASNOX

The principal function of the main routine is to control the logic of the calculation procedure for the prediction of the nitric oxide emissions from gas turbine combustors. In addition, the main routine reads and writes the input data, sets certain values, and performs many related minor calculations.

The main routine calls Subroutines PRIMRY, ZINTER, and DILUTE.

The external input required by the main routine consists of:

- ANNRI
- ANRI
- APR
- ARR
- ATTI
- AXI
- BCON1
- BCON2
- BCON6
- BETAI
- CH2
- EKS
- EK1
- EK2
- EQUIVI
- ERI
- FF
- IDATAI
- IN
- KASEI
- PHII
- HIP
- PPP
- RH0
- RI
- R6
- SI
- SET
- TAUBARI
- TOTAIRI
- VP
- XENDI
- XLI
- ZPI

The external output provided by the main routine consists of:

- ANNRI
- ANRI
- APR
- ARR
- ATTI
- AXI
- BCON1
- BCON2
- BCON6
- BETAI
- CH2
- CUMDIS
- EKS
- EK1
- EK2
- EQUIVI
- ERATI
- FF
- NOZEROI
- PHI
- HIP
- PPP
- RH0
- RI
- R6
- SI
- SET
- TAUBARI
- TOTAIRI
- XENDI

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in the main routine which are not part of COMMON. Singly and doubly subscripted arrays are indicated by their respective indices:

- I - General index of descriptive data
- IJ - Incremental axial station index for combustor air
- J - Element index
<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AAR(IJ)</td>
<td>$(M_A)_X$</td>
<td>Total mass of airflow into combustor liner at position $X$ (cumulative)</td>
<td>lb/sec</td>
</tr>
<tr>
<td>ANNR(IJ)</td>
<td>$R_{X_0}$</td>
<td>Outer radius of liner at position $X$; applies only for annular configuration</td>
<td>in</td>
</tr>
<tr>
<td>AWR(IJ)</td>
<td>$R_{X_1}$</td>
<td>Inner radius of liner at position $X$; applies only for annular configuration</td>
<td>in</td>
</tr>
<tr>
<td>APR(IJ)</td>
<td>$(M_A)_X$</td>
<td>Per cent of total mass of airflow into combustor liner at position $X$ (cumulative)</td>
<td></td>
</tr>
<tr>
<td>ARR(IJ)</td>
<td>$R_X$</td>
<td>Radius of liner at position $X$; applies only for canannular configuration</td>
<td>in</td>
</tr>
<tr>
<td>A:X</td>
<td>$X$</td>
<td>Axial position in the combustor</td>
<td>in</td>
</tr>
<tr>
<td>DELAIR</td>
<td>$\Delta M_{AIR}$</td>
<td>Combustor air scaling factor</td>
<td>lb/sec</td>
</tr>
<tr>
<td>DEX</td>
<td>$\Delta X$</td>
<td>Combustor length</td>
<td>in</td>
</tr>
<tr>
<td>EQUIV</td>
<td>$\phi_p$</td>
<td>Mass mean equivalence ratio in the primary zone (before fuel burns)</td>
<td></td>
</tr>
<tr>
<td>ERAT</td>
<td>$E_{rat}$</td>
<td>Variable for varying $\phi_p$ parametrically yet maintaining constant air-to-fuel ratio in the combustor</td>
<td></td>
</tr>
<tr>
<td>IDATA</td>
<td></td>
<td>Number of sets of kinetic, thermodynamic, and equilibrium data and combustor inlet conditions</td>
<td></td>
</tr>
<tr>
<td>IN</td>
<td></td>
<td>Number of sets of combustor dimensions, operating conditions, and primary zone mixedness parameter</td>
<td></td>
</tr>
<tr>
<td>KASE</td>
<td></td>
<td>Number of sets of airflow distribution data</td>
<td></td>
</tr>
<tr>
<td>PHI(J)</td>
<td>$\phi_j$</td>
<td>Equivalence ratio of an element $j$</td>
<td></td>
</tr>
<tr>
<td>SET(I)</td>
<td></td>
<td>Combustor descriptive data</td>
<td></td>
</tr>
<tr>
<td>TOTAIR</td>
<td>$M_A$</td>
<td>Total mass of air fed into the combustor liner</td>
<td>lb/sec</td>
</tr>
</tbody>
</table>
Analysis Procedure

The step-by-step procedure of the main routine is given below. The Fortran listing of the routine is presented at the conclusion of the step-by-step procedure.

1. Read the input kinetic, thermodynamic, and equilibrium data and the combustor inlet conditions for the case.

2. Set the values of certain parameters.

3. Read the input airflow distribution data.

Step 4 is performed only if the combustor is an annular configuration.

4. Calculate the equivalent can radii as:
   \[ R_x = \left[ (R_x)^2 - (R_x')^2 \right]^{1/2} \]

5. Read the input combustor dimensions, operating conditions, and primary zone mixing parameter.

6. Convert the percentage airflow data to mass flow for each specified axial station by the relationship:
   \[ (\dot{m}_A)_x = (\dot{m}_A)_x^* M_A / 100.0 \]

7. Calculate \( \overline{\varphi}_p \) as
   \[ \overline{\varphi}_p = \varphi_p * \bar{\varphi} \]

8. Calculate \( \overline{\varphi}_p \) as:
   \[ \overline{\varphi}_p = \overline{\varphi}_p * E_{rat} \]

9. Set the values of certain parameters and constants.

10. Write the heading for the airflow distribution data for the case.

11. Calculate the total mass of airflow into the combustor liner for each specified axial station correcting for the effect of \( E_{rat} \).

12. Convert the units of the airflow distribution data to the metric system.

13. Write the input data.

14. Convert the units of the combustor dimensions to the metric system.

15. Using Subroutine PRIMARY, calculate the primary zone exit conditions.
16. Set certain indicators.
Step 17 is performed only if $X_{END} = 0$.
17. Go to step 24.
Step 18 is performed only if $S_0 = 0$.
18. Go to step 23.
19. If $X_{END} < X_L$, reset certain indicators.
20. Using Subroutine ZINTER, perform the intermediate zone calculations.
Step 21 is performed only if the chemical rate of formation of nitric oxide is frozen in the intermediate zone.
21. Go to step 23.
Step 22 is performed only if $X_{END} < X_L$.
22. Go to step 24.
23. Using Subroutine DILUTE, perform the dilution zone calculations.
24. If this is the last set of combustor dimensions, operating conditions, and primary zone mixing parameter for the given airflow distribution, continue to step 25. If not, return to step 5.
25. If this is the last set of combustor airflow distribution data for the given kinetic, thermodynamic, and equilibrium data and combustor inlet conditions, continue to step 26. If not, return to step 3.
26. If this is the last set of kinetic, thermodynamic, and equilibrium data and combustor inlet conditions, continue to step 27. If not, return to step 1.
27. Stop.
PROGRAM GASNOX (INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT)
DIMENSION SET(25), PHI(50), AAR(50), AXX(50), APR(50), ARR(50), ANR(50)
1, ANN(50)
COMMON/DATA1/AIR(50), RR(50), XX(50), FF(50), BCON1(50), BCON2(50), CH2(50)
150, ZP(70), CUMDIS(70), VP, RH(50), BCON6(50), ATT(50), PPP, FN0XP, R1(50)
20, R6(50), EK1(50), EK2(50), A2, A3, XL, CN, BETA, S, PHIP, EKS, XEND, A1
COMMON/OUT1/AVECSG, AVECOG, AVECH2G, AVECSP, AVECO, AVECH2P, AVECSD, AVECOG9, SAS*0060
10, AVCH2D, AVECSF, AVECOF, AVCH2F
COMMON/OOUT/AVENOG, AVEXOF, AVEXOF, AVEFNU, RR0, ILAST
COMMON/OOUT/INDIC1, NO(50), AGET TANBAR, ROBAR, PHPAB, IMEX, XD
1, FBARU, XI, LEN, TAI, INT, TAUIDL, VELOC
COMMON/OOUT/CONCNO(50), DELXD(50), AREAD, ASLOPE, DHFUD, SLOPE (50), TSLLOGA9, 110
1, PENVUP(50), EK0, DMFTU, UMN(50), DDH(50), FP(50), DMFUD, AIRD, DMFDDG, SAS*0120
2, RSHX, SIG, SIGZER, AVEMW, DMODA(50), DMMDM(50), DMDP(50), DMDPP(50), FSA9, 0130
3, PRIME(50), NOE0XD, ANO, A00, DFIIO(50), NOZERO(50), ROOT(50), E(50)
GAS*0140
COMMON/OOUT/IOCT, MSTAR, DOUT5/TAPE5=NNOUTTAPE6=DLJTPUT) GAS*0000
DATA (L) = 170.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
15.0, 50.0, 60.0, 65.0, 70.0, 75.0, 80.0, 85.0, 90.0, 95.0, 105.1, 110.0, GAS*0170
21, 15.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0, 50.0, 55.0, 60.0, 65.0, 70.0, 75.0, 13.5
3.0, 80.0, 85.0, 90.0, 95.0, 100.0, 105.0, 110.0, 115.0, 120.0, 125.0, 130.0, 135.0, 140.0
445.2, 50, 2.0, 2.0, 2.2, 2.0, 2.2, 2.0, 2.2, 2.0, 2.2, 2.0, 2.2, 2.0, 2.2, 2.0
50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0
50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0, 50.0
GAS*0200
DATA (CUMDISI(1)) = 170.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
1.6x7.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
23.4, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
30.8, 94.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0
45.4, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
5.9, 96.0, 97.0, 98.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0
60.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0
70.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0, 99.0
GAS*0220
C**** READ IN AND WRITE OUT THE REQUIRED DATA
GAS*0300
C****
READ(5, 50) IDATA
GAS*0320
DO 925 IIK = 1, IDATA
GAS*0330
READ(5, 400) (SET(I); I=1,15) + PPP, SET(16) + SET(17) + SET(18) + SET(19) + EK5 + GAS*0350
400 FORMAT(12A6/2A61A2, El5.8, 3A6, A4, E15.8)
GAS*0360
DO 940 J = 1, 35
GAS*0370
READ(5, 450) FF(J), PH(J), RH0(J), ATT(J), BCON6(J), BCON2(J), BCON1(J), C5 + GAS*0390
450 FORMAT(12A6/2A61A2, El5.8, 3A6, A4, E15.8)
GAS*0370
1M2(J), R1(J), R6(J), EK1(J), EK2(J)
GAS*0390
NOZERO(J) = 0
GAS*0400
IF (HO(J) = EQ, 0.0, AND, R1(J), EQ, 0.0) NOZERO(J) = 1
GAS*0410
600 CONTINUE
GAS*0420
450 FORMAT(6E12.5)
GAS*0430
READ(5, 50) KASE
GAS*0440
50 FORMAT(16)
GAS*0450
DO 990 II = 1, KASE
GAS*0460
DO 300 IJ = 1, 11
GAS*0470
READ(5, 250) AXX(J), APR(J), ARR(J), ANR(J), ANR(1J)
GAS*0480
250 FORMAT(16)
GAS*0490
XX(J) = AXX(J)
GAS*0500
RR(J) = ARR(J)
GAS*0510
IF (RR(J) = EQ, 0.0, RR(J) = SQRT(ANNR(J)**2.0 - ANR(J)**2.0)
GAS*0510
300 CONTINUE
GAS*0520
250 FORMAT(5E12.5)
GAS*0530
READ(5, 260) IN
GAS*0540
200 FORMAT(16)
GAS*0550
DO 325 K = 1, IN
GAS*0560
READ(5, 410) VP, XL, XEND, EQUIV, BETA, TOTAIR, S, ERAT, TAUBAR
GAS*0570
DO 425 IJ = 1, 11
GAS*0580
AAR(J) = APR(J)**TAUBAR/100.0
GAS*0590
425 CONTINUE
PHIP = EQUIV*BETA
PHIP=PHIP*ERAT
FNXP = 0.0
CN = 5.0
A1 = 0.5
A2 = 0.5
A3 = 1.0
410 FORMAT(6E12.5/6E12.5)
DELAIL=AAR(IJ)*[1.0-1.0/ERAT]
DEX=XX(11)-XX(1)
WRITE(6,100)
WRITE(6,775)
775 FORMAT(///49X,34HCORBUSTOR AIR FLOW CHARACTERISTICS///)
WRITE(6,780)
780 FORMAT(64X,3HCAN,21X,7HANNULAR)
WRITE(6,785)
785 FORMAT(28X,BHDISTANCE,8X,10PERCENTAGE,9X,6HRADIUS,8X,12HINNER RAD
11US,5X,12HOUTER RADIUS)
786 FORMAT(45X,BHAIR FLOW)
WRITE(6,786)
WRITE(6,790)
790 FORMAT(29X,6HINCHES,28X,6HINCHES,11X,6HINCHES,11X,6HINCHES///)
DO 350 IJ=1,11
AIR(IJ)=AAR(IJ)*DELAIL*(XX(11)-XX(IJ))/DEX
WRITE(6,825) AXX(IJ),APR(IJ),ARR(IJ),ANR(IJ)
825 FORMAT(26X,5(E12.5/5X))
AIR(IJ) = AIR(IJ)*D454
IF(K*GT.1) GO TO 350
XX(IJ) = XX(IJ)*2.54
RR(IJ) = RR(IJ)*2.54
350 CONTINUE
WRITE(6,500) K
500 FORMAT(///5X~11HCASE NO. = I6///)
WRITE(6,550)
550 FORMAT(///48X,35HCUMULATIVE NORMAL DISTRIBUTION DATA///)
WRITE(6,615)
615 FORMAT(14X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS///)
15S,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS///)
2HZP,3X,6HCUMDIS///)
DO 120 L=1,10
WRITE(6,110) ZP(L),CUMDIS(L),ZP(L+10),CUMDIS(L+10),ZP(L+20),CUMDIS(L+20),CUMDIS(L+30),ZP(L+30)
10,CUMDIS(L+30),ZP(L+40),CUMDIS(L+40),ZP(L+50),CUMDIS(L+50)
2(L+50),ZP(L+60),CUMDIS(L+60)
110 FORMAT(///5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS,5X,2HZP,3X,6HCUMDIS///)
2HZP,3X,6HCUMDIS///)
DO 120 CONTINUE
WRITE(6,610)
WRITE(6,650)
650 FORMAT(///58X,16MEQUIVLIBRIUM DATA///)
WRITE(6,675) (SET(I),I=1,15),PPP,SET(16),SET(17),SET(18),SET(19),EGAS
15
675 FORMAT(1X,14A6,A2,E15.8/33X,3A6,A4,E15.8///)
WRITE(6,680)
680 FORMAT(1A,123THE FOLLOWING DATA TABLE CONTAINS THE THERMODYNAMIC GAS
PROPERTIES,KINETIC RATE CONSTANTS, AND EQUILIBRIUM COMPOSITIONS FOR GAS
2 EACH ELEMENT THESE GAS PROPERTIES ARE IN ORDER OF PRINTING MIXTURE RATIO AND EQUILIBRIUM GAS
4AT10/1X,11H10,ADIA10FRATE TEMPERATURE,NO,C0,C(S),AND CHGAS
520UNBURNED HYDROCARBONS) EQUILIBRIUM MOL FRACTION, AND THE KINETIC GAS
67/1X,27H PARAMETERS R1, R2, K1, AND K2///)
WRITE(6,690)
DO 756 J = 1, 35
    WRITE(6,100) J, JFF(J), PHI(J), RHO(J), ATT(J), BCON1(J), BCON2(J), BCON3(J)
1J)
    CH2(J), R1(J), R6(J), EK1(J), EK2(J)
700 FORMAT(26X, 12, 3X, 6E12.5)
750 CONTINUE
    WRITE(6,100)
    WRITE(6,850)
850 FORMAT(/ //51X, 31HTHE REST OF THE INPUT VARIABLES///)
    WRITE(6,851) VP
851 FORMAT(16X, 67HTHE LENGTH OF THE INTERMEDIATE ZONE IS, E12.5//)
    WRITE(6,852) XL
852 FORMAT(16X, 67HTHE LENGTH OF THE INTERMEDIATE ZONE IS, E12.5//)
    WRITE(6,853) XEND
853 FORMAT(16X, 67HTHE LENGTH OF THE INTERMEDIATE ZONE AND DILUTION ZONE)
1E(COMBINED) IS, E12.5//)
    WRITE(6,854) EQUIV
854 FORMAT(16X, 67HTHE MEAN PRIMARY ZONE EQUIVALENCE RATIO IS, E12.5//)
    WRITE(6,855) BETA
855 FORMAT(16X, 67HTHE COMBUSTION EFFICIENCY IN THE PRIMARY ZONE IS, E12.5//)
12.5//)
    WRITE(6,856) TOTAIR
856 FORMAT(16X, 67HTHE TOTAL MASS OF AIR FED INTO THE COMBUSTOR IS, E12.6//)
1.5, 9H LB/*SEC.//)
    WRITE(6,857) S
857 FORMAT(16X, 67HTHE DEGREE OF MIXEDNESS IS, E12.5//)
    WRITE(6,858) ERAT
858 FORMAT(16X, 67HTHE COMBUSTION EFFICIENCY IN THE PRIMARY ZONE IS, E12.5//)
    WRITE(6,859) TAUBAR
859 FORMAT(16X, 67HTHE MEAN PRIMARY ZONE RESIDENCE TIME (ONLY APPLIES IF)
1E(VOLUME OF THE PRIMARY ZONE IS ZERO IN INPUT) IS, E12.5//)
2C.)
    VP = VP*2.54**2.54*2.54
790 XL = XL*2.54
790 XEND = XEND*2.54
100 FORMAT(1M1)
C**** PERFORM PRIMARY ZONE CALCULATIONS
C**** CALL PRIMRY
C**** PERFORM INTERMEDIATE ZONE CALCULATIONS
C****
LEN = 0
IF(XEND.EQ.0.0) GO TO 1000
IF(S.EQ.0.0) GO TO 950
IF(XEND.LT.XL) LEN = 1
CALL INTER
C****
C**** PERFORM DILUTION ZONE CALCULATIONS
C****
IF(ILAST.EQ.1) GO TO 950
IF(LEN.EQ.1) GO TO 1000
950 CALL DILUTE
1000 CONTINUE
325 CONTINUE
900 CONTINUE
925 CONTINUE
STOP
END
The function of Subroutine PRIMRY is to calculate the nitric oxide emissions at the primary zone exit of a gas turbine combustor.

Subroutine PRIMRY is called by the main routine (GASNOX); it, in turn, calls Subroutines PRCalc, ZMASS, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON. The internal input consists of:

\[
\begin{align*}
\text{ATT} & \quad \text{BCON1} & \quad \text{BCON2} & \quad \text{BCON6} & \quad \text{Ch2} \\
\text{FNOXP} & \quad \text{PHIP} & \quad \text{PPP} & \quad \text{RHO} & \quad \text{S} \\
\text{TAUBAR} & \quad \text{VP} \\
\end{align*}
\]

The internal output consists of:

\[
\begin{align*}
\text{ANO} & \quad \text{AVCH2A} & \quad \text{AVCH2B} & \quad \text{AVCH2C} & \quad \text{AVCH2P} \\
\text{AVECOD} & \quad \text{AVECOF} & \quad \text{AVECOG} & \quad \text{AVECOP} & \quad \text{AVECSD} \\
\text{AVECSF} & \quad \text{AVECSG} & \quad \text{AVECSP} & \quad \text{AVEWS} & \quad \text{AVENO} \\
\text{AVENOF} & \quad \text{AVENOG} & \quad \text{AVENOP} & \quad \text{AVET} & \quad \text{CONGNO} \\
\text{FNOXG} & \quad \text{INDIC} & \quad \text{PHIBAR} & \quad \text{RHOBAR} & \quad \text{TAUBAR} \\
\text{VELOC} & \quad \text{XO} & \quad \text{XU} \\
\end{align*}
\]

The external output consists of:

\[
\begin{align*}
\text{FELD} & \quad \text{I} & \quad \text{QQNO} & \quad \text{QSUMNO} \\
\end{align*}
\]

**Additional Fortran Nomenclature**

The following table gives the Fortran nomenclature for those symbols used in Subroutine PRIMRY which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH2AV</td>
<td>(\bar{\text{CH}_2})</td>
<td>(e)</td>
<td>Average equilibrium mole fraction of unburned hydrocarbons exclusive of (C) and (CO) in the primary zone</td>
</tr>
<tr>
<td>COAV</td>
<td>(\bar{\text{CO}})</td>
<td>(e)</td>
<td>Average equilibrium mole fraction of (CO) in the primary zone</td>
</tr>
<tr>
<td>CSAV</td>
<td>(\bar{\text{C}}(s))</td>
<td>(e)</td>
<td>Average equilibrium mole fraction of (C) in the primary zone</td>
</tr>
<tr>
<td><strong>Fortran Symbol</strong></td>
<td><strong>Symbol</strong></td>
<td><strong>Description</strong></td>
<td><strong>Units</strong></td>
</tr>
<tr>
<td>------------------</td>
<td>-----------</td>
<td>-----------------</td>
<td>----------</td>
</tr>
<tr>
<td>DELX</td>
<td>$\delta x$</td>
<td>Increment of the combustor length across which the solution is generated</td>
<td>cm</td>
</tr>
<tr>
<td>FELD(1)</td>
<td>$(H_{frac})_i$</td>
<td>Element $i$ mass fraction</td>
<td></td>
</tr>
<tr>
<td>FNOXG</td>
<td>$[NO_o]$</td>
<td>NO formed in the flame front (mass fraction)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$i$</td>
<td>Index of the element</td>
<td></td>
</tr>
<tr>
<td>NPRINT</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NPRINT = 0</td>
<td>if intermediate output is not requested by the user</td>
<td></td>
</tr>
<tr>
<td></td>
<td>NPRINT = 1</td>
<td>if intermediate output is requested by the user</td>
<td></td>
</tr>
<tr>
<td>QNO(I)</td>
<td>$[NO_i]$</td>
<td>Nitric oxide concentration in the element $i$</td>
<td>ppm(vol)</td>
</tr>
<tr>
<td>QSUMND(I)</td>
<td>$\Sigma NO_{-m}$</td>
<td>The cumulative sum of the NO formed up to and including the element $i$</td>
<td>lb/sec</td>
</tr>
<tr>
<td>SUMCHI</td>
<td>$\Sigma CH_{-m}$</td>
<td>Sum of the elemental mass flow rates times their respective unburned hydrocarbon (exclusive of CO and C(s)) equilibrium mole fractions</td>
<td>gm/sec</td>
</tr>
<tr>
<td>SUMCOI</td>
<td>$\Sigma CO_{-m}$</td>
<td>Sum of the elemental mass flow rates times their respective CO equilibrium mole fractions</td>
<td>gm/sec</td>
</tr>
<tr>
<td>SUMCSI</td>
<td>$\Sigma C(s)_{-m}$</td>
<td>Sum of the elemental mass flow rates times their respective C(s) equilibrium mole fractions</td>
<td>gm/sec</td>
</tr>
<tr>
<td>SUMNOI</td>
<td>$\Sigma NO_{-m}$</td>
<td>Sum of the elemental mass flow rates times their respective NO mass fractions</td>
<td>gm/sec</td>
</tr>
<tr>
<td>SUMTI</td>
<td>$\Sigma T_{-m}$</td>
<td>Sum of the elemental mass flow rates times their respective adiabatic flame temperatures</td>
<td>gm-dougl K/sec</td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine PRIMRY is given below.

The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.
1. Convert \([\text{NO} \text{O}]\) to \([\text{NO} \text{O}]\) by 
\[
[\text{NO} \text{O}] = (\text{NO} \text{O}) \times 10^{-6} \times \frac{28.0}{30.0}
\]

2. Set the values of \(X_U, X_D,\) and \(\Delta X\) as:
\[
X_U = 0.0 \\
X_D = 0.0 \\
\Delta X = 0.0
\]

3. Using Subroutine ZMASS, calculate the mass in each element, the mean mixture ratio, the airflow, and the total mass flow.

