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Numerical Calculations of Turbulent Reacting Flow in a Gas-Turbine Combustor

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NUMERICAL CALCULATIONS OF TURBULENT REACTING FLOW IN A GAS-TURBINE COMBUSTOR

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E-3501

SUMMARY

A numerical study for confined, axisymmetrical, turbulent diffusion flames is presented. Local mean gas properties are predicted by solving the appropriate conservation equations in the finite-difference form with the corresponding boundary conditions. The $k-\varepsilon$ two-equation turbulence model is employed to describe the turbulent nature of the flow. A two-step kinetic model is assumed to govern the reaction mechanism. The finite reaction rate is the smaller of an Arrhenius type of reaction rate and a modified version of eddy-breakup model. Reasonable agreement is observed between calculations and measurements, but to obtain better agreement, more work is needed on improvements of the above mathematical models. However, the present numerical study offers an improvement in the analysis and design of the gas turbine combustors.

INTRODUCTION

The design of modern gas turbine combustors is an extremely complex process. Many factors can influence their performance, including combustor geometry, flow properties of oxidant and fuel, flow turbulence, and combustion process. Consequently, methods that could aid in understanding and predicting these phenomena would be very useful in designing more efficient combustors. This report describes numerical calculations of a turbulent reacting flow in a combustion chamber in which the flow is confined and axisymmetric with sudden expansion.

The reacting flow fields considered are gaseous-fueled and are governed by a set of time-averaged conservation equations. Air and natural gas are used as the oxidant and fuel, respectively. In order to close these governing equations, a set of mathematical models are required for the description of various physical processes. Neglecting the radiation effect, two main features need to be modeled: flow turbulence characteristics and chemical reaction. The $k-\varepsilon$ two-equation turbulence model is employed for the description of eddy properties. For the chemical reaction rate, a modified version of eddy-breakup model including kinetic effect, is used.

The objective of present study is to predict the chemical compositions and to compare with measurements and then examine the validity of the mathematical models for combustor problems. It is impossible to obtain analytical solutions, so the computational fluid dynamic techniques are required. A TEACH computer code using the Bounded Skew Hybrid Differencing (BSHD) is used in the present study (refs. 1 and 2). The Pressure-Implicit Split Operation (PISO)

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predictor-corrector procedure (ref. 3) is employed for the calculation of pressure distribution.

GOVERNING EQUATIONS AND BOUNDARY CONDITIONS

The partial differential equations governing the flow considered herein are of the form:

$$\left[\frac{\partial}{\partial x}(\rho U\phi) + \frac{\partial}{r\partial r} r(\rho V\phi)\right] = \frac{\partial}{\partial x}\left(b\frac{\partial \phi}{\partial x}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(rb\frac{\partial \phi}{\partial r}\right) + S_{\phi} \qquad (1)$$

where the corresponding values of dependent variable ϕ, effective exchange coefficient b, and source term S_{ϕ} are given in table I. The equations represent conservation of mass, three components of momentum, turbulent kinetic energy, turbulent dissipation rate, total enthalpy, mass fraction of fuel, mass fraction of CO, and the mixture fraction. The mixture fraction f which is defined as

$$f = \frac{m_{fu} + m_{H_2O}}{r_3}$$

can be considered as the total mass fraction of burned and unburned fuel. r_3 is the mass stoichiometric ratio of H_2O and fuel in the chemical reaction equation.

The effective viscosity is given by

$$\mu_{eff} = \mu_t + \mu_{\ell}$$

where μ_t and μ_{ℓ} are the eddy and laminar viscosities, respectively. μ_t is calculated from the solution of the k-ε turbulence model which will be discussed later. The turbulent Prandtl/Schmidt numbers, σ_H, σ_{fu}, σ_{CO}, and σ_f, are assumed to have a value of 0.9. The source terms, S_{fu}, S_{CO}, and r_2, in the m_{fu} and m_{CO} equations are involved with the combustion model and will be discussed in the later sections.

