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A MODIFIED MATHEMATICAL MODELING

IN GAS TURBINE COMBUSTORS

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ABSTRACT

Computation of the local flow structure, heat transfer, and chemical species concentration in a two dimensional combustor of a gas turbine is described. The prediction is based on a modified TEACH computer program. A simulation of combustion of methane, the assumed fuel, is done in two major steps ($\text{C H}_4 \dots \text{C O} + 2 \text{H}_2 \text{O}$ followed by $\text{C O} + 1/2 \text{O}_2 \dots \text{C O}_2$). In addition formation of other two dominant products, $(\text{NO})^2$ and $(\text{OH})^2$ is traced. Influence of some selected parameters, as air/fuel ratio, velocities ratio, diameters ratio on the performance of the combustor is demonstrated.

INTRODUCTION

The Phenomena

Designers of combustors are aided by experiments, but as an alternative to them, economical design and operation can be facilitated by prior prediction of the flow field. This prediction is found by use of a mathematical model incorporating a numerical solution algorithm of the governing differential transport equations. Strong coupling between the fluid dynamics aspects of a flow and its related chemical kinetics is a merit of consideration during the solution. By sophistication of the mathematical model, a closer approach to the phenomena can be realized.

The Problem

Formation of (C O) , (N O) , and (O H) in the combustion products of methane has considerable influences on the flow parameters inside the combustor, so an analysis for these influences is required. In such analysis, there are two areas of difficulty; the simulation and solution. The simulation should consider the whole aspects of the flow and the mathematical solution should be more quick and cheap than by experiments in real life systems.

Previous Works

Axisymmetric simulation of the flow field in gas turbine combustors had been developed in many works. Some of these simulations give rise to 2-D elliptic flows that considered stream function, or pressure-velocity

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p -u -v formulations, and Gaus-Seidel point by point iterations or line by line SIMPLE (Semi - Implicit Method for Pressure Linked Equation) iterative procedure [1,10] where the line by line method involves tridiagonal matrix (TDM) algorithm. Turbulence simulations were developed in most of the previous works by a way of two equations of a k -a model as in the imperial college TEACH (Teaching Elliptic Axisymmetric Characteristics Heuristically) Computer program [1] .

The simulation of combustion process was done mainly via a simple one step chemical reaction model [7] based on Arrhenious, and breakup concepts for diffusion and premixed situations. Other works in combustion process considers higher degrees of reaction [11], but the solution was devided into two separate algorithms considering weak coupling between the dynamics of the flow and its chemical kinetics.

Outlines of the Paper

This paper introduces a finite difference solution of a 2-D reacting turbulent recirculating flows, in a gas turbine combustors with emphasis on a sophisticated combustion process of methane/air mixture. Formation of (C O), (N O), and (O H) and their inflence on the velocities and temperature fields is demonstrated. The presented algorithm provides simultaneous solution of the equations governing the whole aspects of the flow, and in the same time, it provides the solution with comparatively very small computation time.

Basic equations are presented and molded into a common form in sect.2. The whole solution procedure are dealt with in sect.3, via a discussion of the grid system, finite difference equations, boundary conditions and physical properties evaluation. Results, discussions and conclusions are presented in sect.4.

THEORITICAL MODEL

Governing Equations

The following system of equations , as found in may literatures [1-11] , describe the 2-D reacting turbulent and recirculating flows :

Equations of continuity and momentum

Continuity eqn.

$$\frac{1}{r} \frac{\partial}{\partial r} (r v) + \frac{\partial}{\partial x} (\rho u) = 0 \tag{1}$$

r, x momentum :

$$\rho (v \frac{\partial v}{\partial r} + u \frac{\partial v}{\partial x}) = - \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} (2 r \mu \frac{\partial v}{\partial r}) - 2 \frac{\mu v}{r^2} + \frac{\partial}{\partial x} (\mu (\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x})) \tag{2}$$

$$\rho (v \frac{\partial v}{\partial r} + u \frac{\partial u}{\partial x}) = - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (2 r \mu \frac{\partial u}{\partial r}) + \frac{\partial}{\partial x} (2 \mu \frac{\partial u}{\partial x}) \tag{3}$$