4. Calculate \(\bar{\rho}\) as:
\[
\bar{\rho} = \frac{\bar{\rho}^{\text{MAX}} \cdot \bar{\rho}^{\text{MIN}}}{\bar{\rho}} \\
\bar{\rho} = \bar{\rho}^{\text{MAX}} \\
\text{Step 5 is performed if } V_p \neq 0.0
\]

5. Go to step 8.

6. Calculate \(V_p\) as:
\[
V_p = \frac{\bar{T} \cdot \bar{M}_{D}^{e}}{\bar{\rho}}
\]


8. Calculate \(\bar{T}\) as:
\[
\bar{T} = \frac{V_p \cdot \bar{\rho}}{\bar{M}_{D}^{e}}
\]

9. Calculate \([\text{NO} \text{O}]\)` as:
\[
[\text{NO} \text{O}] = \frac{\text{NO} \text{O}^{\text{MAX}} \cdot \text{NO} \text{O}^{\text{MIN}}}{\text{NO} \text{O}^{\text{MAX}} \cdot T_{L} \cdot 32.057/P} \\
[\text{NO} \text{O}] = \frac{\text{NO} \text{O}^{\text{MAX}} \cdot 30.0}{\text{NO} \text{O}^{\text{MAX}} \cdot T_{L} \cdot 32.057/P} \\
\text{Step 11 is performed only if intermediate output is requested by the user.}
\]

10. Using Subroutine PRCALC, calculate the NO concentration in each element in the distribution.

11. Write the heading identifying the primary zone-elemental exit conditions.
12. For each element in which \( m_i \) is non-zero, calculate
\[
\begin{align*}
\leq & \ \text{NO}_m, \ \leq & \ \text{C}_m, \ \leq & \ \text{CO}_m, \ \leq & \ \text{CH}_m, \\
\leq & \ \text{T}_m, \ \text{and} \ \left( M_{\text{frac}} \right)_i
\end{align*}
\]

as:
\[
\begin{align*}
\leq & \ \text{NO}_m = \left( \frac{\max}{\sum_{i=1}^{\max} [\text{NO}_i](\Delta M_i)_D} \right) \\
\leq & \ \text{C}_m = \left( \frac{\max}{\sum_{i=1}^{\max} [\text{C}_i](\Delta M_i)_D} \right) \\
\leq & \ \text{CO}_m = \left( \frac{\max}{\sum_{i=1}^{\max} [\text{CO}_i](\Delta M_i)_D} \right) \\
\leq & \ \text{CH}_m = \left( \frac{\max}{\sum_{i=1}^{\max} [\text{CH}_i](\Delta M_i)_D} \right) \\
\leq & \ \text{T}_m = \left( \frac{\max}{\sum_{i=1}^{\max} T_i (\Delta M_i)_D} \right) \\
\end{align*}
\]
\[
\left( M_{\text{frac}} \right)_i = \frac{(\Delta M_i)_D}{M_i^*}
\]

Steps 13-14 are performed only if intermediate output is requested by the user.

13. Convert the units of \( \leq \text{NO}-m \) from \( \text{gm/sec} \) to \( \text{lb/sec} \).

14. Convert the units of \( [\text{NO}_i] \) from mass fraction to \( \text{ppm(vol)} = \frac{\text{gm-mole}}{\text{gm}} \).

15. Calculate \( \bar{[\text{NO}]} \), \( \bar{T} \), and \( \bar{M} \) as:
\[
\begin{align*}
\bar{[\text{NO}]} &= \frac{\leq \text{NO}_m}{m_i^*} \\
\bar{T} &= \frac{\leq \text{T}_m}{m_i^*} \\
\bar{M} &= \bar{\sigma} * \bar{T} * 82.057 / \rho
\end{align*}
\]

Steps 16-17 are performed only if intermediate output is requested by the user.

16. Convert the units of \( [\text{NO}_i] \) from \( \text{ppm(vol)} \) to \( \text{ppm(vol)} \).

17. For each element in the distribution, write the element mass fraction, the nitric oxide concentration (ppm-vol),
the cumulative sum of the NO formed up to and including the element, and the element number.

18. Calculate \( \overline{\phi} \) as

\[
\overline{\phi} = \overline{\phi}_p
\]

19. Calculate \( V \) as

\[
V = \frac{M_D^*}{\overline{\rho}^* A} x_D
\]

20. Calculate \( [\overline{\text{NO}_3}], [\overline{\text{NO}_2}], [\overline{\text{NO}^*}] \) as:

\[
[\overline{\text{NO}_3}] = [\overline{\text{NO}_2}] \times 10^6 \times \overline{MW} / 30.0
\]

\[
[\overline{\text{NO}^*}] = [\overline{\text{NO}_2}] \times \overline{\rho}
\]

\[
[\overline{\text{NO}_2}] = [\overline{\text{NO}_2}] \times M_D^* \times 1000 / (\dot{m}_f) x_D
\]

21. Calculate \( (\overline{\text{C}_2})_e, (\overline{\text{CO}})_e, \text{ and } (\overline{\text{CH}_2})_e \) as:

\[
(\overline{\text{C}_2})_e = \frac{\leq C_{(s)} - m}{M_{D}^*}
\]

\[
(\overline{\text{CO}})_e = \frac{\leq CO - m}{M_{D}^*}
\]

\[
(\overline{\text{CH}_2})_e = \frac{\leq CH_2 - m}{M_{D}^*}
\]

22. Calculate \( [\overline{\text{C}_2}]_e, [\overline{\text{CO}}]_e, \text{ and } [\overline{\text{CH}_2}]_e \) as:

\[
[\overline{\text{C}_2}]_e = (\overline{\text{C}_2})_e \times 12 / \overline{MW}
\]

\[
[\overline{\text{CO}}]_e = (\overline{\text{CO}})_e \times 28 / \overline{MW}
\]

\[
[\overline{\text{CH}_2}]_e = (\overline{\text{CH}_2})_e \times 14 / \overline{MW}
\]

23. Calculate \( \{\overline{\text{C}_2}\}_e, \{\overline{\text{CO}}\}_e, \text{ and } \{\overline{\text{CH}_2}\}_e \) as:

\[
\{\overline{\text{C}_2}\}_e = [\overline{\text{C}_2}]_e \times 10^6 \times \overline{MW} / 12
\]

\[
\{\overline{\text{CO}}\}_e = [\overline{\text{CO}}]_e \times 10^6 \times \overline{MW} / 28
\]

\[
\{\overline{\text{CH}_2}\}_e = [\overline{\text{CH}_2}]_e \times 10^6 \times \overline{MW} / 14
\]
24. Calculate $[\tilde{C}(s)]_e^*$, $[\tilde{CO}]_e$, and $[\tilde{CH}_2]_e^*$ as:

$$
[\tilde{C}(s)]_e^* = [\tilde{C}(s)]_e^* \cdot \bar{g}
$$

$$
[\tilde{CO}]_e = [\tilde{CO}]_e^* \cdot \bar{g}
$$

$$
[\tilde{CH}_2]_e^* = [\tilde{CH}_2]_e^* \cdot \bar{g}
$$

25. Calculate $[\tilde{C}(s)]_e^*$, $[\tilde{CO}]_e$, and $[\tilde{CH}_2]_e^*$ as:

$$
[\tilde{C}(s)]_e^* = [\tilde{C}(s)]_e^* \cdot m_D^* \cdot 1000 / (M_F)_{QP}
$$

$$
[\tilde{CO}]_e = [\tilde{CO}]_e^* \cdot m_D^* \cdot 1000 / (M_F)_{QP}
$$

$$
[\tilde{CH}_2]_e^* = [\tilde{CH}_2]_e^* \cdot m_D^* \cdot 1000 / (M_F)_{QP}
$$

26. Using Subroutine PRINTS, write the output for the primary zone.

27. Return.
SUBROUTINE PRI*0000
REAL NO
REAL MSTAR0,MSTARU
DIMENSION QO(N0(50)),OSUMNO(50),FELD(50)
COMMON/OUT1/AVECG,AVECG,AVECS,AVECSP,AVECOP,AVECH2P,AVECSD,AVECOPRI*0070
10,AVCH20,AVECSF,AVECOF,AVECH2F
COMMON/OUT2/AVENOG,AVENOA,AVECOP,AVENOJ,ARRHOF,RTLAST
COMMON/OUT3/INDICNO(N0),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD
1FBARD,XU*1,LEN,TAUDINT,TAUDIL,VELOC
COMMON/OUT4/CONGNO(N0),DELM0(N0),AREAD,ASLOPE,DMFU0,SLOPE(50),TSLOPR
1PE-NOP(50),EKD0,UDMA,DDM(50),S50,DMFU,DMFUD,FB(50),DMFD,DMFEDPR
2,RHUBAR+SIG,STGZER,AVEM,DMDDA(50),DMDDM(50),DMDDP(50),DMDDDPR(N0),FPR
3PRI*0140
COMMON/OUT5/MSTARD,MSTARU
NPHIN=1
INDIC = 1
C**** CONVFRATE FLAME NO UNITS (NOTE MEAN MW TAKEN AS 28.0)
C**** FNOXG=FNOX*1.0E-Q6*(30.0/28.0)
C**** CALCULATE MASS IN EACH ELEMENT
C**** XU = 0.0
C**** XD = 0.0
C**** DELX = 0.0
C**** CALL ZMASS(DELX)
WRITE(6,100)
C**** CALCULATE AVERAGE RHO AND TAU
C**** RHUBAR = 0.0
C**** DO 1000 I = 1,IMAX
C**** IF(S*EQ.0.0.AND.I.LT.IMAX) GO TO 1000
C**** RHOBAR = RHOBAR+RHO(I)*DELW(I)/MSTARD
C**** CONTINUE
C**** IF(VP*NE.0.0) GO TO 1025
C**** VP=TAUBAR*MSTARD/RHOBAR
C**** GO TO 1050
C**** TAUBAR=(VP*RHOBAR/MSTARD)
C**** CONTINUE
C**** DO NO CALCULATIONS
C**** SUMNOI = 0.0
C**** SUMTI = 0.0
C**** SUMCSI = 0.0
C**** SUMCOI = 0.0
C**** SUMCM1 = 0.0
C**** DO 2000 I = 1,IMAX
C**** IF(S*EQ.0.0.AND.I.LT.IMAX) GO TO 2000
C**** CONGNI = 5*CON6(I)*30.0/(RHO(I)*ATT(I)*82.057/PPP)
C**** CONTINUE
C**** CALL PRCALC(FNOXG)
C**** IF(NPRINT.EQ.0) GO TO 2500
C**** WRITE(6,9987)
9987 FORMAT(///,52X,28HPRI*0000,ZONE EXIT CONDITIONS)
WRITE(6,9988)
9988 FORMAT(///,46X,4KMASS,9X,2HNO,8X,8HTOTAL NO,7X,7HELEMENT)
WRITE(6,9989)
9989 FORMAT(44X,8HFRACTION,5X,8HPPM(VOL),5X,6HLB/SEC,10X,3HNO,///)
2500 CONTINUE
DO 3000 I = 1,IMAX
IF(DELMD(I).EQ.0.0) GO TO 3000
SUMNOI = SUMNOI+NO(I)*DELM(DI)
SUMCSI = SUMCSI+BCON1(I)*DELM(DI)
SUMCOI = SUMCOI +BCON2(I)*DELM(DI)
SUMCH1 = SUMCH1+CH2(I)*DELM(DI)
SUMTI = SUMTI+ATT(I)*DELM(DI)
FELD(I) = DELMD(I)/MSTARD
IF(NPRINT.EQ.0) GO TO 3000
QSUMNO(I) = SUMNOI/454*0
QQNO(I) = QQNO(+3E+06/30.0)
WRITE(6,9990) FELD(I),QQNO(I),QSUMNO(I),I
9990 FORMAT(42X#3E12*597X9I3)
3000 CONTINUE
DO 3200 I = 1,IMAX
QQNO(I) = QQNO(I)*AVEMW
3200 CONTINUE
CALL PRINTS
100 FORMAT(1H1)
RETURN
END
APPENDIX V - SUBROUTINE ZINTER

The function of Subroutine ZINTER is to calculate the concentration of nitric oxide at specified axial stations, and at the exit, of the intermediate zone of a gas turbine combustor.

Subroutine ZINTER is called by the main routine (GASNGL): it, in turn, calls Subroutines MINT, CHECKK, RUNKUT, ZMASS, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON.

The internal input consists of:

- ATT
- BCON1
- BCON2
- BCON6
- CH2
- CN
- CONGNO
- EKS
- EK1
- EK2
- FF
- LEN
- NO
- NOZERO
- PPP
- RHO
- RSUBX
- R1
- R6
- TAUBAR
- XD
- XEND
- XL

The internal output consists of:

- ANO
- AQQ
- AVCH2D
- AVCH2F
- AVCH2G
- AVCH2P
- AVECOD
- AVECOF
- AVECOG
- AVECOP
- AVECSD
- AVECSF
- AVECG
- AVECSP
- AVEMW
- AVENFU
- AVENOD
- AVENOF
- AVENOG
- AVENOP
- AVET
- CONGNO
- DMDDA
- DMDDM
- DMDDP
- DMDDPP
- EKKD
- ILAST
- INDIC
- LEN
- NO
- NOP
- PHIBAR
- RHOBAR
- RRO
- TAUBAR
- TAUINT
- VELOC
- XD
- XU

The external output consists of:

- AVNO
- AVRHO
- DDFNO
- E
- J
- XD

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine ZINTER which are not included in COMMON:

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVNO(J)</td>
<td>NO_j</td>
<td>Mass average nitric oxide concentration for a given iteration j at the end of each major step in the combustor</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Description</td>
<td>Units</td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>-----------------------------------------------------------------------------------------------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>AVRHO(J)</td>
<td>Mass average density of the combustion products for a given iteration j at the end of each major step in the combustor</td>
<td>gm/cc</td>
<td></td>
</tr>
<tr>
<td>AVVNOG</td>
<td>Ratio of total nitric oxide mixing out of the elements to the total mass mixing into the elements</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AVVNOG</td>
<td>Mass average nitric oxide concentration for a given iteration at a given axial step in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH2AV</td>
<td>Mass average equilibrium mole fraction of unburned hydrocarbons (exclusive of C(s) and CO) at a given axial station in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CNOLST</td>
<td>Nitric oxide equilibrium concentration for the last incremental step in the intermediate zone</td>
<td></td>
<td></td>
</tr>
<tr>
<td>COAV</td>
<td>Mass average equilibrium mole fraction of carbon monoxide at a given axial station in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CSAV</td>
<td>Mass average equilibrium mole fraction of C(s) at a given axial station in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DDFNO</td>
<td>Measure of difference in the calculated NO levels after successive iterations at a given axial station in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DELTAX</td>
<td>Integration step size (major) in the intermediate zone</td>
<td>cm</td>
<td></td>
</tr>
<tr>
<td>DELX</td>
<td>Increment of the combustor length across which the solution is generated</td>
<td>cm</td>
<td></td>
</tr>
<tr>
<td>DIFNO</td>
<td>Measure of difference in the calculated NO levels after successive iterations at a given axial station in the combustor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DUMMY</td>
<td>Dummy variable</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EK*</td>
<td>Constant - equal to 0.05</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EKILST</td>
<td>Ratio of forward reaction rate constants for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Variable initialized but not used in subroutine*
<table>
<thead>
<tr>
<th><strong>Fortran Symbol</strong></th>
<th><strong>Symbol</strong></th>
<th><strong>Description</strong></th>
<th><strong>Units</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>EK2LST</td>
<td>(K_2)</td>
<td>Ratio of forward reaction rate constants for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EN</td>
<td>(N)</td>
<td>Proportionality constant between (\Delta X) and (\xi X)</td>
<td></td>
</tr>
<tr>
<td>FFF</td>
<td>(F)</td>
<td>Mean mixture ratio for the last step in the intermediate zone</td>
<td></td>
</tr>
<tr>
<td>FURAT</td>
<td>(\Delta \overline{NO}_{\Delta X})</td>
<td>Measure of change in NO concentration for successive steps in the combustor</td>
<td></td>
</tr>
<tr>
<td>GNOMI</td>
<td>([NO]_{gm})</td>
<td>Nitric oxide content of an element (i) at a given axial station in the combustor</td>
<td>(gm)</td>
</tr>
<tr>
<td>IENDZ</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td>IENDZ = 0 for all except the last major integration step in the intermediate zone</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>IENDZ = 1 for the last major integration step in the intermediate zone</td>
<td></td>
<td></td>
</tr>
<tr>
<td>II</td>
<td>(\ell)</td>
<td>Integration increment index</td>
<td></td>
</tr>
<tr>
<td>IIIE</td>
<td>(\ell_{ie})</td>
<td>Counter of number of iterations attempting to satisfy (E_i) criteria</td>
<td></td>
</tr>
<tr>
<td>J</td>
<td>(J)</td>
<td>Number of iterations for each major axial step in the combustor</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>(K)</td>
<td>Number of iterations for each major axial step in the combustor</td>
<td></td>
</tr>
<tr>
<td>KON(1)*</td>
<td></td>
<td>Index</td>
<td></td>
</tr>
<tr>
<td></td>
<td>KON(1) = 0 if integration for the element has not converged</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>KON(1) = 1 if integration for the element has converged</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LSGN</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LSGN = 1 if intermediate zone and not the last step in the zone</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>LSGN = 2 if intermediate zone and the last step in the zone</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>LSGN = 3 if dilution zone</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Variable initialized but not used in subroutine*
<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>N</td>
<td>Proportional y constant between $\Delta X$ and $\Delta^2 X$</td>
<td></td>
</tr>
<tr>
<td>NOAVGS**</td>
<td>$[NO]_{\text{spec}}$</td>
<td>Nitric oxide concentration of the last element in the array</td>
<td></td>
</tr>
<tr>
<td>NONO(I)</td>
<td>$[NO]_{\text{NO}}$</td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>NOSTAR**</td>
<td>$[NO^*]_\text{NO}$</td>
<td>Nitric oxide concentration of the combustion products before air addition at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>NPRINT</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 0 if intermediate output is not requested by the user</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 1 if intermediate output is requested by the user</td>
<td></td>
</tr>
<tr>
<td>OUTNO</td>
<td>$[NO]_{\text{0-1}}$</td>
<td>Total nitric oxide mixing out of the elements at a given axial station in the combustor, intermediate zone</td>
<td>gm/sec-cm</td>
</tr>
<tr>
<td>OUTNO2</td>
<td>$[NO]_{\text{0-2}}$</td>
<td>Total nitric oxide at a given upstream axial station in the combustor intermediate zone</td>
<td>gm/sec</td>
</tr>
<tr>
<td>PINO</td>
<td>$M_{\text{in}}$</td>
<td>Total mass mixing into the elements at a given axial station in the combustor</td>
<td>gm/sec-cm</td>
</tr>
<tr>
<td>Q(I)</td>
<td>$q_i$</td>
<td>Measure of the round-off error for the element i at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>QQ(I)</td>
<td>$q_{iR}$</td>
<td>Measure of the round-off error for the element i at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>RHOLST</td>
<td>$\rho_{\text{LST}}$</td>
<td>Density of combustion product for the last step in the intermediate zone at the mean mixture ratio</td>
<td>gm/cm$^3$</td>
</tr>
<tr>
<td>RHOMI</td>
<td>$\rho'_{R}$</td>
<td>Dummy variable</td>
<td>gm$^2$/cm$^3$</td>
</tr>
<tr>
<td>RILST</td>
<td>$(R_1)_{\text{LST}}$</td>
<td>Forward reaction rate for the first kinetic reaction for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
</tbody>
</table>

**Variable set real but not used in subroutine.
<table>
<thead>
<tr>
<th><strong>Fortran Symbol</strong></th>
<th><strong>Symbol</strong></th>
<th><strong>Description</strong></th>
<th><strong>Units</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>R6LST</td>
<td>( R_6^{LST} )</td>
<td>Forward reaction rate for the sixth kinetic reaction for the last step in the intermediate zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td>( \text{gm-mole/cm}^3\text{-sec} )</td>
</tr>
<tr>
<td>STEPS</td>
<td>( n_{\text{step}} )</td>
<td>Number of remaining integration steps before end of intermediate zone</td>
<td></td>
</tr>
<tr>
<td>STORE1</td>
<td></td>
<td>Dummy variable</td>
<td>( \text{gm-mole/cm}^3\text{-sec} )</td>
</tr>
<tr>
<td>STORE2</td>
<td></td>
<td>Dummy variable</td>
<td>( \text{gm-mole/cm}^3\text{-sec} )</td>
</tr>
<tr>
<td>STORE3</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE4</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE5</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE6</td>
<td></td>
<td>Dummy variable</td>
<td>( \text{deg K} )</td>
</tr>
<tr>
<td>STORE7</td>
<td></td>
<td>Dummy variable</td>
<td>( \text{gm/cm}^3 )</td>
</tr>
<tr>
<td>SUMNO1</td>
<td>( \sum_{\text{NO/C}} )</td>
<td>Summation of the total nitric oxide present at a given axial location in the intermediate zone</td>
<td>( \text{gm} )</td>
</tr>
<tr>
<td>SUM1(J)</td>
<td>( \left( \sum_{\text{1}} \right)_j )</td>
<td>Dummy variable</td>
<td>( \text{gm}^2/\text{cm}^3 )</td>
</tr>
<tr>
<td>SUM2(J)</td>
<td>( \left( \sum_{\text{2}} \right)_j )</td>
<td>Summation of the total nitric oxide present at a given axial location in the intermediate zone at the jth iteration at that point</td>
<td>( \text{gm} )</td>
</tr>
<tr>
<td>TAU</td>
<td>( \overline{T}_{\text{inc}} )</td>
<td>Incremental residence time</td>
<td>( \text{sec} )</td>
</tr>
<tr>
<td>TTLAST</td>
<td>( T_{\text{LST}} )</td>
<td>Adiabatic flame temperature for the last step in the intermediate zone at the mean mixture ratio</td>
<td>( \text{deg K} )</td>
</tr>
<tr>
<td>XI</td>
<td>( X_I )</td>
<td>Integrated length of intermediate zone</td>
<td>( \text{cm} )</td>
</tr>
<tr>
<td>XXX</td>
<td>( X_{XX} )</td>
<td>Axial position in the combustor</td>
<td>( \text{cm} )</td>
</tr>
<tr>
<td>XXXX</td>
<td>( X_{XXX} )</td>
<td>Distance between upstream end of integration interval and end of intermediate zone</td>
<td>( \text{cm} )</td>
</tr>
<tr>
<td>YNOLST</td>
<td>( (\text{NO}_e)^{\text{LST}} )</td>
<td>Equilibrium mole fraction of NO for the last step in the intermediate zone at the mean mixture ratio</td>
<td></td>
</tr>
</tbody>
</table>
Analysis Procedure

The step-by-step procedure of Subroutine ZINTER is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Initialize indicators.
2. Initialize \( \bar{N}_{0} \) as:
   \[ \bar{N}_{0} = 0 \]
3. Set \( k_e \) as:
   \[ k_e = 0.05 \]
4. Calculate \( X_U \) as
   \[ Y_U = X_D \]
5. Initialize \( \bar{R}_{EXT} \) as:
   \[ \bar{R}_{EXT} = 0 \]

Step 6 is performed for each potential array element satisfying the criteria 1 \( \leq i \leq 50 \).

6. Initialize \( q_i \) as:
   \[ q_i = 1.0 \times 10^{-15} \]
7. Calculate \( \Delta X \) as:
   \[ \Delta X \leq 0.1 \times R_{X_D} \]

8. Calculate \( X_L \) as:
   \[ X_L = X_L - X_U \] if intermediate zone calculations end at \( X_L \)
   \[ X_L = X_{END} - X_U \] if intermediate zone calculations end at \( X_{END} \)

Step 9 is performed only if \( \Delta X \leq X_I \)

9. Go to step 12.
10. Recalculate \( \Delta X \) as:
    \[ \Delta X = X_I \]
11. Reset the indicator to indicate that this is the last major integration step in the intermediate zone.