Since the equations are elliptic in form, boundary conditions are required at all the boundaries. Figure 1 shows the geometry of the combustor considered. The flow measurements for this geometry were made by Lewis and Smoot (ref. 4). Some boundary conditions can be obtained from their measurements. Table II shows the measured boundary conditions and the compositions of air and fuel. The inlet velocities are parallel and assumed to have power law distributions. This implies that the flow is nonswirling and the tangential momentum equation can be neglected. The inlet turbulent kinetic energy for air flow was given as 11.765 m^2/s^2, and the corresponding value for fuel flow was measured to be 1.633 m^2/s^2. The dissipation rates are estimated by the following relation:

$$\varepsilon = \frac{C_{\mu} k^{1.5}}{(0.03\ D_1)}$$

where D_i is the diameter of the flow passage. At all walls, the nonslip condition is applied and temperature is provided by the measurements. The gradients of other dependent variables are assumed zero. The dependent variables at the wall are linked to those at the grid node next to the wall by the logarithmic law of the wall. The symmetry axis provides a boundary condition of the form $\partial\phi/\partial r = 0$ except the radial velocity v which is zero at the centerline. At the exit, all gradients are assumed to be zero, i.e., $\partial\phi/\partial x = 0$.

THERMODYNAMIC PROPERTIES

The local density of gas mixture is obtained from the equation of perfect gas

$$P = \frac{\rho\tilde{R}T}{M}$$

where M is the mixture molecular weight calculated from the relation

$$\frac{1}{M} = \sum_i \left(\frac{m_i}{W_i}\right)$$

where m_i and W_i are the mass fraction and molecular weight, respectively, for the ith species. The total enthalpy H is defined as

$$H = \sum_i \int_0^T C_{p_i}\, dT + m_{fu}H_{fu} + (m_{co} + r_2 m_{fu})\, H_{co} + \underbrace{\frac{\rho[U^2 + V^2 + V\theta^2]}{2}}_{\substack{\text{usually neglected}\\ \text{for low-speed flow}}} \qquad (2)$$

where H_{fu} and H_{co} are the heats of reactions for fuel and CO, respectively, corresponding to the two-step overall kinetic equations, and the species specific heat is calculated by

$$C_{p_i} = a_i + b_i T + c_i T^2 + d_i T^3 \qquad (3)$$

The constants a_i, b_i, c_i, and d_i can be found from reference 5. The temperature T is calculated iteratively by using Eqs. (2) and (3).

CHEMICAL KINETICS MECHANISM

The simplest chemical mechanism is the one-step overall kinetic mechanism which is the most convenient for numerical modeling. This approach assumes the oxidation process to occur directly to CO_2 and H_2O. However, it does not account for the characteristics of hydrocarbon oxidation since small amounts of intermediate hydrocarbons and somewhat larger amounts of CO are usually to form prior to significant productions of CO_2 and H_2O.

The next stage of complexity introduced has been the two-step overall kinetic mechanism which separates the highly exothermic oxidation of CO to CO_2 from the less exothermic oxidation of the hydrocarbon to CO (refs. 6 and 7):

$$C_XH_Y + \left(\frac{X}{2} + \frac{Y}{4}\right)(O_2 + nN_2) \rightarrow XCO + \frac{Y}{2} H_2O + \left(\frac{X}{2} + \frac{Y}{4}\right) nN_2$$

$$XCO + \frac{X}{2} (O_2 + nN_2) \rightarrow XCO_2 + \frac{X}{2} nN_2.$$

In the first reaction,

r_1 = (mass of O_2)/(mass of fuel),

r_2 = (mass of CO)/(mass of fuel),

r_3 = (mass of H_2O)/(mass of fuel);

in the second reaction,

r_4 = (mass of O_2)/(mass of CO),

r_5 = (mass of CO_2)/(mass of CO).