Differential Transport Equations for k and e

k-Equation

$$\rho (v \frac{\partial k}{\partial r} + u \frac{\partial k}{\partial x}) = \frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_k \frac{\partial k}{\partial r}) + \frac{\partial}{\partial x} (\Gamma_k \frac{\partial k}{\partial x}) + G_k - \rho \tag{4}$$

ε Equation

$$\rho (v \frac{\partial \epsilon}{\partial r} + u \frac{\partial \epsilon}{\partial x}) = \frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_{\epsilon} \frac{\partial \epsilon}{\partial r}) + \Gamma_{\epsilon} \frac{\partial \epsilon}{\partial x} + C_1 \frac{\epsilon}{k} G_k - C_2 \frac{\rho \epsilon^2}{k} \quad (5)$$

Where C₁ and C₂ are constants with the values recommended as 1.43 and 1.92 the term G_k is given by :

$$G_k = \mu_t (2 (\frac{\partial u}{\partial x})^2 + 2 (\frac{\partial v}{\partial r})^2 + 2 (\frac{v}{r})^2 + (\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x})^2) \quad (6)$$

Energy Equation

$$\frac{1}{r} \left\{ \frac{\partial}{\partial x} (\rho u r h) + \frac{\partial}{\partial r} (\rho v r h) - \frac{\partial}{\partial x} (r \Gamma_h \frac{\partial h}{\partial x}) - \frac{\partial}{\partial r} (r \Gamma_h \frac{\partial h}{\partial r}) \right\} = s_h \quad (7)$$

where

$$\begin{aligned} \Gamma_{\phi} &= 0.09 \mu k^2 / \epsilon G_{\phi} \\ s_{\phi} &= \text{respective source term for } \phi \quad [6] \end{aligned} \quad (8)$$

Reaction Equations

Conservation equation for a chemical species, can be expressed as :

$$\rho (v \frac{\partial m_j}{\partial r} + u \frac{\partial m_j}{\partial x}) = R_j + \frac{1}{r} \frac{\partial}{\partial r} (r \Gamma_j \frac{m_j}{\partial r}) + \frac{\partial}{\partial x} (\Gamma_j \frac{\partial m_j}{\partial x}) \quad (9)$$

Where m_j is the mass fraction of the chemical species j, it may represent air, C₂H₄, CO₂, NO, and OH. The term R_j is the mass rate per unit volume of creation or decay of the species j by chemical reaction.

Fuel Combustion

Predictions of the local mass fractions of fuel C₂H₄, CO₂, H₂O, O₂, and N₂ are provided by a slightly more sophisticated kinetic scheme proceeding via the following steps [3,13] :



All the presented chemical calculations are related to 1 kg of air, so the fuel - air mixture can be rich, or lean according to the value of the equivalence ratio defined by :

$$\xi = (F/A)_{\text{actual}} / (F/A)_{\text{stoichiometric}} \quad (11)$$

Introducing the reaction rates R_{CH₄}, R_{CO} as found imperically in [3], two differential transport equations in the form of equation (9) can be solved for determination of the two parameters y_{C₂H₄} and y_{CO} representing the concentration of the chemical species C₂H₄ and also CO₂.

In addition, algebraic equations resulting from the conservation consideration of the other species air, CO, H₂O and O₂ is furnished as :

$$m_{O_2} = y_{air} - y_{N_2}^o - 3/2 (M_{O_2} / M_{CH_4}) (y_{CH_4}^o - y_{CH_4}) \quad (12)$$

$$- (M_{O_2} / M_{CO_2}) y_{CO_2} - (M_{O_2} / M_{NO}) y_{NO} + (M_{O_2} / M_{OH}) y_{OH}$$

$$m_{H_2O} = 2 (M_{H_2O} / M_{CH_4}) (y_{CH_4}^o - y_{CH_4}) - (M_{H_2O} / M_{CH_4}) \quad (13)$$

$$m_{CO} = (M_{CO} / M_{CH_4}) (y_{CH_4}^o - y_{CH_4}) - (M_{CO} / M_{CO_2}) y_{CO_2} \quad (14)$$

where $y_{CH_4}^o$ and $y_{N_2}^o$ represent the concentration of CH₄ and N₂ at no combustion which can be calculated according the value of the equivalence ratio.