Steps 12 and 13 are performed for each potential array element satisfying the criteria: 1 \( \leq i \leq 50 \).
12. Calculate \( [\text{NO}]_\text{NO} \) and \( q_i \) as:
\[
[\text{NO}]_\text{NO} = [\text{NO}]_0 \\
q_i = q_i
\]
13. Initialize convergence indicators.
Step 14 is performed for each potential integration iteration satisfying the criteria \( 1 \leq j \leq 6 \).
14. Initialize \( (\xi_1)_j \) and \( (\xi_2)_j \) as:
\[
(\xi_1)_j = 0 \\
(\xi_2)_j = 0
\]
15. Set \( x_{xx} \) equal to \( x_D \).
16. Set \( J \) and \( N \) as:
\[
J = 1 \\
N = 5
\]
Step 17 is performed only if \( J = 1 \).
17. Go to step 21.
18. Calculate \( x_U \) and \( x_D \) as:
\[
x_U = x_{xx} \\
x_D = x_U
\]
19. Using Subroutine ZMASS, calculate the elemental and over-all mass flow rates, the mean mixture ratio, and the airflow rate at \( x_D \).
Step 20 is performed for each element in the array satisfying the criteria \( 1 \leq i \leq i_{\text{MAX}} \).
20. Calculate \( [\text{NO}]_i \) and \( q_i \) as:
\[
[\text{NO}]_i = [\text{NO}]_0 \\
q_i = q_i
\]
21. Calculate \( S_X \) as:
\[
S_X = \Delta X / N
\]
22. Calculate \( K_D \) and \( \overline{\text{NO}} \) as:
\[
K_D = C_N / x_L \\
\overline{\text{NO}} = [\text{NO}]_0
\]
23. Set \( I! = 1 \).
24. Initialize \([\text{NO}_0 - 1], [\text{NO}_0 - 2] \) and \([\text{NO}_0 - N]\) as:
   \( [\text{NO}_0 - 1] = 0 \)
   \( [\text{NO}_0 - 2] = 0 \)
   \( [\text{NO}_0 - N] = 0 \)

25. Calculate \(X_D\) as:
   \(X_D = X_0 + S_X\)

Step 26 is performed only if \(I = N\) and if this is the last major integration step in the intermediate zone.

26. Go to step 100.

27. Using Subroutine ZMASS, calculate the elemental and over-all mass flow rates, the mean mixture ratio, and the airflow rate at \(X_D\).

28. Using Subroutine CHECKK, calculate the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it.

29. Set \(i = 1\).

30. Initialize \(\text{ie}\) as:
   \(\text{ie} = 0\)

Step 31 is performed only if \(\frac{d(Sm_i)}{dx} < 0\) and if \((Sm_i)_D = 0\).

31. Calculate \([\text{NC}_0 - 2]\) as:
   \([\text{NC}_0 - 2] = [\text{NC}_0 - 2] + (Sm_i)_D \times [\text{NO}_0 - 1]\)

Step 32 is performed only if \((Sm_i)_D = 0\).

32. Go to step 44.

33. Calculate \((Sm'_i)_C\) as:
   \((Sm'_i)_C = (Sm'_i)_D \times \frac{d(Sm'_i)}{dx} \times x_D / m_u\)

34. Calculate \((Sm''_i)_C\), \((Sm'_{n_i})_C\) and \((Sm''_{n_i})_C\) as:
   \((Sm''_i)_C = \left[ \frac{d(Sm'_i)}{dx} \times x_D + E \times (Sm'_i)_D - R_i \right] \)
   \((Sm'_{n_i})_C = (Sm''_i)_C - (Sm'_{n_i})_C \)
   \((Sm''_{n_i})_C = E - (Sm''_i)_D\)
Step 35 is performed only if $\left( \sum_{m} \right)_c > 0$

35. Go to step 43.

36. Calculate $E_i$ as:
   
   $E_i = 2E_i$

Step 37 is performed only if $E_i = 0$.

37. Calculate $E_i$ as:
   
   $E_i = 0.02$

38. Calculate $l_{ie}$ as:
   
   $l_{ie} = l_{ie} + 1$

Step 39 is performed only if $l_{ie} < 40$.

39. Go to step 34.

40. Write $l_{ie}$ and $E_i$.

41. Reset the appropriate indicator to indicate that intermediate zone calculations end at $X_{END}$.

42. Go to step 125.

43. Calculate $\left[ \text{NO}_2 \right]_{D-1}$ and $M_{ZW}$ as:
   
   $\left[ \text{NO}_2 \right]_{D-1} = \left[ \text{NO}_2 \right]_{D-1} + \left( \sum_{m} \right)_c \times \left[ \text{NO}_2 \right]_c$

   $M_{ZW} = M_{ZW} + \left( \sum_{m} \right)_c + R_c$

44. If this is not the last element in the array satisfying the criteria $1 \leq i \leq i_{MAX}$ increment $i$ as $i = i + 1$ and go to step 30. If this is the last element, go to step 45.

45. Calculate $\left[ \text{NO}_2 \right]_{D-1}$ as:
   
   $\left[ \text{NO}_2 \right]_{D-1} = \left[ \text{NO}_2 \right]_{D-1} + \left[ \text{NO}_2 \right]_{D-2} / S_X$

46. Calculate $rat_1$ as:
   
   $rat_1 = \left[ \text{NO}_2 \right]_{D-1} / M_{ZW}$

47. Initialize $\xi_{NC/L}$ as:
   
   $\xi_{NC/L} = 0$

48. Set $i = 1$.

Step 49 is performed only if $\left( \sum_{m} \right)_D = 0$ or if the chemical rate of production of NO in the element is zero.
49. Go to step 55.

50. Calculate \([\text{NO} \text{mo}]\) as:

\[ [\text{NO} \text{mo}] = \text{rat}_1 \]

51. Using Subroutine RUNKUT, calculate the values of \([\text{NO} \text{mo}]\) and \(q_i\) at \(X_D\).

Step 52 is performed only if \([\text{NO} \text{mo}] < 0\).

52. Calculate \([\text{NO} \text{mo}]\) as:

\[ [\text{NO} \text{mo}] = \text{rat}_2 \]

53. Calculate \(\frac{\text{NO}}{\text{mo}}\) as:

\[ \frac{\text{NO}}{\text{mo}} = \frac{\text{NO}_{\text{mo}}}{m_D} \]

54. Recalculate \(X_U\) as:

\[ X_U = X_D - \delta X \]

55. If this is not the last element in the array satisfying the criteria \(1 \leq i \leq \ell_{\text{MAX}}\), increment \(i\) as \(i = i + 1\) and go to step 49. If this is the last element, go to step 56.

56. Calculate \(\text{NO}\) as

\[ \text{NO} = \frac{\text{NO}_{\text{mo}}}{m_D} \]

57. Set \(X_U\) equal to \(X_D\).

58. If \(11 < N\), increment \(11\) as \(11 = 11 + 1\) and go to step 24 to continue the integration. If not, go to step 59.

59. Set \(i = 1\).

60. Calculate \(D\) and \([\text{NO} \text{mo}]_{\text{gn}}\) as:

\[ D = R_i \times (\Delta m_i)_D \]

\[ [\text{NO} \text{mo}]_{\text{gn}} = [\text{NO} \text{mo}]_D \times (\Delta m_i)_D \]

61. Calculate \((\mathbf{Z}_1)_i\) and \((\mathbf{Z}_2)_i\) as:

\[ (\mathbf{Z}_1)_i = (\mathbf{Z}_1)_j + D \]

\[ (\mathbf{Z}_2)_i = (\mathbf{Z}_2)_j + [\text{NO} \text{mo}]_{\text{gn}} \]

62. If this is not the last element in the array satisfying the criteria \(1 \leq i \leq \ell_{\text{MAX}}\), increment \(i\) as \(i = i + 1\) and go to step 60. If this is the last element, go to step 63.
63. Calculate the mass average density, \( \bar{\rho}_j \), and the mass average nitric oxide concentration \( \bar{\text{NO}}_j \) for the jth iteration as:

\[
\bar{\rho}_j = \frac{(\rho_d)_j}{m^*_D} \\
\bar{\text{NO}}_j = \frac{(\text{NO})_j}{m^*_D}
\]

Step 64 is performed only if intermediate output is requested by the user.

64. Write \( \rho_0, J, \bar{\rho}_j \) and \( \bar{\text{NO}}_j \).

Steps 65-66 are performed only if \( J = 1 \).

65. Calculate \( \text{NO}_{\text{DOM}} \) as:

\[ \text{NO}_{\text{DOM}} = \bar{\text{NO}} \]

66. Go to step 69.

Steps 67-71 are performed only if \( 1 \leq J \leq 5 \).

67. Calculate \( \Delta \text{NO} \) as:

\[ \Delta \text{NO} = \frac{\bar{\text{NO}} - \text{NO}_{\text{DOM}}}{\bar{\text{NO}}} \]

Step 68 is performed only if \( \Delta \text{NO} < 0.01 \).

68. Go to step 74.

69. Reset \( J \) and \( N \) as:

\( J = J + 1 \)
\( N = 2N \)

70. Set \( \text{NO}_{\text{DOM}} = \bar{\text{NO}} \).

71. Go to step 17.

Steps 72-73 are performed only if \( 5 \leq J \leq 6 \).

72. Calculate \( \Delta \text{NO} \) as:

\[ \Delta \text{NO} = \left| \frac{\bar{\text{NO}} - \text{NO}_{\text{DOM}}}{\bar{\text{NO}}} \right| \]

73. Write \( \Delta \text{NO} \), \( N \), and \( \rho_0 \) with the error message indicating that the Runge-Kutta iteration failed to converge to the specified limit.

Step 74 is performed only if \( N = N \) and this is the last major integration step in the intermediate zone.
74. Go to step 119.

75. Calculate \( \text{[CNO]} \), \( \bar{p} \), \( \bar{T} \), \( (\text{C(s)})_e \), \( (\text{CO})_e \) and \( (\text{CH}_2)_e \) as:

\[
\begin{align*}
\text{[CNO]} &= \sum_{i=1}^{i_{\text{max}}} \text{CNO}\_i \times (\Delta m\_i) / \text{m}_D^\text{x} \\
\bar{p} &= \sum_{i=1}^{i_{\text{max}}} p\_i \times (\Delta m\_i) / \text{m}_D^\text{x} \\
\bar{T} &= \sum_{i=1}^{i_{\text{max}}} T\_i \times (\Delta m\_i) / \text{m}_D^\text{x} \\
(\text{C(s)})_e &= \sum_{i=1}^{i_{\text{max}}} (\text{C(s)})\_i \times (\Delta m\_i) / \text{m}_D^\text{x} \\
(\text{CO})_e &= \sum_{i=1}^{i_{\text{max}}} (\text{CO})\_i \times (\Delta m\_i) / \text{m}_D^\text{x} \\
(\text{CH}_2)_e &= \sum_{i=1}^{i_{\text{max}}} (\text{CH}_2)\_i \times (\Delta m\_i) / \text{m}_D^\text{x}
\end{align*}
\]

76. Calculate \( \text{MW} \) as:

\[
\text{MW} = \bar{p} \times \bar{T} \times 82.051 / \rho
\]

77. Calculate \( [\text{C(s)}]_e \), \( [\text{CO}]_e \), and \( [\text{CH}_2]_e \) as:

\[
\begin{align*}
[\text{C(s)}]_e &= (\text{C(s)})_e \times \text{12} / \text{MW} \\
[\text{CO}]_e &= (\text{CO})_e \times \text{28} / \text{MW} \\
[\text{CH}_2]_e &= (\text{CH}_2)_e \times \text{14} / \text{MW}
\end{align*}
\]

78. Calculate \( \{\text{NO}\} \), \( \{\text{NO}^+\} \), and \( \{\text{NO}\} \) as:

\[
\begin{align*}
\{\text{NO}\} &= \text{[NO]} \times 10^6 \times \text{MW} / 30.0 \\
[\text{NO}^+] &= \text{[NO]} \times \bar{p} \\
\{\text{NO}\} &= \text{[NO]} \times \text{m}_D^\text{x} \times \text{1000} / (\bar{T}_p)\_D
\end{align*}
\]
79. Calculate \( \{C(s)\}_e, \{CO\}_e, \) and \( \{CH_2\}_e \) as:

\[
\{C(s)\}_e = \{C(s)\}_e \times 10^6 \times \overline{MW} / 12
\]
\[
\{CO\}_e = \{CO\}_e \times 10^6 \times \overline{MW} / 28
\]
\[
\{CH_2\}_e = \{CH_2\}_e \times 10^6 \times \overline{MW} / 14
\]

80. Calculate \( [\bar{C}(s)]_e, [\bar{CO}]_e, \) and \( [\bar{CH}_2]_e \) as:

\[
[\bar{C}(s)]_e = [\bar{C}(s)]_e \times \bar{R}
\]
\[
[\bar{CO}]_e = [\bar{CO}]_e \times \bar{R}
\]
\[
[\bar{CH}_2]_e = [\bar{CH}_2]_e \times \bar{R}
\]

81. Calculate \( \{\bar{C}(s)\}_e, \{\bar{CO}\}_e, \) and \( \{\bar{CH}_2\}_e \) as:

\[
\{\bar{C}(s)\}_e = \{\bar{C}(s)\}_e \times \bar{M}_D \times 1000 / (\bar{M}_F)_{X_D}
\]
\[
\{\bar{CO}\}_e = \{\bar{CO}\}_e \times \bar{M}_D \times 1000 / (\bar{M}_F)_{X_D}
\]
\[
\{\bar{CH}_2\}_e = \{\bar{CH}_2\}_e \times \bar{M}_D \times 1000 / (\bar{M}_F)_{X_D}
\]

82. Calculate \( \Delta NO_{AX} \) as:

\[
\Delta NO_{AX} = \frac{[\bar{NO}] - [\bar{NO}]_{up}}{[\bar{NO}]}
\]

83. Calculate \( n_{step} \) as:

\[
n_{step} = (x_{END} - x_U) / \Delta x
\]

Step 84 is performed only if \( \Delta NO_{AX} \times n_{step} < 0.05 \)

84. Set the appropriate indicator to indicate that the nitric oxide reaction is frozen at this point in the combustor.
85. Calculate $\alpha_{\text{inc}}$ as:
\[
\alpha_{\text{inc}} = \Delta X \cdot \rho \cdot A_{x_D} / m_D^*
\]

86. Calculate $\alpha_{\text{int}}$ and $\alpha$ as:
\[
\begin{align*}
\alpha_{\text{int}} &= \alpha_{\text{inc}} + \alpha_{\text{inc}} \\
\alpha &= \alpha_{\text{int}} + \alpha_{\text{inc}}
\end{align*}
\]

87. Calculate $V$ as:
\[
V = \frac{m_D^*}{\rho \cdot A_{x_D}}
\]

88. Calculate $\bar{\rho}$ as:
\[
\bar{\rho} = \frac{\bar{F}}{(k_s \cdot (1 - \bar{F}))}
\]

89. Using Subroutine PRINTS, write the output for this axial station in the intermediate zone.

Step 90 is performed only if the nitric oxide reaction is frozen at this point in the combustor.

90. Write a message indicating frozen conditions exist in the combustor.

Step 91 is performed only if the appropriate indicator has been previously set to indicate that the nitric oxide reaction is frozen.

91. Go to step 124.

92. Set $\frac{\bar{N_O}}{U_p}$ as:
\[
\begin{bmatrix}
\frac{\bar{N_O}}{U_p}
\end{bmatrix} = \begin{bmatrix} \bar{N_O} \end{bmatrix}
\]

93. Calculate $(\bar{\rho})_{fr}$ as:
\[
(\bar{\rho})_{fr} = \bar{\rho}
\]

Step 94 is performed only for the last major integration step in the intermediate zone.

94. Go to step 125.
95. Calculate \( x_{XXX} \) as:
\[
x_{XXX} = x_L - x_U \quad \text{if intermediate zone calculations end at } x_L.
\]
\[
x_{XXX} = x_{END} - x_U \quad \text{if intermediate zone calculations end at } x_{END}.
\]
Step 96 is performed only if \( \Delta x \leq x_{XXX} \).
96. Go to step 12.
97. Calculate \( \Delta x \) as:
\[
\Delta x = x_{XXX}
\]
98. Set the appropriate indicator to indicate that this is the last major integration step in the intermediate zone.
99. Go to step 12.
100. Set the appropriate indicator to indicate a dilution zone type calculation is to be applied to the last element in the intermediate zone.
101. Using Subroutine \( \text{?MASS} \), calculate the over-all mass flow rate, the mean mixture ratio, and the airflow rate at \( x_D \).
102. Using Subroutine \( \text{CHECKK} \), calculate the mass flow rate out of an element due to mixing and the total mass flowing into it.
103. Reset the appropriate indicator to indicate intermediate zone calculations.
104. Calculate \( Q \) and \( \sum_{i=1}^{N_{OAN}} \) as:
\[
Q = \sum_{i=1}^{N_{MAX}} q_i \cdot x (\alpha_m_i) / M_D
\]
\[
\sum_{i=1}^{N_{OAN}} = \sum_{i=1}^{N_{END}} (\Delta \rho) D / \rho_D
\]
105. Using Subroutine \( \text{MINT} \), calculate \( (\frac{R}{\rho})_{\text{LS}} \).
106. Using Subroutine \( \text{MINT} \), calculate \( (\rho_D)_{\text{LS}} \).
107. Using Subroutine \( \text{MINT} \), calculate \( (\rho_D)_{\text{LS}} \).
108. Using Subroutine \( \text{MINT} \), calculate \( (\rho_D)_{\text{LS}} \).
109. Using Subroutine \( \text{MINT} \), calculate \( (\rho_D)_{\text{LS}} \).
110. Using Subroutine \( \text{MINT} \), calculate \( (\rho_D)_{\text{LS}} \).
111. Using Subroutine \( \text{MINT} \), calculate \( T_{\text{LS}} \).
112. Calculate \( [\Delta x]_{\text{ER}} \) as:
\[
[\Delta x]_{\text{ER}} = \{(\rho_D)_{\text{LS}}\} \cdot 30.0 / \rho_{\text{LS}} \cdot T_{\text{LS}} \cdot 82.05 \cdot R
\]
113. Set the appropriate indicator to indicate that this is the last step of the intermediate zone calculations.

114. Using Subroutine RUNKUT, compute the values of $\xi_\Delta\xi_{AN}$ and $Q$ at $x_D$.

115. Recalculate $x_U$ as:
$$x_U = x_D - 8x$$

116. Reset the appropriate indicator to signify intermediate zone calculations.

117. Calculate $\bar{\xi}_j$ and $\bar{N}_O_j$ as:
$$\bar{\xi}_j = \xi_{LST}$$
$$\bar{N}_O_j = N_{O_{AN}}$$

118. Go to step 65.

119. Compute $\bar{T}$, $\bar{R}$ and $[N_{O}]$ as:
$$\bar{T} = T_{LST}$$
$$\bar{R} = R_{LST}$$
$$[N_{O}] = [N_{O_{AN}}]$$

120. Using Subroutine MINT, compute $(\xi_{L \Delta \xi})_e$.

121. Using Subroutine MINT, compute $(\xi_{O})_e$.

122. Using Subroutine MINT, compute $(\xi_{CH_2})_e$.

123. Go to step 76.

124. Calculate $N_{O_{AN}}$ as:
$$N_{O_{AN}} = [N_{O}]$$

125. Return.
SUBROUTINE ZINTER
REAL NONO(50),HSTARU,HSTARD,NO,NOAVGS,NOP,NSTAR
DIMENSION AVRNO(10),AVNO(10),KON(10),Q(50),QQ(50),SUM1(10),SUM2(10)

COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(50)
COMMON/OUT1/AVECSG,AVECG,AVECH2G,AVECSP,AVECOP,AVECH2P,AVECSD,AVECSM
COMMON/OUT2/AVENOG;AVENOD,AVENOP,AVENOF,AVENO,AVENF1,AVENO,AVEND1,AVEND2
COMMON/OUT3/INDICNO(50),AVETAU,TBARH,BARPHI,XXD1
COMMON/OUT4/CONGNO(50),DELNO(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLOC
COMMON/OUT5/MSTARU,MSTARU
COMMON/OUT6/REAT90,REAT91

C**** SET INITIAL INDICATORS, CALCULATE DELTAX, CHECK X

NPRINT=0
ILAST=0
LSGN=1
INDIC=2
IEND=0
AVENFU=0.0
EK=5.05
XU=XD
TAUINT =0.0
DO 100 I=1,50
Q(I)=1.0*E-15
100 CONTINUE

DELTAX = 0.1
RSUBX
IF(LEN.EQ.0) XI=XL-XU
IF(LEN.EQ.1) XI=XEND-XU
IF(DELTAX.LE.XI) GO TO 200
DELTAX = XI
IEND = 1
200 CONTINUE

C**** STORE INITIAL VALUES FOR BEGINNING OF EACH MAJOR STEP

250 CONTINUE
DO 300 I=1,50
NONO(I)=NO(I)
QD(I)=Q(I)
KON(I)=0
300 CONTINUE

350 CONTINUE
XXX = XD
J = 1
N=5

C**** SET INITIAL VALUES EQUAL TO STORED VALUES EACH TIME N CHANGES

360 CONTINUE
IF(J.IEQ.1) GO TO 500
XU = X00

CALL LMASS(DELX)
DO 600 I = 1.IMAX
  NO(I) = NONO(I)
  Q(I) = QQ(I)
CONTINUE
500 EN = N
  DELX = DELTAX/EN
  EK=KD=C.I.XL
  AVN06=AYENDS

START THE MAJOR STEPS DOWN THE CONDUCTOR
DO 3000 I=1,N
  OUTNO=O.0
  OUTNO2=O.0
  PINO=0.0
  XO = XU+DELX
  IF(I.EQ.N.AND.1ENDZ.EQ.1) GO TO 2000
  CALL LMASS(DELX)
  CALL CHECKKDELXI

TEST EACH ELEMENT FOR CONVERGENCE
IF NOZERO=1 BYPASS THE NO CALC
DO 2000 I=1.IMAX
  IIE=0
  IF(SLOPE(I).LT.0.5.AND.DAY(I).EQ.0.0) OUTNO2=OUTNO2+UDM(I)*NC(I)
  IF(DIM(I).EQ.0.0) GO TO 2000
  DMDD(I) = UDM(I)*ASLOPE/HSTARE
  DMDDP(I) = SLOPE(I)*E(I)*UDM(I) + RDOT(I)
  DMDDM(I) = DMDDP(I)-DMDDP(I)
  IF(DMDDM(I).LT.0.0) GO TO 700
  E(I)=2.0*E(I)

HENCE E(I) CANNOT EQUAL ZERO
IF(E(I).EQ.0.0) E(I)=0.02
  IIE=IIIE+1
  IF(IIE.LE.40) GO TO 500
  RITE(6.9999) IIE,E(I)
  LEN=1
  GO TO 500
CONTINUE
2000 OUTNO=OUTNO+DMDDP(I)*NO(I)
PINO=PIN0+DMDDP(I)*RDOT(I)
CONTINUE
OUTNO=OUTNO+OUT02/DELX
AVN06=OUTNO/PINO
SU4NO=0.0
GO 4000 I=1,IMAX
IF(DM(IJ).EQ.0.0) GO TO 4000
IF(NODEN0(IJ),EQ.1) GO TO 4000

   XU=XU-DELX
   NNH=NNH*DELM0(IJ)
   SUM01=SUM01*DELMO(IJ)

4000 CONTINUE
   AVVNOG=SUMNO1/MSXARD
   XU=XU

3000 CONTINUE
   DO 3500 J =1,IMAX
   RHO(J) = RHO(I)*DELM0(I)
   GNUM(J) = GNUM(I)*DELM0(I)
   SUM1(J)= SUM1(J)+RHO(J)
   SUM2(J)= SUM2(J)+GNUM(J)

3500 CONTINUE
   AVHNO(IJ)= SUM1(J)/MSXARD
   AVN0(IJ)= SUM2(J)/MSXARD

C------- WRITE CONTROL
C------
   IF(NPRINT,EQ.0) GO TO 3550
   WRITE(6,3500) X(J),AVHNO(IJ)*AVN0(IJ)

3550 CONTINUE
C------- LOGIC CONTROL ON J
C-------
   GO TO (4100,4300,4300,4300,4300,4300,4300,4300),J

4100 DUMMY=AVVNOG
   GO TO 4500

4300 IF(NC=ABS((AVVNOG-DUMMY)/AVVNOG)) THEN
   IF(DIFNC*LT.0.01) GO TO 5000

4500 J= J+1
   N = 2*N
   DUMMY=AVVNOG
   GO TO 360

4600 DIFNO=ABS((AVVNOG-DUMMY)/AVVNOG)
   WRITE(6,4700) DIFNO
   GO TO 4700

4700 FORMAT('H RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED
1ST LIMIT. DIFNO = ',E12.5', N = ',I4, ',5H X = ',E12.5,')