The values of these ratios can be obtained in the following:

$$r_1 = \left(\frac{X}{2} + \frac{Y}{4}\right) \frac{W_{O_2}}{W_{fu}}$$

$$r_2 = X \frac{W_{CO}}{W_{fu}}$$

$$r_3 = \left(\frac{Y}{2}\right) \frac{W_{H_2O}}{W_{fu}}$$

$$r_4 = \left(\frac{1}{2}\right) \frac{W_{O_2}}{W_{CO}}$$

$$r_5 = \frac{W_{CO_2}}{W_{CO}}$$

Here the W's are the molecular weights of the chemical species. With the values of r's, we can calculate the mass fractions of O_2, CO_2, and H_2O from the following:

$$m_{O_2} = R(1 - f) + r_4 m_{CO} + (r_1 + r_2 r_4)(m_{fu} - f), \quad R = 0.233$$

$$m_{CO_2} = r_2 r_5 (f - m_{fu}) - r_5 m_{CO}$$

$$m_{H_2O} = r_3 (f - m_{fu})$$

It is noted that the fuel considered in the present study is a natural gas consisting of several components such as CH_4, C_2H_6, etc., so the calculations of r's described above need to be modified. This can be done without much difficulty.

TURBULENCE AND COMBUSTION MODELS

The $k-\varepsilon$ two-equation turbulence model is used for the closure of Reynolds equations. The eddy viscosity is obtained from the relation

$$\mu_t = \frac{C_\mu \rho k^2}{\varepsilon}$$

Values of the constants associated with the calculation of eddy viscosity using the $k-\varepsilon$ turbulence model are given in the following (ref. 8):

$$C_1 = 1.44, \quad C_2 = 1.92, \quad C_\mu = 0.09, \quad K = 0.42, \quad \sigma_k = 1.0,$$

$$\sigma_\varepsilon = \frac{K^2}{\left\{(C_2 - C_1) C_\mu^{1/2}\right\}},$$

In the near-wall region, equations were introduced to link the values of dependent variables on the wall to those in the logarithmic region (ref. 9).

This turbulence model has been tested previously for many recirculating flows (refs. 10 to 13). The investigation indicated that acceptable agreement was obtained between measured and predicted flow pattern, flame structure, and heat flux.

Equations are required for the reaction rate of fuel and CO. Several models have been proposed to predict burning rate of fuel in turbulent environments. In the present study, an Arrhenius type reaction rate is compared with a modified eddy-breakup rate, and the smaller of the two rates controls the reaction (ref. 7). The corresponding rates for the first reaction is expressed as:

$$S_{fu} = -\text{Min.}(S_1, S_2)$$

where

$$S_1 = F_1 \rho^{1.5} m_{fu}^{0.5} m_{OX} \exp\left(\frac{-E_1}{\tilde{R}T}\right),$$

$$S_2 = C_{R,1}\,\rho\,\frac{\varepsilon}{k}\,\mathrm{Min.}\left(m_{fu},\,\frac{m_{OX}}{i_1}\right)$$

S_1 is the Arrhenius rate of fuel oxidation as controlled by chemical kinetics. The eddy-breakup model of Spalding expresses the rate of oxidation as influenced by turbulence intensity and scale, and concentration of unburned fuel. This model is applicable to premixed flames. However, the combustion in gas-turbine combustors is neither fully premixed nor entirely diffusion controlled, so a term is added in the model to determine the rate of fuel oxidation as controlled by the availability of the oxygen.

Similarly, the reaction rate of CO can be expressed as:

$$S_{co} = -\mathrm{Min.}(S_3,S_4)$$

where

$$S_3 = F_2\rho^2\,m_{CO}m_{OX}\,\exp\left(\frac{-E_2}{\tilde{R}T}\right),$$

$$S_4 = C_{R,2}\,\rho\,\frac{\varepsilon}{k}\,\mathrm{Min.}\left(M_{co},\,\frac{M_{OX}}{i_2}\right)$$

i_1 and i_2 are the stoichiometric ratios of the first and second chemical equations, respectively. The eddy-breakup constants, $C_{R,1}$ and $C_{R,2}$ are set to be 2.0 and 1.0, respectively. The other constant appearing in the Arrhenius equations are the following values (refs. 14 and 15):