NO Formation

Following Iverach [3] and Zeldovich [14], the formation of (NO) can be predicted according to the mechanism.



Introducing the reaction rate R_{NO} as found in [10], for the (NO) reaction, a differential transport equation in the form (2.9) can be solved for the determination of the parameter y_{NO} representing the concentration of the chemical species NO.

OH Formation

According to Iverach et al., [3], the formation of OH can be derived by assuming the reaction :



Reaction rate R_{OH} can be found in a similar procedure followed by Peck et al., [10], by using the equality of the ratios O/O₂ and N/N₂ as found by Iverach et al., [3]. Introducing R_{OH} as the source term in a differential transport equation as (2.9), we may solve to find the concentration y_{OH} .

Concerning the conservation equation for air, it is written with the source term as the rate of consumption of Oxygen as found from equation (11).

The conservation equation for air is solved to determine y_{air} to be substituted in equation (12).

Common Form of the Governing Equation

Common Form of the Governing Equation

Similarity between the differential equations and their diffusion terms allows them all to be put in the common form :

$$\frac{1}{r} \left\{ \frac{\partial}{\partial x} (\rho u r \phi) + \frac{\partial}{\partial r} (\rho v r \phi) - \frac{\partial}{\partial x} \left(r \Gamma_{\phi} \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma_{\phi} \frac{\partial \phi}{\partial r} \right) \right\} = S_{\phi} \quad (17)$$

where ϕ stands for any of the solution parameter $u, v, k, e, h, y_{CH_4}, y_{CO_2}, y_{NO}, y_{OH},$ and y_{air} . Putting $\phi = 1.$, and $S_{\phi} = \Gamma_{\phi} = 0.$, the common form will lead to the continuity equation used for pressure correction. Such similarity for the governing equations for all the field parameters, lead to a repetitive solution of the whole problem which simplifies the solution algorithm to using one subroutine for solving the whole set of equations.

SOLUTION PROCEDURE

Preliminary Remarks

Having a nonlinear system of equations to be solved, and having often irregular boundaries, we get to a conclusion that the analytical solution procedures are inapplicable. So, if the solution can be obtained at all, it will be only through iterative numerical procedures. Of these, the most successful one is that which concentrate attention on a finite number of points within the integration domain, and solve the simultaneous algebraic equations derived from the characterizing differential equations to connect the dependent variable at these points with the values at the neighbouring points and boundaries.

The Staggered Grid

Figure (1) illustrates an integration domain while figure (2) shows some of the rectangular computational mesh surrounding a grid node P(I,J) with its four neighbouring points. The intersections of the solid lines mark the grid nodes where all variables except u and v velocity components are stored. The latter are stored at points which are denoted by the arrows and located midway between the grid intersection.