4800 CONTINUE
5000 CONTINUE
   IF(I1.EQ.N AND IENDZ.EQ.1) GO TO 8500

C------- WRITE THE APPROPRIATE OUTPUT FOR THIS AXIAL STATION
C-------
   AVN0G = .0
   RHOAR = 0.0
   AVET = 0.0
   CSAV = 0.0
   COAV = 0.0
   CH2AV = 0.0
   DO 6000 I =1,IMAX
   AVEN0G = AVEN0G+NO(I)*DELM0(I)
   RHOAR = RHOAR+RHO(I)*DELM0(I)
   AVET = AVET+ATT(I)*DELM0(I)
   CSAV = CSAV+CON1(I)*DELM0(I)
   COAV = COAV+CON2(I)*DELM0(I)

6000 CONTINUE
CH2AV = CH2AV+CH2(I)*DELMD(I)

6000 CONTINUE
AVENG = AVENG/MSTARD
RHOBAR = RHOBAR/MSTARD
AVET = AVET/MSTARD
CSAV = CSAV/MSTARD
COAV = COAV/MSTARD
CH2AV = CH2AV/MSTARD

6500 AVE4M = RHOBAR*AVET*82*057/PPP
AVECSG = CSAV*12*0/AVE4M
AVECO6 = COAV*28*0/AVE4M
AVENTP = AVENG*1.0E+06*AVE4M/30.0
AVENG = AVENG/RHOBAR
AVENG = AVENG/MSTARD*1000+/DMFT
AVECSG = AVECSG*1.0E+06/AVE4M/12.0
AVECO6 = AVECO6*1.0E+06/AVE4M/28.0
AVECH2G = AVECH2G*1.0E-06/AVE4M/14.0

C****
C**** CALCULATE RESIDENCE TIME,Etc.
C****
TAU = DELTAX*RHOBAR*AREA/MSTARD
TAUNIT = TAU/TAU
TAUBAR = TAUBAR+TAU
VELOC = MSTARD/(RHOBAR*AREA)
PHBAR = FBARD/(EKS*(1.0-FBARD))

CALL PRINTS
IF(IILAST.EQ.*) WRITE(699500,9)

9500 FORMAT(///,10X,42HNITRIC OXIDE REACTION FROZEN AT THIS POINT://)

IF(IILAST.EQ.*) GO TO 8600

C****
C**** CONTROL OVERALL STEPS
C****
AVENFU = AVENOF
RRO = RHOBAR
IF(IENDZ.EQ.*) GO TO 9060
IF(len.EQ.0) XXX = XL-XU
IF(len.EQ.1) XXX = XEND-XU
IF(DELTAX.LT.XXXX) GO TO 250
DELTAX = XXX
IENDZ = 1
GO TO 250

C****
C**** COMPUTATION FOR LAST ELEMENT
C****
5000 INDIC = 3
CALL AVE(INDIC
CALL CHECK(INDIC
INDIC = 2
AOQ = 0.0
AND = 0.0
DO 8100 I = 1, IMAX
AQQ = AQQ*Q(I)*DELMD(I)
ANO = ANO*NO(I)*DELMD(I)
8100 FFF = FSTD
AQQ = AQQ/HSTD
ANO = ANO/HSTD
CALL MINT(1, FFF, 35, FF, R1, R1LAST)
CALL MINT(1, FFF, 35, FF, R6, R6LAST)
CALL MINT(1, FFF, 35, FF, EK1, EK1LAST)
CALL MINT(1, FFF, 35, FF, EK2, EK2LS)
CALL MINT(1, FFF, 35, FF, BCON6, YNOLST)
CALL MINT(1, FFF, 35, FF, RHO, RHOLST)
CALL MINT(1, FFF, 35, FF, ATT, TTLAST)
CNOLST = YNOLST*30.0/(RHOLST*TTLAST*82.057/PPP)
STORE1 = R1(I)
STORE2 = R6(I)
STORE3 = EK1(I)
STORE4 = EK2(I)
STORE5 = CONGNO(I)
STORE6 = ATT(I)
STORE7 = RHO(I)
R1(I) = R1LAST
R6(I) = R6LAST
EK1(I) = EK1LAST
EK2(I) = EK2LAST
RHO(I) = RHOLST
ATT(I) = TTLAST
CONGNO(I) = CNOLST
LSGN = 2
CALL RUNKUT(XU, DELX, ANO, AQQ, LSGN, 1)
XU = XU-DELX
R1(I) = STORE1
R6(I) = STORE2
EK1(I) = STORE3
EK2(I) = STORE4
CONGNO(I) = STORE5
ATT(I) = STORE6
RHO(I) = STORE7
AVRHO(J) = RHOLST
AVNO(J) = ANG
LSGN = 1
GO TO 3550
C*** COMPUTE APPROPRIATE AVERAGES
C***
6500 AVET = TTLAST
RHOBAR = RHOLST
AVENOG = ANU
CALL MINT(1, FFF, 35, FF, BCON1*CSAV)
CALL MINT(1, FFF, 35, FF, BCON2*COAV)
CALL MINT(1, FFF, 35, FF, CH2*CM2AV)
GO TO 6500
9999 FOKMAT (10X, 16, 8E12.5)
8600 ANO = AVENOG
9000 RETURN
END
APPENDIX VI - SUBROUTINE DILUTE

The function of Subroutine DILUTE is to calculate the concentration of nitric oxide at specified axial stations, and at the exit of the dilution zone of a gas turbine combustor.

Subroutine DILUTE is called by the main routine (GASNOX); it, in turn, calls Subroutines ZMASS, MINT, RUNKUT, and PRINTS. The subroutine does not require external input but does provide external output. Internal input and output are transmitted through COMMON. The internal input consists of:

AIRD  AND  AQQ  ATT  BCON1  BCON2  CH2  EKS  EK1  EK2  FF  ILAST  PPP  RHO  R6  RSUBX  R1  R6  S  XEND  XD

The internal output consists of:

ANO  AVCH2D  AVCH2F  AVCH2G  AVCH2P  AVECOD  AVECOF  AVECOG  AVECOP  AVECSF  AVECSG  AVECSP  AVMW  AVENFU  AVENOD  AVENOF  AVENOG  AVENOP  AVET  INDIC  NOEQXD  PHIBAR  RRO  TAUBAR  TAUDIL  VELOC  XD  XU

The external output consists of:

DDIFNO  DILL  DNO  J  N  REAT  RHOBAR  XD

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine DILUTE which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIRXX</td>
<td>MA_X</td>
<td>Combustor airflow at axial station X_D</td>
<td>gm/sec</td>
</tr>
<tr>
<td>DDIFNO</td>
<td>[ANO]</td>
<td>Difference in NO concentrations for successive iterations at the end of each major step in the combustor</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>----------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>DELTAX</td>
<td>$\Delta X$</td>
<td>Integration step size (major) in the dilution zone</td>
<td>cm</td>
</tr>
<tr>
<td>DELX</td>
<td>$\Delta X$</td>
<td>Increment of the combustor length across which the solution is generated</td>
<td>cm</td>
</tr>
<tr>
<td>DNO</td>
<td>$[\text{NO}]_{DN}$</td>
<td>Average NO at given axial station (downstream) in the combustor</td>
<td></td>
</tr>
<tr>
<td>DUMMY</td>
<td>$[\text{NO}]_{DUM}$</td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>EK1LST</td>
<td>$(K_1)_{LST}$</td>
<td>Ratio of forward reaction rate constants at a given axial station in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EK2LST</td>
<td>$(K_2)_{LST}$</td>
<td>Ratio of forward reaction rate constants at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EN</td>
<td>$N$</td>
<td>Proportionality constant between $\Delta X$ and $\Delta X$</td>
<td></td>
</tr>
<tr>
<td>FURAT</td>
<td>$[\Delta \text{NO}]_{\Delta X}$</td>
<td>Measure of change in NO concentration for successive steps in the combustor</td>
<td></td>
</tr>
<tr>
<td>IENDD</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>IENDD = 0 for all except the last major integration step in the dilution zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>IENDD = 1 for the last major integration step in the dilution zone</td>
<td></td>
</tr>
<tr>
<td>LLSGN</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LLSGN = 1 if intermediate zone and not the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LLSGN = 2 if intermediate zone and the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LLSGN = 3 if dilution zone</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>$N$</td>
<td>Proportionality constant between $\Delta X$ and $\Delta X$</td>
<td></td>
</tr>
<tr>
<td>NONO</td>
<td>$[\text{NO}]_{NO}$</td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>NPRINT</td>
<td>NPRINT</td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 0 if intermediate output is not requested by the user</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 1 if intermediate output is requested by the user</td>
<td></td>
</tr>
<tr>
<td>Q</td>
<td>q</td>
<td>Measure of the round-off error in the Runge-Kutta integration routine at a given axial station in the combustor</td>
<td></td>
</tr>
<tr>
<td>QQ</td>
<td>qq</td>
<td>Measure of the round-off error in the Runge-Kutta integration routine at a given axial station</td>
<td></td>
</tr>
<tr>
<td>R1LST</td>
<td>(R_1)_LST</td>
<td>Forward reaction rate for the first kinetic reaction at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>gm-mole/cm^3-s</td>
<td></td>
</tr>
<tr>
<td>R6LST</td>
<td>(R_6)_LST</td>
<td>Forward reaction rate for the sixth kinetic reaction at a given axial position in the dilution zone at the mean mixture ratio (see Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>gm-mole/cm^3-s</td>
<td></td>
</tr>
<tr>
<td>STEPS</td>
<td>n_{step}</td>
<td>Number of remaining integration steps before combustor exit</td>
<td></td>
</tr>
<tr>
<td>STORE1</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE2</td>
<td></td>
<td>gm-mole/cm^3-s</td>
<td></td>
</tr>
<tr>
<td>STORE3</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE4</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>TAU</td>
<td>\sigma_{inc}</td>
<td>Incremental residence time</td>
<td></td>
</tr>
<tr>
<td>YOZ</td>
<td>X_{OZ}</td>
<td>Distance between upstream end of integration interval to combustor exit</td>
<td></td>
</tr>
<tr>
<td>XXX</td>
<td>X_{XX}</td>
<td>Axial position in the combustor</td>
<td></td>
</tr>
<tr>
<td>XXXX</td>
<td>X_{XXX}</td>
<td>Distance between upstream end of integration interval and combustor exit</td>
<td></td>
</tr>
<tr>
<td>YCH2XD</td>
<td>(CH_2)<em>eX</em>{0}</td>
<td>Equilibrium mole fraction of unburned hydrocarbon (exclusive of ( \text{CO} ) and ( \text{CO}_2 )) at a given axial station in the dilution zone at the mean mixture ratio</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>YCOXD</td>
<td>(CO)_{exD}</td>
<td>Equilibrium mole fraction of CO at a given axial station in the dilution zone at the mean mixture ratio</td>
<td></td>
</tr>
<tr>
<td>YCSXD</td>
<td>(C_s)_{exD}</td>
<td>Equilibrium mole fraction of C_s at a given axial station in the dilution zone at the mean mixture ratio</td>
<td></td>
</tr>
<tr>
<td>YNOXD</td>
<td>(NO)_{exD}</td>
<td>Equilibrium mole fraction of NO at a given axial station in the dilution zone at the mean mixture ratio</td>
<td></td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine DILUTE is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Initialize indicators.
2. Set $\tilde{[NO]}_DN = \tilde{[NO]}_AN$
3. Go to step 16
4. Calculate $X_U$, $\tilde{Y}_{DIL}$, and $q$ as:
   - $X_U = X_D$
   - $\tilde{Y}_{DIL} = 0$
   - $q = Q$
5. Calculate $\Delta X$ and $X_{DZ}$ as:
   - $\Delta X = 0.1 \times R_{XD}$
   - $X_{DZ} = X_{END} - X_U$
7. Set the indicator to indicate that this is the last step in the combustor and calculate $\Delta X$ as:
   - $\Delta X = X_{DZ}$
8. Initialize dummy variables $M_{\Delta x}$ and $\tilde{[NO]}_{NO}$ as:
   - $M_{\Delta x} \bigg|_{\Delta x} = M_{\Delta x} \bigg|_{X_D}$
   - $\tilde{[NO]}_{NO} = \tilde{[NO]}_{DN}$
9. Initialize \( q_q \) and \( X_{XX} \) as:
   \[
   q_q = q \\
   X_{XX} = X_D
   \]
10. Initialize \( J \) and \( N \) as:
    \[
    J = 1 \\
    N = 20
    \]
11. Initialize \( I_l \) as:
    \[
    I_l = 1
    \]
Step 12 is performed only if \( J = 1 \).
13. Calculate \( M_A|_{X_D} \), \( \phi_j \) and \( [\overline{N_O}]_{DA} \) as:
    \[
    M_A|_{X_D} = M_A|_{XX} \\
    \phi_j = \phi_j \\
    [\overline{N_O}]_{DA} = [\overline{N_O}]_{NO}
    \]
14. Calculate \( S_X \) as:
    \[
    S_X = \Delta X/N
    \]
15. Go to step 19.
16. Set \( N \), \( I_l \), and \( J \) as:
    \[
    N = 10 \\
    I_l = N \\
    J = 6
    \]
17. Calculate \( S_X \), \( \Delta X \) and \( \phi_j \) as:
    \[
    S_X = X_{DA} - X_U \\
    \Delta X = S_X \\
    \phi_j = X_D
    \]
18. Calculate \( [\overline{N_O}]_{AN} \) as:
    \[
    [\overline{N_O}]_{AN} = [\overline{N_O}]_{DN}
    \]
19. Calculate \( X_D \) as:
    \[
    X_D = X_U + S_X
    \]
20. Using Subroutine ZMASS, calculate the over-all mass flow rate, mean mixture ratio, and airflow rate at \( X_D \)
21. Using Subroutine MINT, calculate \( (R_1)_{LST} \)
22. Using Subroutine MINT, calculate \( (R_2)_{LST} \)
23. Using Subroutine MINT, calculate \( (R_3)_{LST} \)
24. Using Subroutine MINT, calculate \( (R_4)_{LST} \)
25. Using Subroutine MINT, calculate $(\frac{N_0}{e})_{XD}$
26. Using Subroutine MINT, calculate $\tilde{p}$
27. Using Subroutine MINT, calculate $\tilde{t}$
28. Using Subroutine MINT, calculate $(C_{(5)})_{e, XD}$
29. Using Subroutine MINT, calculate $(CO)_{e, XD}$
30. Using Subroutine MINT, calculate $(CH_2)_{e, XD}$

Steps 31 and 32 are performed only if the nitric oxide reaction is frozen at this point in the combustor.

31. Calculate $[\overline{NO}]_{DN}$ as:
\[ [\overline{NO}]_{DN} = [\overline{NO}]_{AN} \times \left[ \frac{M^*}{M^*_p} \right] \]

32. Go to step 38.

33. Calculate $[\overline{NO}]_{e, XD}$ as:
\[ [\overline{NO}]_{e, XD} = (N_0)_{e, XD} \]

34. Using Subroutine RUNKUT, calculate the value of $[\overline{NO}]_{DN}$ and $q$

Steps 35 and 36 are performed only if $11 < N$

35. Calculate $11 = 11 + 1$

Step 37 is performed only if intermediate output is requested by the user.

37. Write $X_D$, $J$, $\tilde{r}$, $[\overline{NO}]_{DN}$, $(r)_{REACT}$, $(r)_{DIL}$, $[\overline{NO}]$, and $N$.

Steps 38 and 39 are performed only if $J = 1$

38. Calculate $[NO]_{DUM}$
\[ [NO]_{DUM} = [\overline{NO}]_{DN} \]

39. Go to step 43.

Steps 40-42 are performed only if $1 < J < 5$.

40. Calculate $[\overline{NO}]$ as:
\[ [\overline{NO}] = \left[ \frac{[\overline{NO}]_{DN} - [\overline{NO}]_{DUM}}{[\overline{NO}]_{DUM}} \right] \]

Step 41 is performed only if $[\overline{NO}] < 0.005$.

41. Go to step 48.

42. Reset $[NO]_{DUM}$ as:
\[ [NO]_{DUM} = [NO]_{DN} \]
43. Calculate J and N as
   \[ J = J + 1 \]
   \[ N = 2N \]

44. Go to step 11.

Steps 45 and 46 are performed only if \( J = 5 \).

45. Write the error message stating that the Runge-Kutta
    iteration failed to converge. Write also the value of
    \([\text{ANO}], N, \text{and } x_D\).

46. Go to step 48.

Step 47 is performed only if \( J = 6 \).

47. Set the appropriate indicator to indicate that this is the
    last major step in the combustor.

48. Calculate \( [\text{NO}] \) as
   \[ [\text{NO}] = \frac{[\text{NO}]}{\text{SN}} \]

49. Calculate \( MW \) as
   \[ MW = \frac{\rho * T * 82.0571}{P} \]

50. Calculate \( [\text{C}_2(s)]_e, [\text{CO}]_e, \text{and } [\text{CH}_2]_e \) as:
    \[ [\text{C}_2(s)]_e = (\text{C}_2(s))_{e_x} * 12 / MW \]
    \[ [\text{CO}]_e = (\text{CO})_{e_x} * 28 / MW \]
    \[ [\text{CH}_2]_e = (\text{CH}_2)_{e_x} * 14 / MW \]

51. Calculate \( [\text{NO}]_e, [\text{NO}]_e, \text{and } [\text{NO}]_e \) as:
    \[ [\text{NO}]_e = [\text{NO}]_e + 10^6 * MW / 30.0 \]
    \[ [\text{NO}]_e = [\text{NO}]_e + \rho \]
    \[ [\text{NO}]_e = [\text{NO}]_e + 10^6 * 1000 / (M_d)_{x_3} \]

52. Calculate \( [\text{C}_2(s)]_e, [\text{CO}]_e, \text{and } [\text{CH}_2]_e \) as:
    \[ [\text{C}_2(s)]_e = [\text{C}_2(s)]_e * 10^6 * MW / 12 \]
    \[ [\text{CO}]_e = [\text{CO}]_e * 10^6 * MW / 28 \]
    \[ [\text{CH}_2]_e = [\text{CH}_2]_e * 10^6 * MW / 19 \]
53. Calculate \([\bar{C}\text{cs}]_e\), \([\bar{C}\text{co}]_e\), and \([\bar{C}\text{h}_2]_e\) as:

\[
\begin{align*}
[\bar{C}\text{cs}]_e &= [\bar{C}\text{cs}]_e \cdot \rho \\
[\bar{C}\text{co}]_e &= [\bar{C}\text{co}]_e \cdot \rho \\
[\bar{C}\text{h}_2]_e &= [\bar{C}\text{h}_2]_e \cdot \rho
\end{align*}
\]

54. Calculate \([\bar{C}\text{s}]_e\), \([\bar{C}\text{co}]_e\), and \([\bar{C}\text{h}_2]_e\) as:

\[
\begin{align*}
[\bar{C}\text{s}]_e &= \frac{[\bar{C}\text{cs}]_e \cdot \bar{M}_S^* \cdot 1000}{[\bar{M}_f]_{\text{AD}}} \\
[\bar{C}\text{co}]_e &= \frac{[\bar{C}\text{co}]_e \cdot \bar{M}_S^* \cdot 1000}{[\bar{M}_f]_{\text{AD}}} \\
[\bar{C}\text{h}_2]_e &= \frac{[\bar{C}\text{h}_2]_e \cdot \bar{M}_S^* \cdot 1000}{[\bar{M}_f]_{\text{AD}}}
\end{align*}
\]

Steps 55 and 56 are performed only if the nitric oxide reaction is frozen at this point in the combustor.

55. Calculate \(\bar{M}_D^*\) as:

\[
\bar{M}_D^* = \frac{1}{2} (\bar{M}_D^* + \bar{M}_D^*)
\]

56. Calculate \(\bar{P}\) as:

\[
\bar{P} = \frac{1}{2} (\bar{P} + \bar{P})_{\text{rr}}
\]

57. Calculate \(\bar{\Theta}_{\text{inc}}\) as:

\[
\bar{\Theta}_{\text{inc}} = A_x \cdot \bar{P} \cdot A_{\text{AD}} / \bar{M}_D^*
\]

58. Calculate \(\bar{\Theta}_{\text{DIL}}\) and \(\bar{\Theta}\) as:

\[
\begin{align*}
\bar{\Theta}_{\text{DIL}} &= \bar{\Theta}_{\text{DIL}} + \bar{\Theta}_{\text{inc}} \\
\bar{\Theta} &= \bar{\Theta} + \bar{\Theta}_{\text{inc}}
\end{align*}
\]

59. Calculate \(V\) as:

\[
V = \bar{M}_D^* / \bar{P} \cdot A_{\text{AD}}
\]

60. Calculate \(\bar{\Theta}\) as:

\[
\bar{\Theta} = \bar{P} / (k_s (1 - \bar{P}))
\]
61. Calculate $\Delta \bar{N}_\text{O}_\text{A}$ as:

$$\Delta \bar{N}_\text{O}_\text{A} = \frac{\bar{N}_\text{O}_\text{D} - \bar{N}_\text{O}_\text{UP}}{\bar{N}_\text{O}_\text{D}}$$

62. Calculate $n_{\text{step}}$ as:

$$n_{\text{step}} = \frac{(X_{\text{END}} - X_\text{D})}{\Delta X}$$

Step 63 is performed only if $(\Delta \bar{N}_\text{O}_\text{A} \times n_{\text{step}}) < 0.05$

63. Set the appropriate indicator to indicate that the nitric oxide reaction is frozen at this point in the combustor.

64. Using Subroutine PRINTS, write the output for this axial station in the dilution zone.

65. Reset $\bar{N}_\text{O}_\text{D}$ as:

$$\bar{N}_\text{O}_\text{D} \text{UP} = \bar{N}_\text{O}_\text{D}$$

66. Reset $(\bar{\rho})_{\text{rr}}$ as:

$$(\bar{\rho})_{\text{rr}} = \bar{\rho}$$

Step 67 is performed only if the appropriate indicator indicates that this is the last step in the dilution zone.

67. Go to step 75.

Step 68 is performed only if the nitric oxide reaction is frozen at this point in the combustor.

68. Write a message indicating frozen conditions exist in the combustor.

Step 69 is performed only if the appropriate indicator has been previously set to indicate that the nitric oxide reaction is frozen.

69. Go to step 16.

70. Calculate $X_{\text{XXX}}$ as:

$$X_{\text{XXX}} = X_{\text{END}} - X_\text{D}.$$  

Step 71 is performed only if $\Delta X < X_{\text{XXX}}$

71. Go to step 8.
72. Calculate $\Delta x$ as:
   $\Delta x = x_{XXX}$

73. Set the appropriate indicator to indicate that this is the last step in the dilution zone.

74. Go to step 8.

75. Return.
SUBROUTINE DILUTE
REAL MSTD, NO, NOEQ, MSTD, MSTD
COMMON/DATA/AIR(50), RR(50), XX(50), FF(50), BCON1(50), BCON2(50), CH2(50) DIL0020
150, ZP(70), CUMDIS(70), VP, RH0(50), BCON6(50), ATT(50), PPP, FNOXP, R1(50) DIL0030
2-, RX(50), EK1(50), EK2(50), A2, A3, XL, CN, BETA, S, PHI, EKS, XEND, A1
COMMON/OUT1/AVEC5G, AVECOS, AVECSP, AVECH2, AVECS, AVECDIL DIL0050
10, AVECM2, AVECSC, AVECO, AVECHF
COMMON/OUT2/AVENUG, AVEND, AVEND, AVENF, AROIL, ILAST
COMMON/OUT3/INDEX, NO(50), AVE, TAOBAR, PHBAR, IMAX, XD, DIL0080
1FBARD, XU, XU, TAU, TAUDIO, ILAST
COMMON/OUT4/CONNO(50), DELNO(50), AREAD, ASPACE, DMFUD, SLOPE(50), TSD03DIL0100
1PENOP(50), EKNO, DMFT, UDM(50), DDM(50), F(50), D4FUD, AIRD, DMFEDDIL0110
2-, RSUBX, SIG, SIG2, AVENA, AVMF, DDDA(50), DMDM(50), DHDP(50), HDHDP(50), FDIL0120
3PRIME(50), NOEQ, AO, AQ, DIFNO(50), NOZERO(50), RDOT(50), E(50) DIL0130
COMMON/OUT5/MSTD, MSTD
COMMON/CUT6/REAL DIL

C*** SET INITIAL INDICATORS, CALCULATE DELTAX, CHECK X
C***
NPRINT=0
L3GN=3
INDIC=3
IEND=0
IF(S.EQ.0.0) ILAST=0
DNO = ANO
IF(ILAST.EQ.1) GO TO 2000
XU=XU
TAUDIL=0.0
Q=AQQ
DELTAX=0.1*RSUBX
XZ=XEND=XU
IF(DELTAX.LE.XZ) GO TO 200
DELTAX=XZ
IEND=1
200 CONTINUE
C*** STORE INITIAL VALUES FOR BEGINNING OF EACH MAJOR STEP
C***
CONTINUE
1ATXX = AIRD
NONO = DNO
QQ=Q
XX = XD
J=1
Q=20
DIFNO = 0.0
C*** SET INITIAL VALUES EQUAL TO STORED VALUES EACH TIME N CHANGES
C***
300 II=1
IF(J.EQ.1) GO TO 400
440 = 41XX
XU=XX
Q=QQ
DNO = NONO
400 EN=N
DELM=DELTAX/EN
C*** START THE MAJOR STEPS DOWN THE CONSUMTOR
C***
GO TO 2500
2000 V=10
II=N
J=6
DELX=XEND-XD
DELTAX=DELX
XU=XD
ANO=DNO
2500 DD 3000 II=1,N
XD=XU+DELX
CALL ZMASS(DELX)
C*=** CALCULATE NO AT XD
C**** CALL MINT(1,FBARD,35,FF,R1,R1LST)
CALL MINT(1,FBARD,35,FF,R6,R6LST)
CALL MINT(1,FBARD,35,FF,Ek1,Ek1LS)
CALL MINT(1,FBARD,35,FF,Ek2,Ek2LST)
CALL MINT(1,FBARD,35,FF,BCON5,YNOXD)
CALL MINT(1,FBARD,35,FF,RHO,RHOBAR)
CALL MINT(1,FBARD,35,FF,ATT,AVET)
CALL MINT(1,FBARD,35,FF,BCON1,YCSXD)
CALL MINT(1,FBARD,35,FF,BCON2,YC0XD)
CALL MINT(1,FBARD,35,FF,CH2,YCH2XD)
IF(ILAST.EQ.1) DNO=ANO*MSTARU/MSTARD
IF(ILAST+EQ.1) GO TO 4000
STORE1 = R1(1)
STORE2 = R6(1)
STORE3 = Ek1(1)
STORE4 = Ek2(1)
R1(1) = R1LST
R6(1) = R6LST
Ek1(1) = Ek1LST
Ek2(1) = Ek2LST
NOE=XD/YNOXD*30.0/(RHOBAR*AVET*82.057/PPP)
CALL RUNKUT(XU,DELX,DNO,G,LSGN,1)
R1(1) = STORE1
R6(1) = STORE2
Ek1(1) = STORE3
Ek2(1) = STORE4
3000 CONTINUE
C**** WRITE CONTROL
C**** IF(NPRINT.EQ.0) GO TO 4000
WRITE(6,3500) XD,J,RHOBAR,DNO,REAT,DILL
WRITE(6,9997) DDIFNO,N
3500 FORMAT(9H XCM) = +E12.5*4J = +16.16*HAVE. RHO(GM/CC) = +E12.5*17HDI
1AVE. NO(GM/CM) = +E12.5*5X*2E12.5)
C**** LOGIC CONTROL ON J
C**** 4000 CONTINUE
GO TO (4100*4300,4300,4300*4600,4800)* J
4100 DUMMY = DNO
GO TO 4500
4300 DDIFNO = ABS((DNO-DUMMY)/DNO)
IF(DDIFNO.LT.0.005) GO TO 5000
DUMMY = DNO
4500 J=J+1
DILL*0600
DILL*0610
DILL*0620
DILL*0630
DILL*0640
DILL*0650
DILL*0660
DILL*0670
DILL*0680
DILL*0690
DILL*0700
DILL*0710
DILL*0720
DILL*0730
DILL*0740
DILL*0750
DILL*0760
DILL*0770
DILL*0780
DILL*0790
DILL*0800
DILL*0810
DILL*0820
DILL*0830
DILL*0840
DILL*0850
DILL*0860
DILL*0870
DILL*0880
DILL*0890
DILL*0900
DILL*0910
DILL*0920
DILL*0930
DILL*0940
DILL*0950
DILL*0960
DILL*0970
DILL*0980
DILL*0990
DILL*1000
DILL*1010
DILL*1020
DILL*1030
DILL*1040
DILL*1050
DILL*1060
DILL*1070
DILL*1080
DILL*1090
DILL*1100
DILL*1110
DILL*1120
DILL*1130
DILL*1140
DILL*1150
DILL*1160
DILL*1170
DILL*1180
DILL*1190
N=2*N
GO TO 300

4600 WRITE(6,4700) DDIFFNO,N,XD
4700 FORMAT('///',%9.5H RUNGE-KUTTA ITERATION FAILED TO CONVERGE TO SPECIFIED LIMIT. DDIFFNO = ',E12.5',5H N = ',I4.5',5H X = ',E12.5',5H CMS///')
GO TO 5000

4800 IENDU = 1
5000 CONTINUE

WRITE THE APPROPRIATE OUTPUT FOR THIS AXIAL STATION

AVENOF = DNO
AVECSG=AVEMH*12.0/AVEMW
AVECG=AVEMH*29.0/AVEMW
AVCH2G=AVCH2D*14.0/AVEMW
AVCH2P=AVCH2G*1.0E06*AVEMW/30.0
AVEND=AVENOF*RHOBAR
AVEND=AVENOF*MASTARD/1000.0/DIMFT
AVETP=AVETG*1.0E06*AVEMW/12.0
AVECOP=AVECGP*1.0E06*AVEMW/28.0
AVCH2P=AVCH2G*1.0E06*AVEMW/14.0
AVECG=AVECGP*RHOBAR
AVECO=AVECGP*RHOBAR
AVECSF=AVECSGP*HSTARD/1000.0/DIMFT
AVEC0F=AVECGP*HSTARD/1000.0/DIMFT
AVCH2E=AVCH2GP*HSTARD/1000.0/DIMFT

CALCULATE RESIDENCE TIMES, ETC

IF(ILAST.EQ.1) MASTARD = 0.5*(MASTARD+HSTARD)
IF(ILAST.EQ.1) RHOBAR=0.5*(RHOBAR+RRD)
TAU = DELTAX*RHOBAR*AREAD/HSTARD
TAUDIL=TAUDIL+TAU
TAUBAR=TAUBAR+TAU
VELOC=HSTARD*(RHOBAR*AREAD)
PHIBAR=FBARD/(EKS*(1.0-FBARD))
FUAT=AVENOF-AVENFU)/AVENOF
STEPS=(XEND-XU)/DELTAX
IF(FUAT*STEPS.LT.0.05) ILAST = 1
CALL PRINTS

CONTROL OVERALL STEPS

AVENFU=AVENOF
RRD=RHOBAR
IF(IENDU.EQ.1) GO TO 9000
IF(ILAST.EQ.1) WRITE(6,5500)
9500 FORMAT('///',%9.5H 42NMICROREX REACTION FROZEN AT THIS POINT///')

IF(ILAST.EQ.1) GO TO 2000
XXX=XEND-XU
IF(DELTAX.LT.XXX) GO TO 250
DELTAX=XXX
IENDU=1
GO TO 250

9000 RETURN

9997 FORMAT(20X,E10.3,15)
END
APPENDIX VII - SUBROUTINE PRCALC

The function of Subroutine PRCALC is to calculate the average nitric oxide level at the exit of the primary zone for each mixture ratio element.

Subroutine PRCALC is called by Subroutine PRIMRY; it, in turn, calls Subroutine MINY. Subroutine PRCALC does not require external input and does not provide external output except for an error message and diagnostic data table. External output is written directly onto the output-tape unit. Internal input and output are transmitted through COMMON and as arguments of the subroutine. The internal input consists of:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BCON1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BCON2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BCON6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CONGNO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DELMD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EK1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EK2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FBARD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FF</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FNODG</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IMAX</td>
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<td></td>
</tr>
<tr>
<td>NOZERO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PPP</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RHO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R6</td>
<td></td>
<td></td>
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<tr>
<td>S</td>
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</table>

The internal output consists of:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AQQ</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AVET</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NO</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NOEQXD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RHOBAR</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TAUBAR</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The external output consists of:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALPHA2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DUMMY</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LIMIT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SUMTNO</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRCALC which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AAA(i)</td>
<td>$\alpha_2$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the end of the integration interval</td>
<td></td>
</tr>
<tr>
<td>ALPHAD(i)</td>
<td>$\alpha_D$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element i at the end of the integration interval</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>----------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>ALPHAT(I)</td>
<td>$\alpha_j$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the mean primary zone residence time</td>
<td></td>
</tr>
<tr>
<td>ALPHAU(I)</td>
<td>$\alpha_u$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the start of the integration interval</td>
<td></td>
</tr>
<tr>
<td>ALPHA1</td>
<td>$\alpha_1$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the start of the integration interval</td>
<td></td>
</tr>
<tr>
<td>ALPHA2</td>
<td>$\alpha_2$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the end of the integration interval</td>
<td></td>
</tr>
<tr>
<td>ALPHD</td>
<td>$\alpha_d$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the end of the integration interval</td>
<td></td>
</tr>
<tr>
<td>ALPHU</td>
<td>$\alpha_u$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for a mixture element $i$ at the end of the integration interval</td>
<td></td>
</tr>
<tr>
<td>DALP</td>
<td>$\Delta \alpha$</td>
<td>Integration interval</td>
<td></td>
</tr>
<tr>
<td>DALPHA</td>
<td>$\Delta \alpha$</td>
<td>Integration interval</td>
<td></td>
</tr>
<tr>
<td>DUMMY(I)</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>EK1LST</td>
<td>$(K_1)_\text{LST}$</td>
<td>Ratio of forward reaction rate constants at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EK2LST</td>
<td>$(K_2)_\text{LST}$</td>
<td>Ratio of forward reaction rate constants at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)</td>
<td></td>
</tr>
<tr>
<td>EN</td>
<td>$r$</td>
<td>Integration step size control</td>
<td></td>
</tr>
<tr>
<td>ERR</td>
<td>$\varepsilon_{\text{err}}$</td>
<td>Convergence limit</td>
<td></td>
</tr>
<tr>
<td>FNOXG</td>
<td>[NO$_x$]</td>
<td>NO formed in the flame front (mass fraction)</td>
<td></td>
</tr>
<tr>
<td>FT</td>
<td>$f_k$</td>
<td>Fractional mass in an element that has a residence time $dt$ about $k$</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>----------------</td>
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<td>-------------</td>
<td>--------</td>
</tr>
<tr>
<td>P7FTD</td>
<td>$\left(\xi_{\text{e}}\right)_p$</td>
<td>Accumulated mass fraction leaving element before $t_0$</td>
<td></td>
</tr>
<tr>
<td>FTU</td>
<td>$(\xi_{\text{e}})_u$</td>
<td>Accumulated mass fraction leaving element before $t_u$</td>
<td></td>
</tr>
<tr>
<td>INDEX</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$INDEX = 0$ at start of iteration</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$INDEX = 1$ if convergence criteria not satisfied</td>
<td></td>
</tr>
<tr>
<td>J</td>
<td></td>
<td>Counter:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$J &lt; 6$ if convergence occurs on $\xi_{\text{e}}$-NO</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$J = 6$ if convergence limit is not satisfied on $\xi_{\text{e}}$-NO</td>
<td></td>
</tr>
<tr>
<td>JJ</td>
<td></td>
<td>Counter:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$JJ \leq 20$ if convergence test on $(\xi_{\text{e}})_{\text{rem}}$ applied</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$JJ &gt; 20$ if convergence test on $(\xi_{\text{e}})_{\text{rem}}$ not applied</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$K = 1$ if first integration step</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>$K \neq 1$ if other than first integration step</td>
<td></td>
</tr>
<tr>
<td>LIMIT</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LIMIT $\leq 10$ if convergence occurs</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LIMIT $\geq 10$ if convergence criteria not satisfied</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td></td>
<td>Integration step size control</td>
<td></td>
</tr>
<tr>
<td>REMAIN (1)</td>
<td>$(\xi_{\text{e}})_{\text{rem}}$</td>
<td>Fraction of mass remaining in element i after convergence criteria satisfied</td>
<td></td>
</tr>
<tr>
<td>RLIST</td>
<td>$(R)_{\text{LST}}$</td>
<td>Forward reaction rate for the first kinetic reaction for an element at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
<tr>
<td>R6LST</td>
<td>$(R)_{\text{LST}}$</td>
<td>Forward reaction rate for the sixth kinetic reaction for an element at mean primary zone mixture ratio (See Volume 2, Section 2 or Ref 3)</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
<tr>
<td>STORE1</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>STORE2</td>
<td></td>
<td>Dummy variable</td>
<td>gm-mo.e/cm³-sec</td>
</tr>
<tr>
<td>STORE3</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>STORE4</td>
<td></td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>SUMT (i)</td>
<td>Σ_t</td>
<td>Sum to time t of the mass fractions in an element i</td>
<td></td>
</tr>
<tr>
<td>SUMTNO (i)</td>
<td>Σ_t,NO</td>
<td>Sum to time t of the products of the mass fraction and NG concentrations in an element i</td>
<td></td>
</tr>
<tr>
<td>TD</td>
<td>t_D</td>
<td>Time at end of integration interval</td>
<td>sec</td>
</tr>
<tr>
<td>TIMEN</td>
<td>t_n</td>
<td>Characteristic time used to calculate (F_i)_p</td>
<td>sec</td>
</tr>
<tr>
<td>TT</td>
<td>t_τ</td>
<td>Dummy variable</td>
<td>sec</td>
</tr>
<tr>
<td>TTS</td>
<td>t_τS</td>
<td>Time at end of integration interval</td>
<td>sec</td>
</tr>
<tr>
<td>TTU</td>
<td>t_τU</td>
<td>Time at start of integration interval</td>
<td>sec</td>
</tr>
<tr>
<td>TU</td>
<td>t_τU</td>
<td>Time at start of integration interval</td>
<td>sec</td>
</tr>
<tr>
<td>YCH2XD</td>
<td>e, x_p</td>
<td>Equilibrium mole fraction of unburned hydrocarbons exclusive of C(s) and CO for an element at the mean primary zone mixture ratio</td>
<td></td>
</tr>
<tr>
<td>YCOXD</td>
<td>e, x_p</td>
<td>Equilibrium mole fraction of CO for an element at the mean primary zone mixture ratio</td>
<td></td>
</tr>
<tr>
<td>YCSXD</td>
<td>e, x_p</td>
<td>Equilibrium mole fraction of C(s) for an element at the mean primary zone mixture ratio</td>
<td></td>
</tr>
<tr>
<td>YNOXD</td>
<td>e, x_p</td>
<td>Equilibrium mole fraction of NO for an element at the mean primary zone mixture ratio</td>
<td></td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine PRCAŁC is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.
1. Estimate $(\alpha_2)_i$ as:

$$(\alpha_2)_i = 0.5$$

2. Calculate $(\alpha_0)_i$ as:

$$
(\alpha_0)_i = \begin{cases}
0 & \text{if } [NOC_i] = 0 \\
\frac{[NO_i]}{[NOC_i]} & \text{if } [NOC_i] \neq 0
\end{cases}
$$

Step 3 is performed only if the chemical reaction rate is not significant.


4. Using Subroutine PRRAT, calculate a value of time which corresponds to the estimate of $(\alpha_2)_i$.

5. Calculate $t_{err}$ as:

$$t_{err} = 1 - \frac{t_e}{\bar{t}}$$

Steps 6 and 7 are performed only if $|t_{err}| < 0.05$.

6. Reestimate $(\alpha_2)_i$.

Step 7 is performed only if the number of iterations on $(\alpha_2)_i$ are less than 10.

7. Go to step 4.

8. Calculate $(\alpha_3)_i$ as:

$$(\alpha_3)_i = (\alpha_2)_i$$

Step 9 is performed only if the number of iterations on $(\alpha_3)_i$ equal 10.

9. Write the value of $(\alpha_2)_i$.

10. If this is not the last element in the array, go to step 1.

11. Initialize $n$ as:

$$n = 10$$

Step 12 is performed only if $(\alpha_0)_i < 0$.

12. Go to step 50.

Step 13 is performed only if the chemical reaction rate is not significant.

14. Calculate \((\Delta x)_{i}\) and \(t_{0}\) as:

\[
(\Delta x)_{i} = (\Delta y)_{i} / n
\]

\[t_{0} = 0\]

15. Calculate \((\alpha_{D})_{i}\) as:

\[
(\alpha_{D})_{i} = (\alpha_{0})_{i} + (\Delta x)_{i}
\]

Step 16 is performed only if \((\alpha_{D})_{i} > 1.0\).

16. Recalculate \((\alpha_{D})_{i}\) as:

\[
(\alpha_{D})_{i} = 1.0
\]

Steps 17 through 27 are performed only if \(S_{o} = 0\).

17. Using Subroutine MINT, calculate \((R_{1})_{i}ST\)

18. Using Subroutine MINT, calculate \((R_{2})_{i}ST\)

19. Using Subroutine MINT, calculate \((k_{1})_{i}ST\)

20. Using Subroutine MINT, calculate \((k_{2})_{i}ST\)

21. Using Subroutine MINT, calculate \([N_{D}]_{e}x_{D}\)

22. Using Subroutine MINT, calculate \(P\)

23. Using Subroutine MINT, calculate \(T\)

24. Using Subroutine MINT, calculate \([C_{D}]_{e}x_{D}\)

25. Using Subroutine MINT, calculate \([K_{D}]_{e}x_{D}\)

26. Using Subroutine MINT, calculate \([H_{D}]_{e}x_{D}\)

27. Calculate \((N_{D})_{e}x_{D}\) as:

\[
(N_{D})_{e}x_{D} = \frac{[N_{D}]_{e}x_{D} \times 30.0 \times P}{R \times T \times 82.057}
\]

28. Using Subroutine PRRAT, calculate \((\alpha_{D})_{i}\).

Step 29 is performed only if \(S_{o} = 0\).

29. Calculate \(Q_{i}\) as:

\[Q_{i} = 0\]

Steps 30 through 32 are performed only for the first integration step.

30. Calculate \((f_{e})_{i}\) as:

\[f_{e}(t_{0}) = 0\]

31. Reset \((\alpha_{0})_{i}\) and \(t_{0}\) as:

\[
(\alpha_{0})_{i} = (\alpha_{D})_{i}
\]

\[t_{0} = t\]
32. Go to step 15.
33. Calculate $t_0$ as:
   \[ t_0 = t \]
34. Calculate $t_n$ as:
   \[ t_n = \frac{1}{2} (t_0 + t_2) \]
35. Calculate $(\xi_n)_b$ as:
   \[ (\xi_n)_b = 1 - \exp(-t_n/\alpha) \]
36. Calculate $(\xi_e)_b$, $(\xi_e)_o$, $\Xi_e$, and $\Xi_{e-no}$
37. Reset $(\sigma_o)_e$ and $t_0$ as:
   \[ (\sigma_o)_e = (\sigma_o)_o \]
   \[ t_0 = t_0 \]

Step 38 is performed if the convergence criteria on $(\xi_e)_{\text{elem}}$ are not satisfied but those on $\Xi_{e-no}$ are.
38. Go to step 45.

Step 39 is performed if $tt < 5\hat{\tau}$

Steps 40 through 42 are performed if the convergence criteria on $\Xi_{e-no}$ are not satisfied.
40. If the number of iterations on $\Xi_{e-no}$ equal 6 go to step 43.
41. Reset $n$ as:
   \[ n = 2n \]
42. Go to step 14.
43. If the number of iterations on $\Xi_{e-no}$ are equal to 6, write a diagnostic statement identifying element and the last two values of $\Xi_{e-no}$
44. Calculate $(\Delta\xi)_e$ as:
   \[ (\Delta\xi)_e = 5(\Delta\xi)_e \]
45. Calculate $(\xi_e)_{\text{elm}}$ as:
   \[ (\xi_e)_{\text{elm}} = 1 - \Xi_e \]
Step 46 is performed if \( \varepsilon_{\text{e-no}} < 10^{-5} \)

46. Go to step 48.

Step 47 is performed only if the number of iterations on \( (F_e)_\text{iter} \) are less than or equal to 20.

47. If convergence criteria on \( (F_e)_\text{iter} \) are not satisfied, reset \( (u)_i \) as:

\[
(u)_i = (u_0)_i
\]

and go to step 15.

48. Calculate \( \varepsilon_{\text{e-no}} \) and \( \varepsilon_{\text{e:no}} \)

49. Reset \( n \) as:

\[
n = n/8
\]

50. If this is not the last element in the array, go to step 12.

51. Return.
SUBROUTINE PRCALC(FNOXG)

REAL NO

DIMENSION SUMTNC(50),SUMMNY(50),SUMT(50),REMAIN(50),ALPHAT(50),ALPHA,

1(50),ALPHAD(50)

COMMON/DATA1/AIR(50),R1(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(50),

150),ZP(70),CUMDIS(70),VP,RNO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50),

2),KE(50),EK2(50),AXL,CHN,BETA,SPHIP,KEK,XEND,A1

COMMON/OUT3/INDICNO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,IX,

IFBAR=XB,LENU,TAINT,TAUDL,VELOC

COMMON/OUT4/CNGNO(50),DELT4D(50),READ,ASLOPE,DMFUO,SLFOE(50),TSLOR,P

1),DEP(50),KKK,DMFT,UDM(50),1DM(50),FB(50),DMFUD,AMF,DEMFFED

2),R5UBA SIG SIGZER,AVEM*,DMDDA(50),DMDDM(50),DMDDP(50),FPRC

3PRIME(50),NOEGXD,AND,AQAP,DIFNO(50),NOZERO(50),RDOT(50),E(50)

C*** SET INDICES, INITIAL VALUES, ETC.

TTJ = 0

TTS=0.0

DO 5 I = 1,50

NO(I) = 0.0

50 CONTINUE

DO 1000 I = 1,IMAX

ALPHA2=0.5

LIMIT = 0

IF(CNGNO(I),EQ,0.0) ALPHAU(I) = 0.0

IF(CNGNO(I),NE,0.0) ALPHAU(I) = FNOXG/CNGNO(I)

IF(NOZERO(I),EQ,1) GO TO 1000

ALPHA1 = ALPHAU(I)

DALP=ALPHA1

C*** CALCULATE THE VALUE OF ALPHA-TAU

100 TT = TTU

LIMIT=LIMI

CALL PRRAT(ALPHA1,ALPHA2,TT,T)

AAA=ALPHA2

ERA=(1.0/(TT/TAUBAR))

IF(ABS(ERR)-.0.05) 300,200,200

200 ALPHAS=AAA*(AAA-DALP)*(TAUBAR-XX)/(TT-TTS)

IF(ALPHAS,LE,0.0) ALPHAS = AAA/2.

IF(ALPHAS,GT,0.0) ALPHAS=1.2*AAA

IF(ALPHAS,GT,0.0) ALPHAS=0.998

DALP=AAA

TTS=TT

IF(LIMIT.LT,10) GO TO 100

300 ALPHAT(I)=ALPHAS

IF(LIMIT,LT,10) WRITE(6,99997) ALPHA2,LIMIT

1000 CONTINUE

C*** BEGIN NO CALCULATIONS FOR THE ITH ELEMENT

CALL PRRAT(ALPHA1,ALPHA2,TT,T)

AAA=ALPHA2

ERA=(1.0/(TT/TAUBAR))

IF(ABS(ERR)-.0.05) 300,200,200

200 ALPHAS=AAA*(AAA-DALP)*(TAUBAR-XX)/(TT-TTS)

IF(ALPHAS,LE,0.0) ALPHAS = AAA/2.