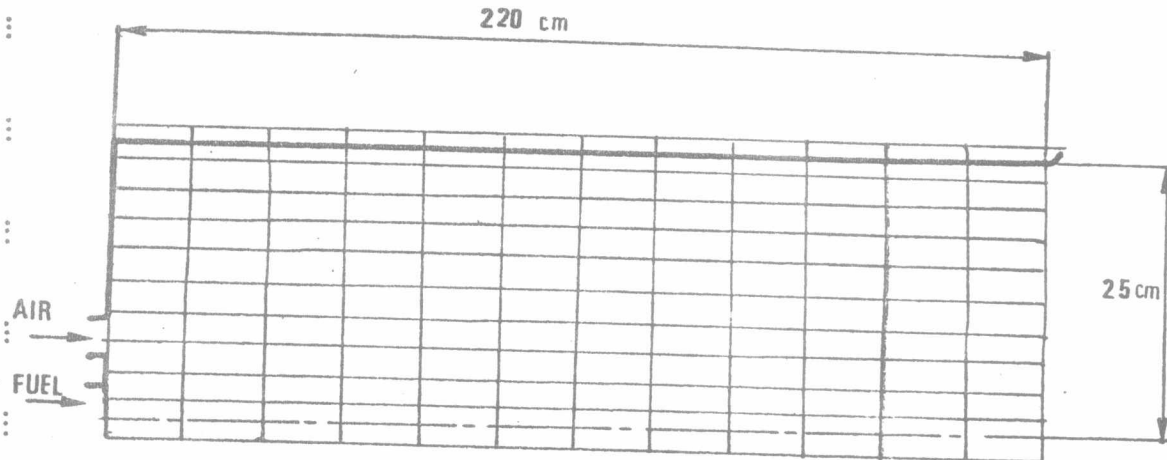


Fig.1. Schematic of the staggered grid.

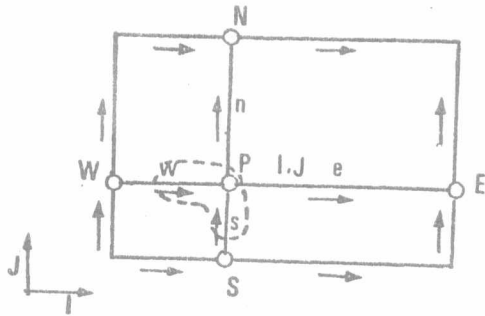


Fig.2. Computation Mesh.

Such grid arrangement places the velocities between the pressure that derives them so it became easier to calculate the local values of pressure gradients. Boundaries are located midway between mesh lines, so that normal velocities are located directly on the boundaries.

Finite Difference Equations

Finite difference equation for the general dependent variable ϕ can be found by integrating the equation (17) over the entire domain for ϕ in question, and then expressing the resulting terms through grid point values.

The source term S_{ϕ} is integrated over the control volume by assuming that the values of ϕ and ϕ at P, prevail over the entire control volume. Such volume integral is linearized in the form: $S_p^{\phi} \phi_p + S_u^{\phi}$, [11], where S_p^{ϕ} should be negative to aid the convergence of the iteration process [8]. There is introduced also, a false source stabilizing term which had no effect on the final solution obtained but alleviates situations that sometimes arise when mass flows at some stage do not satisfy continuity equation. Such situations sometimes yield all coupling coefficients to be zero and the finite difference equations to be singular. Such false source term is evaluated as :

$$S_{false} = | \dot{m}_{net} | (\phi_p^{old} - \phi_p) \tag{18}$$

where \dot{m}_{net} is the net outflow of mass from a cell control volume at certain stage in the computation. When the convection and diffusion terms in equation (17) are integrated over the control volume, they give rise to the integral of the convective and diffusive fluxes across the control volume surfaces, via application of Gauss' divergence theorem. Expressing these integrals in a 'hybrid' scheme as a combination of the central and upwind differences [8], the following general equation is obtained :

$$a_p^{\phi} \phi_p = \sum_j a_j^{\phi} \phi_j + S_u^{\phi} \tag{19}$$

where

$$a_p^{\phi} = \sum_j a_j^{\phi} - S_p^{\phi} \tag{20}$$

where ϕ_j = sum over N, S, E, and W points,

So, equation (19) represent the finite difference scheme that is utilized

in solution for the determination of the enthalpy, turbulence parameters, and chemical species concentrations at the nodal points of the control volume. Similar equation is involved in velocity field (u, v) solution but it is coupled with continuity equation (for pressure correction) through application of SIMPLE [8] algorithm.

The source term in the used scheme is the dominant factor. Starting with the energy equation, the source term for enthalpy is written simply as:

$$S_u^h = \sum_j c_j h_j^o \quad (21)$$

where :

$$h_j^o = H_{CH_4} Y_{jCH_4} + H_{CO} Y_{jCO} + H_{NO} Y_{jNO} + H_{H_2O} Y_{jH_2O} + H_{HO} Y_{jHO} \quad (22)$$

Hence :

$$a_p^h h_p = \sum_j a_j h_j + \sum_j c_j^h h_j^o \quad (23)$$

where : H is the enthalpy of formation of the denoted compounds, \sum_j is the sum over N, S, E, and W points, and C_j represent the convection terms.