IF(ALPHAS,GT,0.0) ALPHAS=1.2*AAA

IF(ALPHAS,GT,0.0) ALPHAS=0.998

DALP=AAA

TTS=TT

IF(LIMIT.LT,10) GO TO 100

300 ALPHAT(I)=ALPHAS

IF(LIMIT,LT,10) WRITE(6,99997) ALPHA2,LIMIT

1000 CONTINUE

C*** SET ADDITIONAL INDICES, INITIAL VALUES, ETC.
INDEX = 0
J = 1
JJ=1
SUMY(I) = 0.0
1150 DALPHA=ALPHAT(I)/EN
SUMTNU(I) = 0.0
SUMT(I) = 0.0
K = 0
ALPHA=ALPHAU(I)
TU=0.0
1200 ALPHD=ALPHU*DALPHA
C**** PRRAT OVERWRITTEN IF ALPHD GT 0.99
C**** IF(ALPHD GT 1.0) ALPHD = 1*
TT=TT
C**** SPECIAL CASE S=0.0 IN PRIMARY ZONE
C**** IF(S NE.0.0) GO TO 1210
CALL MINT(1,FBARD,35,FF,R1,R1LST)
CALL MINT(1,FBARD,35,FF,R6,R6LST)
CALL MINT(1,FBARD,35,FF,Ek1,Ek1LST)
CALL MINT(1,FBARD,35,FF,Ek2,Ek2LST)
CALL MINT(1,FBARD,35,FF,BCON6,YNOXD)
CALL MINT(1,FBARD,35,FF,ROBAR)
CALL MINT(1,FBARD,35,FF,ATTAVET)
CALL MINT(1,FBARD,35,FF,BCON1,YSXD)
CALL MINT(1,FBARD,35,FF,BCON2,YYYYXD)
CALL MINT(1,FBARD,35,FF,CH2,YCH2X)
STORE1 = R1(I)
STORE2 = R6(I)
STORE3 = Ek1(I)
STORE4 = Ek2(I)
R1(I) = R1LST
R6(I) = R6LST
Ek1(I) = Ek1LST
Ek2(I) = Ek2LST
N0EQXD=YNOXD*30.0/(ROBAR*AVET*82.057/PPP)
1210 CALL PRRAT(ALPHU,ALPHD,TT,T)
C**** IF(S NE.0.0) GO TO 1220
C**** R1(I) = STORE1
C**** R6(I) = STORE2
C**** Ek1(I) = STORE3
C**** Ek2(I) = STORE4
AQQ=0.0
C**** 1220 CONTINUE
K = K+1
IF(K NE.1) GO TO 1251
FTU=0.0
ALPHA=ALPHD
TU=TT
GO TO 1200
1251 TT=TT
TIME=TIME+0.5*(TU+TD)
FTE=1.0*EXP(-TIME/TAUBAR)
FT=FTE*FTU
FTU=FID
TU=TD
ALPHA=ALPHD
SUMTN(I) = SUMTN(I) + FT
SUMTN(I) = SUMTN(I) + ALPHU*CONGNO(I)*FT

IF(INDEX.EQ.1) GO TO 1400
IF(TAUBAR.LT.5*TAUBAR) GO TO 1200
IF(ABS((SUMTN(I)-DUMMY(I))/SUMTN(I)) .LE. 0.01 ) GO TO 1300
IF(J.EQ.6) GO TO 1300
EN = 2*EN
DUMMY(I) = SUMTN(I)
J = J+1
GO TO 1150

1300 IF(J.NE.6) GO TO 1350
WRITE(6,9000) SUMTN(I)*DUMMY(I)*I
9000 FORMAT(5SH,POTENTIAL ERROR DUE TO LACK OF CONVERGENCE,SUMTN(I)=,E15.8,2X,PRIOR VALUE OF SUMTN(I)=,E15.8,2X,3Hi=,12///)
DALPHA=5.0*DALPHA

1400 REMAIN(I) = 1-SUMTN(I)
IF(REMAIN(I)*CONGNO(I) .GT. 0.001*SUMTN(I)) INDEX = 1
IF(SUMTN(I) .LT. 1.0E-05) GO TO 1500
JJ=JJ+1
IF(JJ.GT.20) GO TO 1500
IF(REMAIN(I)*CONGNO(I) .GT. 0.001*SUMTN(I)) DALPHA=ALPHAT(I)
IF(REMAIN(I)*CONGNO(I) .GT. 0.001*SUMTN(I)) GO TO 1200

1500 SUMTN(I) = SUMTN(I) + (CONGNO(I)*ALPHU*REMAIN(I))

4000 CONTINUE
5000 CONTINUE
9997 FORMAT(35F,E12.5,I6)
RETURN
END
APPENDIX VIII - SUBROUTINE PRRAT

The function of Subroutine PRRAT is to solve the analytical expression relating nitric oxide concentration to time.

Subroutine PRRAT is called by Subroutine PRCALC; it does not call any other subroutines. Subroutine PRRAT does not require external input and does not provide external output. Internal input and output are transmitted through COMMON and as arguments of the subroutine. The internal input consists of:

CONGNO, EK1, EK2, FINIS
INIT, R1, R6, RHO, TIME

The internal output consists of:
TIME

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRRAT which are not included in COMMON:

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A</td>
<td>Constant</td>
<td>cm$^2$/gm-mole</td>
</tr>
<tr>
<td>B</td>
<td>B</td>
<td>Constant</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
<tr>
<td>D</td>
<td>D</td>
<td>Constant</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
<tr>
<td>DUMMY C</td>
<td>C$^1$</td>
<td>Dummy variable</td>
<td>cm$^3$-sec/gm-mole</td>
</tr>
<tr>
<td>DUMMYA C</td>
<td>C$^2$</td>
<td>Dummy variable</td>
<td>cm$^3$-sec/gm-mole</td>
</tr>
<tr>
<td>DUMMYB C</td>
<td>C$^3$</td>
<td>Dummy variable</td>
<td>gm-mole/cm$^3$-sec</td>
</tr>
<tr>
<td>E</td>
<td>E</td>
<td>Constant</td>
<td></td>
</tr>
<tr>
<td>FINIS (αfin)$^i$</td>
<td></td>
<td>Ratio of NO concentration to NO concentration at equilibrium for an element of mixture ratio F and pressure P at the end of the integration interval</td>
<td></td>
</tr>
</tbody>
</table>
The step-by-step procedure of Subroutine PRRAT is given below.

The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. If \( \alpha_{\text{fin}} \) is greater than 0.99, then \( t_f = 10 t_c \). Go to step 10.

2. Calculate \( A = \frac{Z_{\text{NO}}}{P : [\text{NO}]_0} \).

3. Calculate \( B = \frac{(R_i)_c}{1 + (K_i)_c} \).

4. Calculate \( D = (R_i)_c + B \).

5. Calculate \( E = B (K_i)_c \).

6. Calculate \( C_1 = \frac{E(I) - D}{E^2 - D^2} \).

7. Calculate \( C_2 = \frac{E - (R_i)_c \times D}{E^2 - D^2} \).

8. Calculate \( C_3 = \frac{1 + (K_i \alpha_{\text{fin}})_c \left[ 1 - (\alpha_{\text{init}})_c \right]}{1 + (K_i \alpha_{\text{init}})_c \left[ 1 - (\alpha_{\text{fin}})_c \right]} \).

9. Calculate \( t_f = t_0 + \frac{1}{A} \left[ \frac{1}{2} C_1 \ln C_3 + \left[ C_2 \ln \left[ \frac{(D + E)(\alpha_{\text{fin}})_c)(1 - (\alpha_{\text{init}})_c^2)^{1/2}}{(D + E)(\alpha_{\text{fin}})_c)(1 - (\alpha_{\text{fin}})_c^2)^{1/2}} \right] \right] \).

10. Return.
SUBROUTINE PRRAT(INIT,FINIS,TIME,I)

REAL INIT

COMMON/DATA1/AIR(50),RH(50),XX(50),FF(50),BCTRL(50),BON2(50),CH2(7000)
150),ZP(50),CUMDIS(50),VP,RHO(50),BON6(50),AF(50),PRP,FNOX,PR1(50)
21),R6(50),EK1(50),EK2(50),AZ,A3,XL,CM,BETA,SPHIP,EK5,END:AL

COMMON/OUT4/CONGNO(50),DELMD(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLOP(0050)

PE,NOP(50),EKOD,DMFT,UDML(50),DF(50),DMFUO,AIRD,DMFEDPRP(0060)
2,RSUBX,SIG,SIGER,AVEMH,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50),FPRP(0070)
PRIME(50),NOEQX,ANO,AQQ,NOEQFNO(50),NOZERO(50),RDOT(50),SUEA(50)

**** CALCULATE CONSTANTS

*CALCULATE TIME

IF(FINIS.GT.0.99) GO TO 2000
A = (2.0*30.0/RHO(I)*CONGNO(I))
B = R6(I)/(1.*EK2(I))
D = R1(I)*B
E = D*EK1(I)

DUMMY = (E*EK1(I)-D)/(E*E-D*D)
DUMMYA = (E*EK1(I)*D)/(E*E-D*D)

DUMMYa = ((1.*FINIS)*(1.-INIT))/((1.-FINIS)*(1.)*INIT))
TIME = (1./A)*((0.5*DUMMY*ALOG(DUMMYB))+(DUMMYA*ALOG(((D*E*FINIS)))*0.230)
1SQRT(1.-INIT*INIT))/((D*E*FINIS)**SQRT(1.-FINIS*FINIS)))*TIME

GO TO 1000

2000 TIME = 10.0*TIME
1000 RETURN

END
APPENDIX IX - SUBROUTINE MINT

The function of Subroutine MINT is to provide an interpolated value of a tabulated function of one variable assuming a linear, logarithmic, or exponential relationship.

Subroutine MINT is called by Subroutines PRCALC, ZINTER, DILUTE, CALCBC, and ZMASS; it does not call any other subroutines. Subroutine MINT does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine. The internal input consists of:

\[ \text{ILN} \quad \text{NTAB} \quad X \quad \text{XTAB} \quad \text{YTAB} \]

The internal output consists of:

\[ \text{Y} \]

**Fortran Nomenclature**

The following table gives the Fortran nomenclature for those symbols used in Subroutine MINT. Since the subroutine may be used with any consistent set of units, the units of the symbols are not specified.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>a</td>
<td>Coefficient in the expression for ( Y ) as a function of ( X )</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>b</td>
<td>Coefficient in the expression for ( Y ) as a function of ( X )</td>
<td></td>
</tr>
<tr>
<td>ILN</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \text{ILN}=1 ) if linear interpolation is required</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \text{ILN}=2 ) if logarithmic interpolation is required</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \text{ILN}=3 ) if exponential interpolation is required</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>n</td>
<td>Index of the tabular entry</td>
<td></td>
</tr>
<tr>
<td>NTAB</td>
<td>N</td>
<td>Number of tabular entries</td>
<td></td>
</tr>
<tr>
<td>N1</td>
<td>n_1</td>
<td>Index of the tabular entry preceding ( X )</td>
<td></td>
</tr>
<tr>
<td>N2</td>
<td>n_2</td>
<td>Index of the tabular entry following ( X )</td>
<td></td>
</tr>
</tbody>
</table>
### Fortran Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>Value of the independent variable at which interpolation is required</td>
<td></td>
</tr>
<tr>
<td>XTAB(N)</td>
<td>Tabular entries of the independent variable</td>
<td></td>
</tr>
<tr>
<td>X1</td>
<td>Value of the independent variable at n1</td>
<td></td>
</tr>
<tr>
<td>X2</td>
<td>Value of the independent variable at n2</td>
<td></td>
</tr>
<tr>
<td>Y</td>
<td>The value of the dependent variable to be interpolated</td>
<td></td>
</tr>
<tr>
<td>YTAB(N)</td>
<td>Tabular entries of the dependent variable</td>
<td></td>
</tr>
<tr>
<td>Y1</td>
<td>Value of the dependent variable at n1</td>
<td></td>
</tr>
<tr>
<td>Y2</td>
<td>Value of the dependent variable at n2</td>
<td></td>
</tr>
</tbody>
</table>

### Analysis Procedure

The step-by-step procedure of subroutine MINT is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. If there is only one tabular entry, set \( Y = Y_1 \) and return.
2. If linear or logarithmic interpolation is specified, exclude extrapolation; that is, set \( Y = Y_1 \) if \( X < X_1 \), set \( Y = Y_n \) if \( X > X_n \) and return.
3. Determine the tabular entries \( n_1 \) and \( n_2 \) between which \( X \) lies.
4. Exclude those cases for which the interpolation formulas will degenerate, that is, set \( Y = \frac{1}{2}(Y_{n_1} + Y_{n_2}) \) if \( X_{n_1} = X_{n_2} \) or, set \( Y = Y_{n_1} \) if \( Y_{n_1} = Y_{n_2} \).
5. If linear interpolation is specified, set \( Y = a + bX \).
where \( a = y_{n_1} - b x_{n_1} \)

and \( b = (y_{n_2} - y_{n_1}) / (x_{n_2} - x_{n_1}) \)

and return.

6. If logarithmic interpolation is specified, set

\[
Y = e^{a + b/x}
\]

where

\[
a = \ln(y_{n_1}) - b / x_{n_1}
\]

and

\[
b = \ln(y_{n_2} / y_{n_1}) / (1/x_{n_2} - 1/x_{n_1})
\]

and return.

7. If exponential interpolation is specified, set

\[
Y = a / x^b
\]

where

\[
a = y_{n_1} (x_{n_1})^b
\]

and

\[
b = \ln(y_{n_1} / y_{n_2}) / \ln(x_{n_2} / x_{n_1})
\]

and return.
SUBROUTINE HINT(ILN,X,NTAB,XTAB,YTAB,Y)
C     INTERPOLATION OF A FUNCTION OF ONE VARIABLE USING A MULTIPLICITY
C     OF METHODS
DIMENSION XTAB(1),YTAB(1)
C     CHECK IF THERE IS ONLY ONE TABULAR ENTRY
IF (NTAB.NE.1) GO TO 10
Y=YTAB(1)
RETURN
C     CHECK FOR EXTRAPOLATION IF Y=A*B*X OR LN(Y)=A+B/X IS BEING USED
10 IF (ILN.EQ.3) GO TO 50
IF (X.GT.XTAB(1)) GO TO 20
Y=YTAB(1)
RETURN
20 IF (X.LT.XTAB(NTAB)) GO TO 50
Y=YTAB(NTAB)
RETURN
C     FIND THE TABULAR ENTRIES BETWEEN WHICH X LIES
50 DO 100 N=2,NTAB
   IF (X.GT.XTAB(N)) GO TO 100
   N2=N
   GO TO 200
100 CONTINUE
N2=NTAB
200 N1=N2-1
   X1=XTAB(N1)
   X2=XTAB(N2)
   Y1=YTAB(N1)
   Y2=YTAB(N2)
C     CHECK FOR SPECIAL CASES
   IF (X1.NE.X2) GO TO 300
   Y=0.5*(Y1+Y2)
   RETURN
300 IF (Y1.NE.Y2) GO TO 400
   Y=Y1
   RETURN
400 GO TO (500,600,700),ILN
C     INTERPOLATE FOR Y USING Y=A*B*X
500 B=(Y2-Y1)/(X2-X1)
   A=Y1-B*X1
   Y=A*B*X
   RETURN
C     INTERPOLATE FOR Y USING LN(Y)=A+B/X
600 B=ALOG(Y2/Y1)/(1.0/X2-1.0/X1)
   A=ALOG(Y1)-B/X1
   Y=EXP(A+B/X)
   RETURN
C INTERPOLATE FOR Y USING \( Y = \frac{A}{X^B} \)

700 \( B = \frac{\text{ALOG}(Y_1/Y_2)}{\text{ALOG}(X_2/X_1)} \)
\( A = Y_1^B \)
\( Y = \frac{A}{X^B} \)
RETURN
END
APPENDIX X - SUBROUTINE CALCBC

The function of Subroutine CALCBC is to calculate the value of the mass flow coefficient at each axial station in the combustor primary and intermediate zones.

Subroutine CALCBC is called by Subroutine ZMASS; it, in turn, calls Subroutine MINT. Subroutine CALCBC does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

CUMDIS MSTARD ZP ZPD

The internal output consists of:

C

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine CALCBC which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>$C_X_D$</td>
<td>Mass flow coefficient</td>
<td>gm/sec</td>
</tr>
<tr>
<td>P1</td>
<td>$P_1$</td>
<td>Value of the cumulative normal distribution at Zp</td>
<td></td>
</tr>
<tr>
<td>P2</td>
<td>$P_2$</td>
<td>Value of the cumulative normal distribution at -Zp</td>
<td></td>
</tr>
<tr>
<td>ZPD</td>
<td>$Z_P$</td>
<td>Limit of integration of the cumulative normal distribution</td>
<td></td>
</tr>
</tbody>
</table>

Analysis Procedure

The step-by-step procedure of Subroutine CALCBC is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Using Subroutine MINT, calculate $P_1$

2. Calculate $P_2$ as:

$$P_2 = 1 - P_1$$
3. Calculate $C_{X_D}$ as:

$$C_{X_D} = m_D^x/(P_1 - P_2)$$

4. Return:
SUBROUTINE CALCBC(ZPO,C)
REAL MSTAR,MSTARU
COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(CAL*0020
150),ZP(70),CUMDIS(70),VP,RP0(50),VCON6(50),ATT(50),PPP,FNXP,R1(50)
CAL*0030
21*R6(50),EK1(50),EK2(50),A2,3*XL*CN,BETA,4,PHIP,EK2,XEND,A1
CAL*0040
COMMON/OUT5/MSTAR,MSTARU
CALL MINT(1,ZPO,ZP,CUMDIS,P1)
P2 = 1.-P1
C = MSTAR/(P1-P2)
RETURN
END
APPENDIX XI - SUBROUTINE CHECKK

The function of Subroutine CHECKK is to calculate the proportionality constant between the mass flow rate out of an element due to mixing and the total mass flowing into it. Subroutine CHECKK is called by Subroutine ZINTER; it does not call any other subroutines. Subroutine CHECKK does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

\[ A2 \quad A3 \quad CN \quad DELX \quad DMFUO \]
\[ IMAX \quad MSTARU \quad SLOPE \quad UDM \quad XD \]
\[ XL \quad XU \]

The internal output consists of:

\[ E \quad EKKD \quad RDOT \]

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine CHECKK which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>DELX</td>
<td>( \delta x )</td>
<td>Integration interval</td>
<td>cm</td>
</tr>
<tr>
<td>DUMMYA</td>
<td>( \mu )</td>
<td>Dummy variable</td>
<td>( \text{cm}^{-1} )</td>
</tr>
<tr>
<td>RDOTT</td>
<td>( \hat{R}_T )</td>
<td>Total rate of change of unburned fuel with axial position in the combustor</td>
<td>( \text{gm/sec-cm} )</td>
</tr>
</tbody>
</table>

Analysis Procedure

The step-by-step procedure of Subroutine CHECKK is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate \( K_D \) as:
\[ K_D = C_N / X_L \]

2. Calculate \( \hat{R}_T \) as:
\[ \hat{R}_T = (\tilde{m}_0)(A_3) \left[ \left( \frac{X_D}{X_L} \right)^{A_2} - \left( \frac{X_U}{X_L} \right)^{A_2} \right] / \delta X \]
3. For the element in question, calculate $E_i$ and $R_i$ as:

$$E_i = K_0$$

$$R_i = R_T \frac{(S_m)_0}{m^*_U}$$

Step 4 is performed only if $(S_m)_0 = 0$

4. Go to step 7.

5. Calculate $\psi_c$ as:

$$\psi_c = - \left[ \frac{\partial (S_m)_0}{\partial x} - R_i \right] / (S_m)_0$$

Step 6 is performed only if $\psi_c > K_D$

6. Calculate $E_i$ as:

$$E_i = 1.1 Q_i$$

7. If this is the last element to be considered go to step 8.
   If not, return to step 3.

8. Return.
SUBROUTINE CHECKK(DELX)

REAL MSTARU
DIMENSION DUMMYA(50)
COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(CHK*0030)
150,ZP(70),CUMDIS(70),VP,RHO(50),BCON6(50),ATT(50),PPP,FNOXP,R1(50)CHK*0040
2),R6(50),EK1(50),EK2(50),A2,A3,XL,CN,BETA,SPHIP,EKS,XEND,A1
COMMON/OUT3/INDIC(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XX,
1FBARD,XU,LEN,TUIDT,TAUDIL,VELOC
COMMON/OUT4/CONGNO(50),AREAD,ASLOPE,DMFUO,SLOPE(50),TSLOCHK*0080
1PE,NOP(50),EKKD,DMFT,UDM(50),DDM(50),FB(50),DMFU5,AIRD,DMFFEDCHK*0090
2,RSUBA,SIG,SIGZER,AVEMW,DMDDA(50),DMDDM(50),DMDDP(50),DMDDPP(50)CHK*0100
3,PRIME(50),NOED,XD,ANO,AQQ,DFENO(50),NOZERO(50),RDOT(50),E(50)
COMMON/OUT5/MSTARDMSTARU

C**** CALCULATE K
C**** EKKD=CN/XL
C**** CHECK K VALUE
C****
RDOTT = DNFUO*A3 *((XO/XL)**A2) - (XU/XL)**A2))/DELX
DO 1000 I=1,IMAX
E(I)=EKKD
RDOT(I) = RDOTT*UDM(I)/MSTARU
IF(UDM(I),EQ,0,0) GO TO 1000
DUMMYA(I) = -(SLOPE(I)-RDOT(I))/UDM(I)
IF(DUMMYA(I)) .GE. EKKD) E(I)=1.1*DUMMYA(I)
1000 CONTINUE
RETURN
END
APPENDIX XII - SUBROUTINE RUNKUT

The function of Subroutine RUNKUT is to obtain the solution of a first-order ordinary differential equation by the Gill variation of the Runge-Kutta method.

Subroutine RUNKUT is called by Subroutine ZINTER and DILUTE; it, in turn, calls Subroutine DERIV. The subroutine does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine. The internal input consists of:

DELX  I  LSGN  Q  XD  Y

The internal output consists of:

Q  XU  Y

Fortran Nomenclature for Subroutine RUNKUT

The following table gives the Fortran nomenclature for those symbols used in Subroutine RUNKUT. Since the subroutine may be used with any consistent set of units, the units of the symbols are not specified. The subscript K, where it appears, is the index of the step in the Runge-Kutta solution.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(K)</td>
<td>a&lt;sub&gt;i&lt;/sub&gt;</td>
<td>A set of constants used to determine DIFF</td>
<td></td>
</tr>
<tr>
<td>B(K)</td>
<td>b&lt;sub&gt;i&lt;/sub&gt;</td>
<td>A set of constants used to determine DIFF</td>
<td></td>
</tr>
<tr>
<td>C(K)</td>
<td>c&lt;sub&gt;i&lt;/sub&gt;</td>
<td>A set of constants used to determine Q</td>
<td></td>
</tr>
<tr>
<td>D(K)</td>
<td>d&lt;sub&gt;i&lt;/sub&gt;</td>
<td>A set of constants used to determine X</td>
<td></td>
</tr>
<tr>
<td>DELX</td>
<td>h</td>
<td>Increment in the independent variable across which the differential equation is to be solved</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>DELY</td>
<td>k_i</td>
<td>Product of YPRIME and DELX at each stage of the solution</td>
<td></td>
</tr>
<tr>
<td>DIFF</td>
<td>ΔY</td>
<td>The change in the value of the dependent variable at each stage of the solution</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>l</td>
<td>Index of element</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>l</td>
<td>Index of the stage of the solution</td>
<td></td>
</tr>
<tr>
<td>LSGN</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=1 if intermediate zone and not the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=2 if intermediate zone and the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=3 if dilution zone or dilution zone type calculation</td>
<td></td>
</tr>
<tr>
<td>Q</td>
<td>q_i</td>
<td>Quantity used to calculate DIFF at each stage of the solution; the value of Q in the final stage of the solution is a measure of the round-off error in Y</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>x_i</td>
<td>Value of the independent variable at each stage of the solution</td>
<td></td>
</tr>
<tr>
<td>Y</td>
<td>y_i</td>
<td>Value of the dependent variable at each stage of the solution</td>
<td></td>
</tr>
<tr>
<td>YPRIME</td>
<td>f(x_i,x_i)</td>
<td>Value of ( \frac{dy}{dx} ) at each stage of the solution</td>
<td></td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine RUNKUT is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate the value of the independent variable at the given stage if the solution as

   \[ x_L = x_{L-1} + h(\Delta L) \]

2. Using Subroutine DERIV, calculate the value of \( f(x_L, y_L) \) at the given stage of the solution.
3. Calculate $k_L$ at the given stage of the solution as:

$$
k_L = \frac{x_i}{y_i} \cdot \frac{h}{h}
$$

4. Calculate the change in the dependent variable at the given stage of the solution as:

$$
\Delta y = a_L + (k_L - b_L)(b_i)
$$

5. Calculate the value of the dependent variable at the given stage of the solution as:

$$
y_L = y_{i-1} + \Delta y
$$

Step 6 is performed only if $y_{i-1} < 0$. If $y_{i-1} > 0$ go to step 7.