Boundary Condition

Conditions are specified on the entire boundary around the solution domain. All variables are given definite fixed values at the inlet (Dirichlet conditions), and at the outlet all variables are given zero normal gradient conditions (Neumann condition). In the pressure correction equation, it is enforced zero normal gradient condition on p' . In the energy equation, the enthalpy h is given zero normal gradient specification entirely around the flow domain, considering adiabatic wall condition. In stating the boundary conditions for the conservation equations for air and fuel, the inlet boundary conditions are evaluated in such a way that the total mass of inlet air sums to 1 kg/s, and for fuel, it sums to $\xi (F/A)$ stoichiometric kg/s.

Physical Properties

Departure of the calculated products composition from the initial guess leads to change of the estimated molecular weight at each iteration step. Similarly, departure of the calculated temperature field from the initial approximation leads to change of the flow properties. Hence, updating of the flow properties is done after each iteration step, where density correction is done through direct application of the equation of state, and viscosity updating is done by application of simplified effective viscosity model as introduced by Gosman [1].

Solution Procedure

The solution procedure used here has been found by various works and has undergone a process of continuous development in the light of the experience gained from each study to the form which is presented here. In solution of the problem under consideration, we have 10 finite difference equations which are solved iteratively, coefficient and source terms updating is carried out prior to each iteration. The Tri-Diagonal Matrix

(TDM) algorithm [4,8], is used for finding solution of each equation separately in the iteration procedure. At this kind of iteration the experience gained [5,8] imply the use of some degree of relaxation with a relaxation factor of the value 0.5-0.9.

The convergence of solution is decided by the point residuals that measures the departure from exactness of the variable ϕ at the point P. A residual term is defined for each variable at each point and at each iteration by the equation:

$$R_p^\phi = a_p^\phi \phi_p - \sum_j a_j^\phi \phi_j - S_u^\phi \quad (24)$$

At each iteration step the value of R is evaluated for each point, and if there is no value for this term, at any point, exceeding a certain reference value, after a finite number of iteration procedures, then the iteration procedure is terminated and the equations are considered to be finally solved.

RESULTS AND DISCUSSIONS

In order to demonstrate the capability of the program in simulating diffusion flames with emphasis on dissociation, calculations which deal with application of the code to specific combustor design will be presented. Fuel is assumed to be injected in at the center, and air is introduced through an annulus surrounding the injection core with no swirl. Adiabatic conditions on the surrounding walls are assumed.

General Predictions

General predictions about the effect of air/fuel ratio, fuel to air velocities, and diameter ratios are found. As standard base case, the combustor conditions being studied is one in which both injected fuels and air velocities are equal, and the fuel/air ratio equal to the stoichiometric one and $d/L = 0.1$.

Fig.3. displays the velocity vectors showing the magnitude and directions of gases flow, and the corresponding plot of temperature contours is shown in Fig.4. The location of flame front is indicated by sweep temperature gradients.

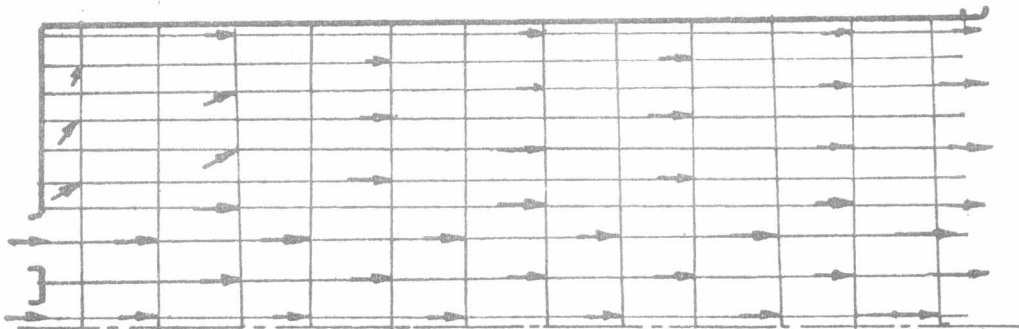


Fig.3. Velocity Vectors showing magnitude & directions of the flow.