6. Set $y_L = 0$.

7. Calculate $q_i$ as:

$$
q_i = q_{i-1} + 3(\Delta y) - (c_L)(k_L)
$$

8. If this is the last stage of the solution, go to step 9. If not, return to step 1.

9. Return.
SUBROUTINE RUNKUT(X, DELX, Y, Q, SGN, I)
DIMENSION A(4), B(4), C(4), D(4)
DATA (A(I), I=1,4)/0.5029289321.70710680.1666667/
1/2+1.010+2.0 (C(I), I=1,4)/0.50.29289321.70710680.5/
2(D(I), I=1,4)/0.050.50.05/ 
C*** RUNKUT - SOLUTION OF A FIRST ORDER ORDINARY DIFFERENTIAL EQUATION 
C*** BY THE GILL VARIATION OF THE RUNGE-KUTTA METHOD 
C*** 
DO 100 K=1,4
X = X+D(K)*DELX
CALL DERIV(X, Y, YPRIME, SGN, I)
DELY = YPRIME*DELX
DIFF = A(K)*(DELY+B(K)*Q)
Y = Y+DIFF
IF(Y.LT.0.0) Y=0.0
100 Q = Q+3.0*DIFF-C(K)*DELY
RETURN
END
APPENDIX XIII - SUBROUTINE DERIV

The function of Subroutine DERIV is to calculate the rate of formation of nitric oxide with respect to axial distance in the combustor intermediate or dilution zone.

Subroutine DERIV is called by Subroutine RUNKUT; it does not call any other subroutines. Subroutine DERIV does not require external input and does not provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

- AREAD
- ASLOPE
- CONGNO
- DDM
- DMDDP
- E
- EK1
- EK2
- FNOXP
- I
- LSGN
- MSTARD
- NO
- NOEQXD
- NOP
- NOZERO
- ROOT
- R1
- R6
- SLOPE
- UDM
- XD
- Y

The internal output consists of:

- DILL
- REAT
- YPRIME

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine DERIV which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFLAME</td>
<td>( \frac{\partial c}{\partial \gamma} )</td>
<td>Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to formation of &quot;prompt NO&quot;</td>
<td>cm(^{-1})</td>
</tr>
<tr>
<td>DMIXT</td>
<td>( \frac{\partial c}{\partial \gamma} )</td>
<td>Total rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing</td>
<td>cm(^{-1})</td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>----------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>DMIX1</td>
<td>$\dot{c}_{mix}^i$</td>
<td>Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing into the element</td>
<td>cm$^{-1}$</td>
</tr>
<tr>
<td>DMIX2</td>
<td>$\dot{c}_{mix}^i$</td>
<td>Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mass change mixing term</td>
<td>cm$^{-1}$</td>
</tr>
<tr>
<td>DMIX3</td>
<td>$\dot{c}_{mix}^i$</td>
<td>Rate of change of elemental NO concentration with axial position in the combustor intermediate zone due to mixing out of the element</td>
<td>cm$^{-1}$</td>
</tr>
<tr>
<td>FNOXG</td>
<td></td>
<td>NO formed in the flame front (mass fraction)</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>$i$</td>
<td>Index of element</td>
<td></td>
</tr>
<tr>
<td>LSGN</td>
<td></td>
<td>Indicator:</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=1 if intermediate zone and not the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=2 if intermediate zone and the last step in the zone</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>LSGN=3 if dilution zone or dilution zone type calculation</td>
<td></td>
</tr>
<tr>
<td>RAT</td>
<td>$\left{ \begin{array}{l} F_D \ \frac{F_D}{P} \end{array} \right}$</td>
<td>Ratio of NO concentration to NO concentration at equilibrium for an element of mixture ratio $F$ and pressure $P$ at axial position $X_D$; ratio of NO concentration to NO concentration at equilibrium at axial position $X_D$</td>
<td></td>
</tr>
<tr>
<td>X</td>
<td>$X_D$</td>
<td>Axial position (downstream) in the combustor</td>
<td>cm</td>
</tr>
<tr>
<td>Y</td>
<td>$\left{ \begin{array}{l} [NO]<em>{X_D} \ [NO]</em>{X_D} \end{array} \right}$</td>
<td>Nitric oxide concentration for an element of mixture ratio $F$ and pressure $P$ (mass fraction) at $X_D$; nitric oxide concentration at $X_D$</td>
<td></td>
</tr>
</tbody>
</table>
### Fortran Symbol	Symbol Description	Units
YPRIME $\left[ \frac{\partial [NO]}{\partial x} \right]_x$ Rate of change of elemental NO concentration with axial position in the combustor intermediate zone; rate of change of NO concentration with axial position in the combustor dilution zone cm$^{-1}$

#### Analysis Procedure

The step-by-step procedure of Subroutine DERIV is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Calculate $\nabla [NO]$.

Steps 2 through 5 are performed only in the dilution zone or for a dilution zone type calculation.

2. If $\nabla [NO]_\text{XD} = 0$, then calculate $\left[ \frac{\partial [NO]}{\partial x} \right]_x$ as:

$$\left[ \frac{\partial [NO]}{\partial x} \right]_x = 0$$

3. If $\nabla [NO]_\text{XD} = 0$, go to step 18.

4. Calculate $(\zeta_D)$ as:

$$\zeta_D = \frac{[NO]_\text{XD}}{[NO]_\text{e} \cdot x_D}$$

5. Go to step 9.

6. Calculate $\left[ \frac{\partial [NO]}{\partial x} \right]_x$ as:

$$\left[ \frac{\partial [NO]}{\partial x} \right]_x = 0$$

Step 7 is performed only if $[NO]_\text{e} = 0$ or if the chemical reaction rate is not significant.

7. Go to step 18.

8. Calculate $(\zeta_D)_\text{e}$ as:

$$\zeta_D = \frac{[NO]_\text{e} \cdot x_D}{[NO]_\text{e} \cdot x_D}$$
9. Calculate \((\hat{r})_{\text{react}}\).
Steps 10 through 13 are performed in the intermediate zone except for the last step in the zone.

10. Calculate \((\hat{r}_{\text{mix}})_1, (\hat{r}_{\text{mix}})_2, (\hat{r}_{\text{mix}})_3\) and \((\hat{r})_{\text{flame}}\).

11. Calculate \((\hat{r}_{\text{mix}})_{\text{TOT}}\) as:
\[
(\hat{r}_{\text{mix}})_{\text{TOT}} = (\hat{r}_{\text{mix}})_1 - (\hat{r}_{\text{mix}})_2 - (\hat{r}_{\text{mix}})_3 + (\hat{r})_{\text{flame}}
\]

12. Calculate \[
\left[ \frac{\partial \hat{r}}{\partial x} \right]_{x_{\text{p}}} = \left( \frac{\partial (\hat{r}_{\text{mix}})_{\text{TOT}}}{\partial x} \right)_{x_{\text{p}}} + \left( \frac{\partial (\hat{r})_{\text{react}}}{\partial x} \right)
\]

Steps 14 and 15 are performed only for the last step in the intermediate zone.

14. Calculate \[
\left[ \frac{\partial \hat{r}}{\partial x} \right]_{x_{\text{d}}} = \left( \frac{\partial (\hat{r})_{\text{react}}}{\partial x} \right)
\]

15. Go to step 18.
Steps 16 and 17 are performed in the dilution zone or for a dilution zone type calculation.

16. Calculate \((\hat{r})_{\text{DIL}}\).

17. Calculate \[
\left[ \frac{\partial \hat{r}}{\partial x} \right]_{x_{\text{d}}} = \left( \frac{\partial (\hat{r})_{\text{react}}}{\partial x} \right) + \left( \frac{\partial (\hat{r})_{\text{DIL}}}{\partial x} \right)
\]

18. Return.
SUBROUTINE DERIV(X,Y,YPRIME,LSGN,I)
REAL *STARD,MSTARU,NOP,NOEQXD,NO
COMMON/DATA1/AIR(50),RR(50),XX(50),FF(50),BCON1(50),BCON2(50),CH2(50)
150),ZP(70),CHMDIS(70),VP,RKO(50),BCON6(50),ATT(50),POP,FNOXP,R1(50)
21,R6(50),E1,K(50),EK2(50),A2*,A3,XL,BETA,SPHIP,EKS,XEND,A1
COMMON/OUT3/INDIC,NO(50),AVET,TauBAR,RHODAR,PHIBAR,TMAX,XD
1FBARD,XU,LEN,TAUINT,TAUDIL,VELOC
COMMON/OUT4/CONGNO(50),DELMD,AREAD,ASLOPE,DMMFO,SLOPE(50),TSLODER
1PE,NOP(50),EKKO,DMFT,UMO(50),DDM(50),FB(50),DMFJD,AIRD,DMMFEDER
2,RSUBX,SIG,SIGER,AVEM,DMDDA(50),DMDDM(50),DMDDP(50),FJER
3PRIME(50),NOEQXD,ANO,AQ0,DFNO(50),NOZERO(50),RDOT(50),E(50)
COMMON/OUT5/STARD,MSTARU
COMMON/OUT6/REAT,
FNOXP = FNOXP*1.0E-06*(30.0/28.0)
IF(LSGN.NE.3) GO TO 500
IF(NOEDO.EQ.0.0) YPRIME = 0.0
IF(NOEQXD.EQ.0.0) GO TO 4000
RAT = Y/NOEDO
GO TO 750
500 CONTINUE
YPRIME = 0.0
IF(CONGNO(I).EQ.0.0) OR NOZERO(I).EQ.1) GO TO 4000
RAT = Y/CONGNO(I)
750 CONTINUE
YPRIME = ((2.0*3.0)/(MSTARD/AREAD)) * (1.0-RAT*RA) * ((R1(I)/(1.0+(RA)
1*EK(I))) * (R6(I)/(1.0*EK2(I))))
REAT = YPRIME
GO TO (1000,2000,3000)*LSGN
1000 DMIX1 = (DMDDP(I)+RDOT(I))*NOP(I)
DMIX2 = E(I)+DMFT(I)+NO(I)
DMIX3 = SLOPE(I)+NO(I)
DFLAME = FNOXP+RDOT(I)
DMIX = DMIX1+DMIX2+DMIX3+DFLAME
DMIX = DMIX/DMFT(I)
YPRIME = DMIX*REAT
GO TO 4000
2000 YPRIME = REAT
GO TO 4000
3000 DILL = -(Y/MSTARD)*ASLOPE
YPRIME = YPRIME*DILL
4000 RETURN
END
APPENDIX XIV - SUBROUTINE ZMASS

The function of Subroutine ZMASS is to determine the mass flow in each element of the distribution function at a prescribed axial station in a gas turbine combustor. In addition, ZMASS calculates the mean mixture ratio, total mass flow, and the airflow rate at each of these axial stations.

Subroutine ZMASS is called by Subroutines PRIMRY, ZINTER, and DILUTE; it, in turn, calls Subroutines CALCBC and MINT. The subroutine does not require external input but does provide external output. Internal input and output are transmitted as arguments of the subroutine and through COMMON. The internal input consists of:

- AIR
- AL
- A2
- A3
- BETA
- CUMDIS
- DDM
- DELX
- EKS
- FF
- INDIC
- MSTARD
- PHIP
- PPP
- RR
- S
- VP
- XD
- XL
- XU
- XX
- ZP

The internal output consists of:

- AIRD
- AREAD
- ASLOPE
- DDM
- DELMD
- DMFFED
- DMFTE
- DMFUD
- DMFUO
- FB
- FBARD
- IMAX
- MSTARD
- MSTARU
- NOZERO
- SIG
- SIGZER
- SLOPE
- TSLOPE
- UDM

The external output consists of:

- AFR
- DDM
- FEDF
- FULOAD
- IHIGHD
- ILOWD

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols used in Subroutine ZMASS which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A</td>
<td>Lower integration limit for the evaluation of the cumulative normal distribution integral</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>ADDM</td>
<td>((\bar{G}_m)_A)</td>
<td>Dummy variable</td>
<td>gm/sec</td>
</tr>
<tr>
<td>AFR</td>
<td>A/F</td>
<td>Over-all air-to-fuel ratio</td>
<td></td>
</tr>
<tr>
<td>AIRI</td>
<td>((\bar{\dot{m}}_A)_I)</td>
<td>Airflow rate at the primary zone exit</td>
<td>gm/sec</td>
</tr>
<tr>
<td>AIRU</td>
<td>((\bar{\dot{m}}_A)_U)</td>
<td>Airflow rate at the upstream axial integration limit of the combustor</td>
<td>gm/sec</td>
</tr>
<tr>
<td>S</td>
<td>B</td>
<td>Upper integration limit for the evaluation of the cumulative normal distribution integral</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>(C_{X_0})</td>
<td>Mass flow coefficient</td>
<td>gm/sec</td>
</tr>
<tr>
<td>DELX</td>
<td>(\delta X)</td>
<td>Increment of the combustor length across which the solution is generated</td>
<td>cm</td>
</tr>
<tr>
<td>DUMMY</td>
<td>((FB)_{DUM})</td>
<td>Dummy variable</td>
<td></td>
</tr>
<tr>
<td>FEDF</td>
<td>((\bar{m}_f)_f)</td>
<td>Total mass of fuel fed into the combustor</td>
<td>lb/hr; lb/sec</td>
</tr>
<tr>
<td>FJLOAD</td>
<td>(\omega)</td>
<td>Fuel loading</td>
<td>lb/sec-ft^3-atm^2</td>
</tr>
<tr>
<td>I</td>
<td>i</td>
<td>Index of the element</td>
<td></td>
</tr>
<tr>
<td>IHIGHD</td>
<td>((i_{\text{HIGH}})_D)</td>
<td>Subscript of the mass element with the highest equivalence ratio (downstream end of integration interval)</td>
<td></td>
</tr>
<tr>
<td>IHIGHU</td>
<td>((i_{\text{HIGH}})_U)</td>
<td>Subscript of the mass element with the highest equivalence ratio (upstream end of integration interval)</td>
<td></td>
</tr>
<tr>
<td>ILOWD</td>
<td>((i_{\text{LOW}})_D)</td>
<td>Subscript of the mass element with the lowest equivalence ratio (downstream end of integration interval)</td>
<td></td>
</tr>
<tr>
<td>ILOWU</td>
<td>((i_{\text{LOW}})_U)</td>
<td>Subscript of the mass element with the lowest equivalence ratio (downstream end of integration interval)</td>
<td></td>
</tr>
<tr>
<td>IN</td>
<td></td>
<td>Counter; indicates first mass element with zero mass at upper end of equivalence ratio distribution function</td>
<td></td>
</tr>
<tr>
<td>KKOUNT</td>
<td>(K_{KOUNT})</td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(KKOUNT = 0) if (FB(I) \leq 2\bar{F}) for the element (i)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(KKOUNT = 1) if (FB(I) &gt; 2\bar{F}) for the element (i)</td>
<td></td>
</tr>
<tr>
<td>Fortran Symbol</td>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>---------------</td>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>KOUNT</td>
<td>K_COUNT</td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>KOUNT = 0 if the element i has no mass</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>KOUNT = 1 if the element i contains mass</td>
<td></td>
</tr>
<tr>
<td>NN</td>
<td>Nn</td>
<td>Number of elements in the array</td>
<td></td>
</tr>
<tr>
<td>NNN</td>
<td>N_n</td>
<td>Number of last mixture ratio boundary</td>
<td></td>
</tr>
<tr>
<td>NPRINT</td>
<td></td>
<td>Indicator</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 0 if intermediate output is not requested by the user</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>NPRINT = 1 if intermediate output is requested by the user</td>
<td></td>
</tr>
<tr>
<td>P1</td>
<td>Pi</td>
<td>Constant - equal to $3.14159265$</td>
<td></td>
</tr>
<tr>
<td>P1</td>
<td>P_1</td>
<td>Value of the normal distribution integral from $-\infty$ to $A$</td>
<td></td>
</tr>
<tr>
<td>P2</td>
<td>P_2</td>
<td>Value of the cumulate normal distribution integral from $-\infty$ to $B$</td>
<td></td>
</tr>
<tr>
<td>SDDM</td>
<td>$\Sigma_{n}m_{i}$</td>
<td>Sum of the element mass flows</td>
<td>gm/sec</td>
</tr>
<tr>
<td>ZPD</td>
<td>Z_{P,n}</td>
<td>Limit of integration of the cumulative normal distribution</td>
<td></td>
</tr>
</tbody>
</table>

**Analysis Procedure**

The step-by-step procedure of Subroutine ZMASS is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

Step 1 is performed only for the primary zone.

1. Calculate $\mathbf{I_{LOW}}_D$ and $\mathbf{I_{HIGH}}_D$ as:
   \[
   \begin{align*}
   \mathbf{I_{LOW}}_D &= 0 \\
   \mathbf{I_{HIGH}}_D &= 50 \\
   \end{align*}
   \]
2. Calculate $\mathbf{I_{LOW}}_U$ and $\mathbf{I_{HIGH}}_U$ as:
   \[
   \begin{align*}
   \mathbf{I_{LOW}}_U &= \mathbf{I_{LOW}}_D \\
   \mathbf{I_{HIGH}}_U &= \mathbf{I_{HIGH}}_D \\
   \end{align*}
   \]
3. Initialize $N_n$
4. Calculate $N_{nn}$ as:
   \[
   N_{nn} = N_n + 1
   \]
5. Initialize \( \aleph m_A \) as:
\[
\aleph m_A = 0
\]

6. Using Subroutine MINT, calculate \( (\dot{m}_A)_X \)

7. Using Subroutine MINT, calculate \( (\dot{m}_A)_X \)

8. Using Subroutine MINT, calculate \( \dot{m}_A \)

9. Using Subroutine MINT, calculate \( \dot{R}_X \)

10. Calculate \( A \) as:
\[
A_X = \frac{\Pi R^2}{\dot{m}_A}
\]

11. Calculate \( (\dot{m}_F)_{\text{red}} \) as:
\[
(\dot{m}_F)_{\text{red}} = k_3 \times q_1 \frac{(\dot{m}_A)_X}{R^2}
\]

Step 12 is only performed in the intermediate and dilution zones.

12. Calculate the fuel loading, \( \psi \) as:
\[
\psi = (\dot{m}_F)_{\text{red}} \times 2.5 \times 0.3 \times V_F \times \frac{\rho}{\rho}
\]

Step 13 is performed only in the intermediate zone and if \( \dot{m}_u = 0 \).

13. Write the fuel loading, \( \psi \).

14. Calculate \( (\dot{m}_F)_o \) and \( (\dot{m}_F)_f \) as
\[
(\dot{m}_F)_o = (\dot{m}_F)_f \times (1 - R)
\]
\[
(\dot{m}_F)_f = (\dot{m}_F)_{\text{red}} \times 2.5 \times q_1
\]

15. Calculate the overall air-to-fuel ratio \( A/F \) as:
\[
A/F = \frac{\dot{m}_A}{(\dot{m}_F)_{\text{red}}}
\]

16. Readjust the units on \( (\dot{m}_F)_f \) from lb/sec to lb/hr.

Step 17 is only performed for the primary zone.

17. Write \( (\dot{m}_F)_f \) and \( A/F \).

Step 18 is performed only in the dilution zone.

18. Calculate \( (\dot{m}_R)_X \) as:
\[
(\dot{m}_R)_X = 0
\]

Step 19 is performed only in the primary and intermediate zones.

19. Calculate \( (\dot{m}_R)_X \) as:
\[
(\dot{m}_R)_X = (\dot{m}_R)_o \left[ 1 - A_3 \left( \frac{X_D}{X_L} \right)^2 \right]
\]
20. Calculate \((\dot{M}_x)_{xD}\) as:
\[
(\dot{M}_x)_{xD} = (\dot{M}_F)_{fed} - (\dot{M}_F)_{xD}
\]

21. Calculate \(M^*_{U}\) as:
- \(M^*_{U} = 0\) in the primary zone
- \(M^*_{U} = M^*_{D}\) in the intermediate and dilution zones

22. Calculate \(M^*_{D}\) as:
\[
M^*_{D} = (\dot{M}_F)_{xD} + M_A|_{xD}
\]

23. Calculate \(\bar{F}\) as:
\[
\bar{F} = \frac{(\dot{M}_F)_{xD}}{M^*_{D}}
\]

Step 24 is only performed in the primary zone.

24. Calculate \(c_0\) as:
\[
c_0 = S_0 \cdot \bar{F}
\]

25. Calculate \(c\) as:
\[
c = c_0 \left[ 1 - \left( \frac{X_F}{X_L} \right)^{A_1} \right]
\]

Steps 26 and 27 are performed only in the dilution zone:

26. Recalculate \(c\) as:
\[
c = 0
\]

27. Go to step 91.

Step 28 is performed only if \(S_0 = 0\).


29. Calculate \(Z_{F, xD}\) as:
\[
Z_{F, xD} = \frac{\bar{F}}{c}
\]

30. Using Subroutine CALCBC, calculate \(C_{xD}\).

Step 31 is performed only in the intermediate and dilution zones.

31. Go to step 36.

32. Calculate \((F_B)_1\) as:
\[
(F_B)_1 = 0
\]

Step 33 is performed for each boundary \(i\) satisfying the criteria 
\[
2 - \xi \leq N_h
\]
33. Calculate \((F_B)_i\) as:
\[
(F_B)_i = \frac{1}{2} (F_i + F_{i-1})
\]

34. Calculate \((F_B)_{NN}\) as:
\[
(F_B)_{NN} = 2*F_n - (F_B)_{NN}
\]

35. Go to step 41.

Steps 36 and 37 are performed for each element \(i\) satisfying the criteria \(1 \leq i \leq i_{\text{MAX}}\).

36. Calculate \((\Sigma m_i)_U\) as:
\[
(\Sigma m_i)_U = 0 \quad \text{in the primary zone}
\]
\[
(\Sigma m_i)_U = (\Sigma m_i)_D \quad \text{in the intermediate and dilution zones}
\]

37. Calculate \((\Delta m_i)_D\) as:
\[
(\Delta m_i)_D = 0
\]

Step 38 is performed only if \(i_{\text{MAX}} = N_n\).

38. Go to step 41.

Steps 39 and 40 are performed for each element \(i\) in the array satisfying the criteria \((i_{\text{MAX}} + 1) \leq i \leq N_n\).

39. Calculate \((\Delta m_i)_D\) as:
\[
(\Delta m_i)_D = 0
\]

40. Calculate \((\Sigma m_i)_U\) as:
\[
(\Sigma m_i)_U = 0
\]

41. Calculate \(i_{\text{MAX}}\) as:
\[
i_{\text{MAX}} = 50
\]

Step 42 is performed only for the special case that \(S_o = 0\) in the primary zone.

42. Go to step 44.

43. Go to step 49.

Steps 44 through 48 are performed for each element \(i\) in the array satisfying the criteria \(1 \leq i \leq i_{\text{MAX}}\).

44. Calculate \((\Sigma m_i)_D\) and \((\Delta m_i)_D\) for the next element as:
\[
(\Sigma m_i)_D = 0
\]
\[
(\Delta m_i)_D = 0
\]

Step 45 is performed only if \((F_B)_i < F\).
45. Go to step 44.
46. Recalculate $i_{\text{MAX}}$ as:
   
   $$i_{\text{MAX}} = i - 1$$

47. Calculate $(\sum m_i)_D$ and $(\sum m_i)_D$ as:
   
   $$(\sum m_i)_D = m_{i_D}$$
   
   $$(\sum m_i)_D = m_{i_D}$$

48. Go to step 92.
49. Initialize the indicators $K_{\text{COUNT}}$ and $K_{\text{KOUNT}}$ as:

   $$K_{\text{COUNT}} = 0$$
   $$K_{\text{KOUNT}} = 0$$

Steps 50-85 are performed for each element $i$ in the array satisfying the criteria $2 \leq i \leq N_{nn}$.

Steps 50 and 51 are performed only if the element $i$ is equal to $N_{nn}$.

50. Calculate $i_{\text{MAX}}$ as:

   $$i_{\text{MAX}} = N_{nn} - 1$$

51. Go to step 75.

Step 52 is performed only if $(F_b)_i \leq 2\bar{F}$.

52. Go to step 54.

53. Calculate $(F_{b,i})_{\text{DUM}}$, $(F_b)_i$, $i_{\text{MAX}}$, and $K_{\text{KOUNT}}$ as:

   $$(F_{b,i})_{\text{DUM}} = (F_b)_i$$

   $$(F_b)_i = 2\bar{F}$$

   $$i_{\text{MAX}} = i - 1$$

   $$K_{\text{KOUNT}} = 1$$

54. Calculate the distribution integration limits as:

   $$A = \left[ (F_{b,i})_i - \bar{F} \right] / \sigma$$

   $$B = \left[ (F_{b,i-1})_{i-1} - \bar{F} \right] / \sigma$$

Steps 55 and 56 are performed only if $A > 0$.

55. Using Subroutine MINT, calculate $P_1$, the value of the normal distribution integral from $-\infty$ to $A$. 
56. Go to step 60.
57. Calculate \( A \) as:
   \[ A = -A \]
58. Using Subroutine MINT, calculate the value of the normal distribution integral from \(-\infty\) to \( A \)
59. Recalculate \( P_1 \) as
   \[ P_1 = 1 - P_1 \]
   Steps 60 and 61 are performed only if \( B \geq 0 \).
60. Using Subroutine MINT, calculate \( P_2 \), the value of the normal distribution integral from \(-\infty\) to \( B \).
61. Go to step 65.
62. Calculate \( B \) as:
   \[ B = 1 - B \]
63. Using Subroutine MINT, calculate \( P_2 \), the value of the normal distribution integral from \(-\infty\) to \( B \).
64. Recalculate \( P_2 \) as:
   \[ P_2 = 1 - P_2 \]
65. Calculate \( (S_{ml})_D \) as:
   \[ (S_{ml})_D = C_x \cdot (P_1 - P_2) \]
   Step 66 is performed only if \( (S_{ml})_D \geq 0 \).
66. Set \( (I_{LOW})_D \) equal to 1.
   Step 67 is performed only if \( (I_{LOW})_D \geq 0 \).
67. Go to step 69.
   Step 68 is performed only if \( (S_{ml-2})_D = 0 \) and \( (S_{ml-1})_D > 0 \).
68. Set \( (I_{LOW})_D \) equal to \( i-1 \).
   Step 69 is performed only if \( (S_{ml-1})_D > 0 \).
69. Reset \( K_{COUNT} \) as:
   \[ K_{COUNT} = 1 \]
   Step 70 is performed only if \( (S_{ml-1})_D = 0 \) and if \( K_{COUNT} = 1 \).
70. Go to step 77.
   Step 71 is performed only if \( (i-1) = i_{MAX} \).
71. Go to step 74.
72. Calculate $\leq S_m$ as:

$$\leq S_m = \leq S_m + (S_m l-1)_D$$

73. Go to step 83.

74. Calculate $(S_m)_D$ as:

$$(S_m)_D = (S_m l-1)_D$$

75. Calculate $(S_m l-1)_D$, $(\Delta m l-1)_D$, and $(I_{high})_D$ as:

$$(S_m l-1)_D = m^{*}_D - \leq S_m$$

$$(\Delta m l-1)_D = (S_m l-1)_D$$

$$(I_{high})_D = D-1$$

76. Go to step 81.

77. Calculate $(S_m l-2)_D$, $(S_m l-2)_D$, and $(\Delta m l-1)_D$ as:

$$(S_m l-2)_D = m^{*}_D - \leq S_m + (S_m l-2)_D$$

$$(\Delta m l-2)_D = (S_m l-2)_D$$

$$(\Delta m l-1)_D = 0$$

78. Calculate $(I_{high})_D$ and $l_{MAX}$ as:

$$(I_{high})_D = D-2$$

$$l_{MAX} = D-2$$

Step 79 is performed only if $K_{COUNT} = 1$.

79. Calculate $(F_B)_{l_{MAX}+2}$ as:

$$(F_B)_{l_{MAX}+2} = (F_B)_{D+2}$$

80. Reset $K_{COUNT} = 0$.

Step 81 is performed only if $l_{MAX} > n_{nn}$.

81. Go to step 85.

82. Go to step 86.
83. Calculate \((S_{m_{i-1}})^{D}\) as:
\[
(S_{m_{i-1}})^{D} = (S_{m_{i-1}})^{D}
\]
Step 84 is performed only if \(I_{\text{MAX}} < 50\).

84. Go to step 86.

85. If this is the last element in the array, continue to step 86. If not, return to step 50 with \(i = i + 1\).

Steps 86-87 are performed only if intermediate output is requested by the user.

Step 86 is performed for each element in the array satisfying the criteria \(1 \leq i \leq I_{\text{MAX}}\).

86. Write \((S_{m_{i}})^{D}\).

87. Write \((I_{\text{LOW}})^{D}\) and \((I_{\text{HIGH}})^{D}\).

Step 88 is performed if \(K_{\text{COUNT}} = 1\).

88. Calculate \((F_{o})_{I_{\text{MAX}}+1}\) as:
\[
(F_{o})_{I_{\text{MAX}}+1} = (F_{o})_{D_{\text{SUM}}}
\]

Step 89 is performed only in the primary zone.

89. Go to step 92.

Step 90 is performed for each element in the array satisfying the criteria \(1 \leq i \leq I_{\text{MAX}}\).

90. Calculate \(\left[ \frac{\partial (S_{m_{i}})}{\partial x} \right]_{x_{D}}\) as:
\[
\left[ \frac{\partial (S_{m_{i}})}{\partial x} \right]_{x_{D}} = \frac{(S_{m_{i}})^{D} - (S_{m_{i}})^{U}}{S_{x}}
\]

91. Calculate \(\left[ \frac{\partial M_{A}}{\partial x} \right]_{x_{D}}\) and \(\left[ \frac{\partial M_{B}}{\partial x} \right]_{x_{D}}\) as:
\[
\left[ \frac{\partial M_{A}}{\partial x} \right]_{x_{D}} = M_{A|x_{D}} - \left( M_{A|x_{U}} \right) \frac{S_{x}}{S_{x}}
\]
\[
\left[ \frac{\partial M_{B}}{\partial x} \right]_{x_{D}} = M_{B|x_{D}} - \left( M_{B|x_{U}} \right) \frac{S_{x}}{S_{x}}
\]

92. Return.
SUBROUTINE ZMASS(DElX)

REAL MSTARU, MSTARD
COMMON/DATA1/ AIR(50), XX(50), FF(50), BCON1(50), BCON2(50), CH2(50)
COMMON/OUT3/ INDC(50)

10 IF(INDIC.IOE.1) GO TO 10

100 IF(INDIC.IOE.1) GO TO 100

C**** CALCULATE AIR FLOW AND COMBUSTOR AREA

C****
NPRINT=0
IF(INDIC.NE.1) GO TO 10
ILOWD=C
IHIGHD=50
10 ILOWU=ILOWD
IHIGHU=IHIGHD
NN=35
NNN=NN+1
SDDM=0.0
CALL MINT(I+5.511,11,XX*AIR*AIRI)
CALL MINT(I+XU+11,XX*AIR*AIRU)
CALL MINT(I+XD+11,XX*AIR*AIRD)
CALL MINT(I+XD+11,XX*RR*RSUBX)
AREA = PI*RSUBX*RSUBX

C**** CALCULATE FUEL FLOW RATES AND DISTRIBUTION CHARACTERISTICS

C****
DMFED = EKS*PHIP*AIRI/BETA
IF(INDIC.IOE.1) FULOAD=DMFED*12.0**3.0**2.5**3.0/(454.*VP*PPP*2.0)
IF(INDIC.IOE.2) AND. MSTARU.EQ.O.0) WRITE(6,8500) FULOAD

8500 FORMAT(///,1X,20HTHE FUEL LOADING IS;E12.5,28H LB./SEC.-CU. FT.=-ZMA*0360)

1ATMO.*ATMO.)
DMFUO = DMFED*(1.0-BETA)
FEDF = DMFED/454.
AFR = AIR(11)/DMFED
FEDF = FEDF/3600.
IF(INDIC.IOE.1) WRITE(6,9100) FEDF
IF(INDIC.IOE.1) WRITE(6,9150) AFR
IF(INDIC.IOE.3) DMFUD = O.O
IF(INDIC.IOE.3) GO TO 100
DMFUD = DMFUO*(I.-A3*(XD/XL)**A2)

C****

100 DMFT = DMFED-DMFUO
IF(INDIC.IOE.1) MSTARU = O.O
IF(INDIC.IOE.1) MSTARU = MSTAR
MSTARD = DMFT*A1-D
FEPARD = DMFT/MSTARD
IF(INDIC.IOE.1) SIGZER=S*FEPARD
SIGZ = SIGZER/(I.-A3*(XD/XL)**A1)
IF(INDIC.IOE.3) SIG = O.O
IF(INDIC.IOE.3) GO TO 8000
IF(SIG.EQ.0.0) GO TO 500

C****
C**** CALCULATE DISTRIBUTION CHARACTERISTICS AND:

C****
C****
ZPO = FBARD/SIG
CALL CALCBC(ZPO*C)

C**** CALCULATE BOUNDARIES AT WHICH EACH F VALUE APPLIES

C**** 500 CONTINUE
IF(INDIC.EQ.1) GO TO 1500
FB(1) = 0.0
DO 1000 I = 2:NN
1000 FB(I) = 0.5*(FF(I-1)+FF(I))
FB(NNN) = 2.0*FF(NNN)-FB(NNN)
GO TO 3000

C**** STORE MASS FLOWS AT PREVIOUS STATION

C**** 1500 CONTINUE
DO 2000 I = 1:IMAX
IF(INDIC.EQ.1) UDM(I) = 0.0
IF(INDIC.EQ.1) UDM(I) = DDM(I)
DELMD(I) = 0.0
2000 CONTINUE
IF(IMAX.EQ.NN) GO TO 2200
IN = IMAX + 1
DO 2100 I = IN, NN
DELMD(I) = 0.0
2100 UDM(I) = 0.0
2200 CONTINUE

C**** CALCULATE IMAX

C**** 3000 CONTINUE
IMAX = 50

C**** SPECIAL CASE S=0.0 IN PRIMARY ZONE

C**** IF(S.EQ.0.0.AND.INDIC.EQ.1) GO TO 2300
GO TO 2500

2300 DO 2400 I = 1:IMAX
DDM(I) = 0.0
DELMD(I) = 0.0
NOZERO(I) = 1
IF(FB(I) .LT. FBARD) GO TO 2400
IMAX = I + 1
DDM(I-1) = MSTD
DELMD(I-1) = MSTD
NOZERO(I-1) = 0
GO TO 9000
2400 CONTINUE

2500 CONTINUE
KOUNT = 0
KKOUNT = 0
DO 5000 I = 2:NNN
IF(I.EQ.NNN) IMAX = NNN - 1
IF(I.EQ.NNN) GO TO 4800
IF(FB(I) .LT. (2.0*FBARD)) GO TO 4000
DUMMY = FB(I)
FB(I) = 2.0*FBARD
IMAX = I + 1
KKOUNT = 1
4000 CONTINUE
**C**** CALCULATE THE ELEMENT MASSES

**C****

\[ A = \frac{(F_B(I) - F_BRAD)}{\Sigma Z} \]
\[ B = \frac{(F_B(I - 1) - F_BRAD)}{\Sigma Z} \]

IF(A .GE. 0.0) CALL MINT(1, A, 70, ZP, CUMDIS, P1)
IF(A .LT. 0.0) GO TO 4500

\[ A = -A \]

CALL MINT(1, A, 70, ZP, CUMDIS, P1)

P1 = 1.0 - P1

4500 IF(B .GE. 0.0) CALL MINT(1, B, 70, ZP, CUMDIS, P2)
IF(B .LT. 0.0) GO TO 4800

B = B

CALL MINT(1, B, 70, ZP, CUMDIS, P2)

\[ P2 = 1.0 - P2 \]

4800 DDM(I-1) = C*(P1 - P2)
IF(DDM(I-1) .LT. 0.0) ILOWD = 1
IF(ILOWD .LT. 0.0) GO TO 4850
IF(DDM(I-2) .LT. 0.0) KOUNT = 1
IF(DDM(I-1) .LT. 0.0) AND KOUNT .EQ. 1) GO TO 4900
IF(I .LT. 1) EQ. IMAX) GO TO 4875

SDM = SDDM + DDM(I-1)

GO TO 4950

4875 ADDM = DDM(I-1)

4880 DDM(I-1) = MSTARD - SDDM
DELMD(I-1) = DDM(I-1)
IHIGHD = I - 1
GO TO 4925

4900 DDM(I-2) = MSTARD - SDDM + DDM(I-2)
DELMD(I-2) = DDM(I-2)
DELMD(I-1) = 0.0
IHIGHD = I - 2
IMAX = I - 2
IF(KKOUNT .EQ. 1) FB(IMAX + 1) = DUMMY
KCOUNT = 0

4925 CONTINUE
IF(IMAX .LT. NNN) GO TO 5000
GO TO 6000

4950 DELMD(I-1) = DDM(I-1)
IF(IMAX .LT. 50) GO TO 6000

5000 CONTINUE

6000 CONTINUE
IF(NPRINT .EQ. 1) WRITE(6, 9999) (DDM(I), I = 1, IMAX)
IF(NPRINT .EQ. 1) WRITE(6, 9998) ILOWD, IHIGHD
IF(KKOUNT .EQ. 1) FB(IMAX + 1) = DUMMY

C****

**C****

**C****

IF(INDDC .EQ. 1) GO TO 9000
DO 7000 I = 1, IMAX
SLOPE(I) = (DDM(I) - UDM(I)) / DELX

7000 CONTINUE

8000 CONTINUE
ASLOPE = (AIRN - AIRU) / DELX
TSLOPE = (MSTARD - MSTARU) / DELX

9100 FORMAT(///, 10X, 58HTHE COMPUTED TOTAL MASS OF FUEL FED INTO THE CZMA*1760
10MBUSOR IS \( E12.5,8H \LB./HR.///)\n
9150 FORMAT(10X, 42HTHE COMPUTED OVERALL AIR-TO-FUEL RATIO IS , E12.5;///)
9998 FORMAT(5X,20I5//)
9999 FORMAT(10X,10E10.3/)
9000 RETURN
END
APPENDIX XV - SUBROUTINE PRINTS

The function of Subroutine PRINTS is to provide the written output of the calculated results of the program.

Subroutine PRINTS is called by Subroutines PRIMRY, ZINTER, and DILUTE; it does not call any other subroutine. Subroutine PRINTS does not require external input and does provide external output. Internal input is transmitted through COMMON. There is no internal output. The internal input consists of:

- AVCH2D
- AVCH2F
- AVCH2P
- AVECOD
- AVECOF
- AVECOP
- AVECSD
- AVECSF
- AVECSP
- AVENOF
- AVENOP
- AVET
- INDIC
- PHIBAR
- RHOBAR
- TAUBAR
- XD

Additional Fortran Nomenclature

The following table gives the Fortran nomenclature for those symbols in Subroutine PRINTS which are not included in COMMON.

<table>
<thead>
<tr>
<th>Fortran Symbol</th>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVCH2</td>
<td>$\text{CH}_2^*$</td>
<td>Equilibrium concentration of unburned hydrocarbons exclusive of $\text{C}_\text{s}$ and CO at $X_D$.</td>
<td>lb/ft$^3$</td>
</tr>
<tr>
<td>AVECO</td>
<td>CO$^*$</td>
<td>Equilibrium concentration of CO at $X_D$.</td>
<td>lb/ft$^3$</td>
</tr>
<tr>
<td>AVECS</td>
<td>$\text{C}_\text{s}$</td>
<td>Equilibrium concentration of $\text{C}_\text{s}$ at $X_D$.</td>
<td>lb/ft$^3$</td>
</tr>
<tr>
<td>AVENO</td>
<td>NO$^+$</td>
<td>Concentration of NO at $X_D$.</td>
<td>lb/ft$^3$</td>
</tr>
<tr>
<td>AVENO$_2$</td>
<td>NO$_2$</td>
<td>Equivalent concentration of NO$_2$ at $X_D$.</td>
<td>lb/1000 lb fuel burned</td>
</tr>
<tr>
<td>AVETF</td>
<td>T</td>
<td>Temperature at $X_D$.</td>
<td>deg F</td>
</tr>
<tr>
<td>DENOM</td>
<td></td>
<td>Constant</td>
<td>ft$^2$ - cm$^3$ - lb</td>
</tr>
<tr>
<td>IPRINT</td>
<td></td>
<td>Indicator</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IPRINT = 0 if intermediate zone heading is to printed</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>IPRINT = 1</td>
<td>-</td>
</tr>
</tbody>
</table>
### Fortran Symbol | Description | Units
---|---|---
if intermediate zone heading is not to be printed | IPRINT = 2 |  |
if dilution zone heading is not to be printed |  |  |
RHOBA | Mean density of combustion products | lb/ft$^3$
T| $t$ | msecs
XOUT | Axial position downstream in the combustor | in

**Analysis Procedure**

The step-by-step procedure of Subroutine PRINTS is given below. The Fortran listing of the subroutine is presented at the conclusion of the step-by-step procedure.

1. Convert $X_D$ from cm to in.
2. Convert $t$ from secs to msecs.
3. Convert NO, CO, $C(s)$, and CH$_2$ concentrations from gm/cc to lb/ft$^3$.
4. Convert NO concentration at $X_D$ to the equivalent NO$_2$ concentration.
5. Convert $\rho$ from gm/cc to lb/ft$^3$.
6. Convert $T$ from deg K to deg F.
7. If this is the primary zone, write the primary zone heading and output. Go to step 12. If it is not the primary zone, go to step 8.
8. If this is the intermediate zone and the first written output for the zone, write the heading for the intermediate zone. If not, go to step 9.
9. If this is the intermediate zone, write the output at $X_D$. Go to step 12. If it is not the intermediate zone, go to step 10.
10. If this is the dilution zone and the first written output in the zone, write the heading for the dilution zone. If not, go to step 11.
11. If this is the dilution zone, write the output for the dilution zone at $X_D$. Go to step 12.

12. Return.
SUBROUTINE PRINTS
REAL NO, PRT*
COMMON/OUT1/AVECSG,AVECOG,AVCH2G,AVECSP,AVECOP,AVCH2P,AVECSO,AVECOPRT*0020
1D,AVCH2D,AVECSF,AVECOF,AVCH2F
COMMON/OUT2/AVENOD,AVENOP,AVENOF,AVENFU,RHO,ILAST
COMMON/OUT3/INDIC,NO(50),AVET,TAUBAR,RHOBAR,PHIBAR,IMAX,XD,*
COMMON/OUT4/CONGNO(50),DELmD0(50),AREAO,ASLOPE,FUOSLOPE(5L),TSLOPRT
COMMON/OUT5/PENOP(50),EKKOMFTUDM(50),001(50),FD(50),BARDXUL,TAU.DIL,VELOC
COMMON/OUT6/SUB8ASIGSIGZER,AVEMW,DMDD(50),DMDDP(50),DMDDPP(50),FRPT
3PRIME(50),NOEQXD,ANO,AQG,DIRNO(50),NOZERO(50),RDOT(50),E(50)
NPRINT=0
IF(INPRINT.EQ.1) IPRINT=0
XOUT=XD/2*54
TTUHAR=TAUBAR*1000.
AVENO=AVENOD/DENOM
AVECO=AVECDO/DENOM
AVCH2=AVCH2D/DENOM
AVEN02 = AVENO*46.0/30.0
RHOBA=RHOBAR/DENOM
AVETF=((AVET-273.16)*1.0*32.0)
GO TO (1000,1020,1030),INDIC
1000 CONTINUE
WRITE(6,1010)
1010 FORMAT(1H,)
WRITE(6,1020)
1020 FORMAT(48H THIS IS THE MAIN PRINTOUT FOR THE PRIMARY ZONE /////)
GO TO 4000
2000 IF(IPRINT.EQ.1) GO TO 5500
WRITE(6,1010)
WRITE(6,2020)
2020 FORMAT(53H THIS IS THE MAIN PRINTOUT FOR THE INTERMEDIATE ZONE 1////////)
3000 IF(IPRINT.EQ.2) GO TO 5500
WRITE(6,1010)
WP=TE(6,3020)
3020 FORMAT(49H THIS IS THE MAIN PRINTOUT FOR THE DILUTION ZONE /////)
3040 IF(INPRINT.EQ.1) WRITE(6,9999)
WRITE(6,5000)
5000 FORMAT(1X,6HX(IN+),1X,3HPHI,1X,1HT,6X,3HRHO,3X,3H Tau,6X,2HNO,9X,3HPRT)
1N02. 9X,4HC(S), 6X,4HC(S), 8X,2HCO, 9X,2HCO, 8X,3HCH2, 8X,3HCH2)
WRITE(6,5100)
5100 FORMAT(8X,4HAVE,,1X,5HDEG F,3X,4HAVE,,2X,4HAVE,,5X,3HPPM,6X,7HLBS
1PER,7X,3HPPM,5X,7HLBS PER,7X,3HPPM,5X,7HLBS PER, 6X,3HPPM,7X,7HLBS)
WRITE(6,5200)
5200 FORMAT(1X,7HLB/CUFT,1X,4HMSEC,4X,5H(VOL),5X,7H1000 LB,6X,5H(VOL),1
X,7H1000 LB,6X,5H(VOL),4X,7H1000 LB,5X,5H(VOL),4X,7H1000 LB)
WRITE(6,5300)
BURNED)
5500 WRITE(6,6000)XOUT,PHIBAR,AVETF,RHOBAR,TAUBAR,AVENOP,AVENO2,AVECSPRT
1AVECSF,AVECOP,AVECSO,AVECOPRT
6000 FORMAT(1X,F5.2,1X,F4.2,1X,F5.0,1X,F6.4,1X,F6.4,1X,F6.4,1X,F6.4,1X,B(6E10,31X))
IF(NPRINT.EQ.1) WRITE(6,9999)( NO(I),I=1,IMAX)
9999 FORMAT(10X,4H **,8E12.4)
RETURN
END
APPENDIX XVI - METHOD OF CALCULATION OF AIR DISTRIBUTION CHARACTERISTICS

Air enters the combustor liner at discrete positions over the whole length of the liner. The bulk of such flow normally enters perpendicular to the direction of the mainstream product flow and has then to be deflected and entrained before it can mix with the combustion products. This action requires a finite time (i.e., distance) to occur, and its effect upon the nitric oxide formation process has to be considered. A method has been developed, therefore, to take account of this effect. The method is consistent with the mixing assumptions made in the flow model described in this report; it has been applied to all combustors considered in this report and is described below.

The flow behavior at each port shown in the figure above is assumed to behave as follows:

Port 1 All air entering at this position is assumed to mix with the products in the primary zone.

Port 2 Some fraction of the air, f, mixes with the primary zone and the remainder is entrained according to the law described for port 4.
Port 3 Cooling air mixes according to the relationship

\[ M_X = M_3 \left( \frac{\text{Distance from port 3 to } X}{\text{Distance from port 3 to } X_L} \right)^{0.5} \]

and that part which mixes before the primary zone exit \((X = 0)\), is assumed to burn in the primary zone.

Port 4

and 5 Both cooling and combustion air mix according to the relationship shown above, i.e.,

\[ M_X = M_4 \left( \frac{(X-X_L)}{(X_L-X_4)} \right)^{0.5} \]

Port 6

and 7 This air enters the dilution zone so it is assumed that instantaneous mixing occurs (see Section 2.5). All these independent mass flows are then summed at a particular position along the combustor to give the total airflow contained with the combustion products at that point. For example:

- Air burning in the primary zone \( M_{pz} \) is given by,
  \[ M_{pz} = M_0 = M_1 + fM_2 + M_3 \]
  \( x = 0 \)

- Air at position \( X \) \((0 < X < X_L)\)
  \[ M_X = (1-f)M_2 + M_3 + M_4 + M_5 + M_{pz} \]

- Air at position \( X, (X_7 < X < X_6)\)
  \[ M_X = \sum_{1}^{5} M_n + M_7 \]

This method was applied to combustors A and B studied in this report and in each case the value of \( f \), the fraction of air entering the primary zone from the first row of air ports, was assumed to equal one third. For Combustor A this value corresponded to the value recommended by the designers, but in the case of Combustor B, the value was estimated based on the design features. Errors in the predictions of nitric oxide emission levels from this latter estimate can be expected to be negligible as the total airflow through port 2 represents less than two per cent of the total airflow.