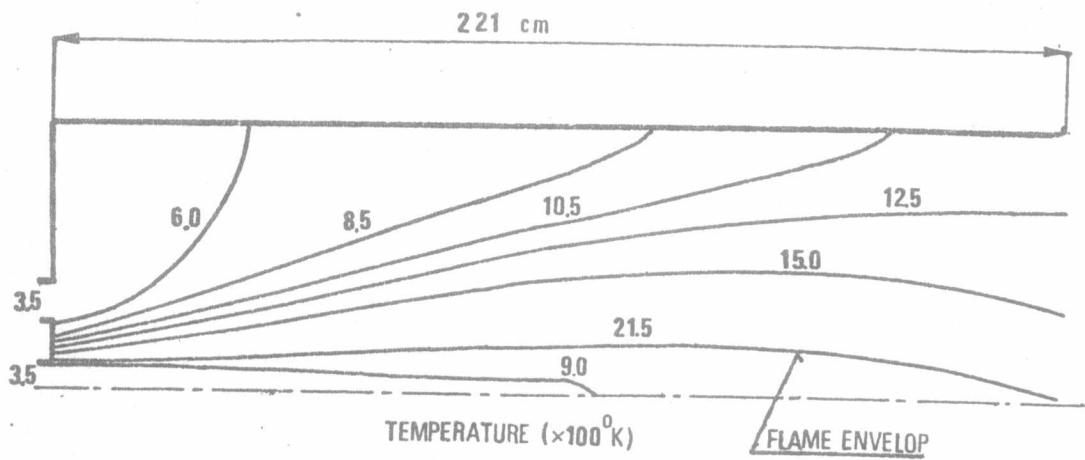


Fig. 4. Temperature distribution, $V_F = V_{Air}, \xi = 1$

In Fig. 5. is plotted the concentration profiles for CO, OH, and NO at the end of the first quarter of the combustor and at the exhaust section.

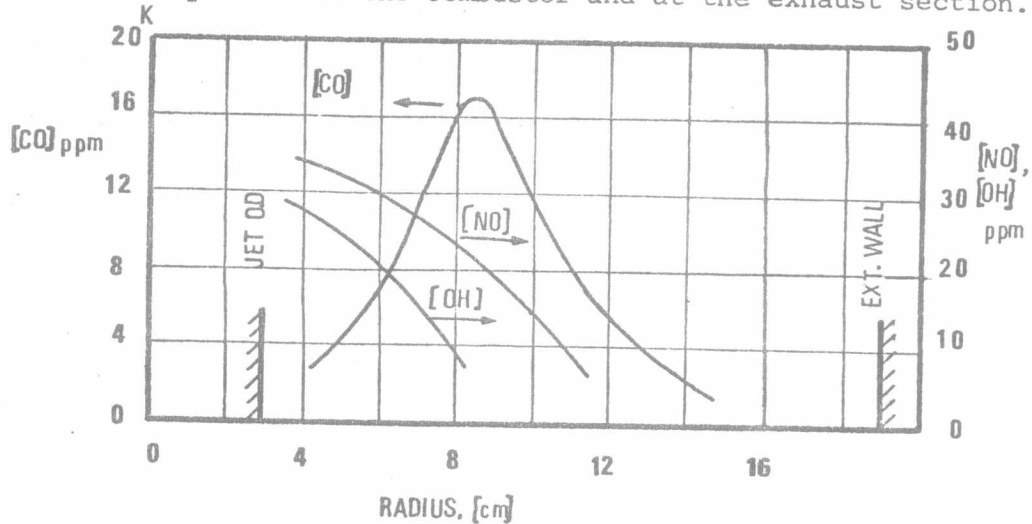


Fig. 5.a. CO, OH, and NO profiles at the first quarter plane.

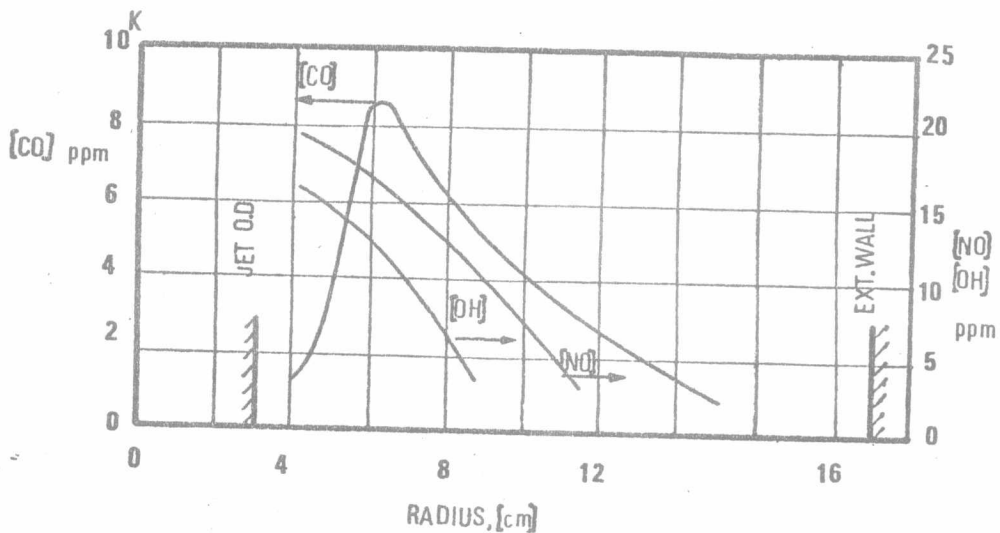


Fig. 5.b. CO, OH, and NO profiles at exhaust section

Deviations of other considered cases from the previously base case were taken into consideration. Results from such preliminary studies provide a direction from experimental verification. The experimental analysis of such pheremens are to be published through a pioneering works in Cairo University and the comparison will be published in future works.

CONCULSIONS

Development of a primitive -variable finite difference technique that consider the whole aspects of a fluid flow, fluid dynamic and chemical kinetics, of a chemically reacting recirculating flow in a gas turbine combustor is described. The solution algorithm involves a staggered grid system for axial and radial velocities, a line relaxation technique for the efficient solution of equations, a two step kinetic model for methane combustion, and simplified kinetic models for calculation the other dominant combustion products.

By this procedure it was possible calculate the influence of the fuel/air ratio, velocity ratio, and diameter ratio on the general performance of combustors including tracing of pollutants and other combustion products. Prediction by this procedure allows some results to be obtained more quickly in fraction of amminute by the use of Cyber 10, and correctly than currently possible by the almost exclusive use of experimental means.

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NOMENCLATURE

a_j, a_p	: Coefficients in the finite difference equation
C_1, C_2, C_D	: Constant in turbulence model
C_p	: Specific heat at constant Pressure
H	: Heat of combustion
h	: Stagnation enthalpy
k	: Kinetic energy of turbulence
M	: Molecular weight of mixture
m_j	: Mass fraction of species j
p	: Pressure
R_j	: Mass rate of reaction of species
r	: Radial Co-ordinate in the cylind. polar system
S	: Stoichiometric mass ratio
S_ϕ, S_p, S_u	: Source term; and its linearized components
T	: Absolute temperature
u, v	: Velocity components in the axial and radial directions
Γ_ϕ	: Exchange coefficient for variable ϕ
σ_ϕ	: Effective Prandtl or Schmidt number for variable ϕ
K	: Constant in the log-law
ϵ	: Dissipation of K
ϕ	: General dependent variable
τ	: Shear Stress
μ_t	: turbulent viscosity
ρ	: time - mean density.

SUBSCRIPTS

eff	: effective
fu	: fuel
i	: Species
j	: neighbouring points
p	: at point p
t	: turbulence
w	: at the wall.