$$F_1 = 3.3\mathrm{x}10^{14},\quad \frac{E_1}{\tilde{R}} = 27\ 000\ \mathrm{K},$$

$$F_2 = 2.2\mathrm{x}10^{8},\quad \frac{E_2}{\tilde{R}} = 12\ 500\ \mathrm{K},$$

SOLUTION PROCEDURE

The governing equations and the associated boundary conditions are solved by a TEACH computer code using the Bounded Skew Hybrid Differencing (BSHD) method (refs. 1 and 2). The pressure distribution is estimated by the Pressure-Implicit Split Operation (PISO) predictor-corrector technique (ref. 3). Calculations are performed with a nonuniform grid distribution comprising 60 by 47 nodes with concentration of the nodes in the near-wall region and centerline regions. The values of the underrelaxation parameters for each dependent variable ϕ are listed in table III. The solutions are assumed to be convergent when the maximum residual is reduced by three orders of magnitude for any node for any ϕ equation. The numerical calculations are performed on a CRAY1 computer with CPU time of around 56.7 min. About 3960 iterations are required to obtain convergent solutions for the present calculations.

RESULTS AND DISCUSSION

The numerical predictions compared with measured data are shown in figures 2 to 9. From figure 2, we observe that the calculations and measurements for the mixture fraction distributions are in good agreement except in the regions near the centerline and in the recirculating regions close to the corner. The calculations overpredict and underpredict, respectively, the mixture fraction in these two regions. However, it is noted that in the developing region near the centerline, large radial concentration gradients exist. The measured (or collected) sample represents the average species concentration over the area of the probe inlet, so the magnitude of the error can be up to 22 percent while the error is negligible for the radial positions outside 3 cm or for axial positions aft 25 cm (ref. 4). With these measurements corrected, the discrepancies between calculations and measurements are expected to be reduced in the developing region. The calculated CH_4 and O_2 concentration profiles in figures 3 and 4, respectively, show that the reaction rates are slower than observed, especially in the two regions mentioned above. Consequently, the concentration of CO_2 and H_2O (figs. 5 to 8) are underpredicted in both the recirculating region near the corner and developing region in the centerline. In far downstream, the predicted H_2O profiles are somewhat higher than the measured data probably due to the neglect of H_2 as one of the intermediate products. The concentration profiles of CO_2 and CO (figs. 7 to 9) indicate that the reaction rate for CO_2 is too low and that the radial spread of CO profiles is underpredicted. Two temperature profiles are shown in figure 9. Since the reaction model used in the present study underpredicts the chemical reaction rate, the calculated temperature is lower than the measured data in the centerline developing region.

According to the above investigations, we can conclude that the overall discrepancy between the calculations and the measurement are due to the inappropriate mathematical modeling in the centerline developing region and the corner recirculation region. Except for these regions, acceptable agreement between numerical and measured data is made using the k-ε turbulence model and reaction model used in this study.

CONCLUSIONS

In the present study, a numerical calculation for turbulent combusting flow in a confined sudden expansion gas-turbine combustor has been investigated. The local mean gas properties are predicted and compared with measurements. The species concentration distributions are reasonably well predicted except in the centerline developing region and corner recirculation region. Some factors which may cause prediction error are:

1. Inappropriate combustion model.

2. Weakness of turbulence model.

3. Inappropriate chemical mechanism by using two-step overall kinetics.

4. Neglect of minor intermediate species.

5. Assumption of equal diffusivities of all chemical species.

6. The numerical error from the computer code itself.

It is believed that the major discrepancy between calculations and measurement is due to items 1 and 2. Research in these areas is still a challenge to us. However, more accurate turbulence model and combustion model are an urgent need in improvement of numerical study.

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TABLE I. - GOVERNING EQUATIONS CORRESPONDING TO EQUATION (1)

Conservation of	ϕ	b	S_ϕ
Mass	1	0	0
Axial momentum	U	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial U}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\mu_{eff}r\frac{\partial V}{\partial x}\right)-\frac{\partial P}{\partial x}$
Radial momentum	V	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{eff}\frac{\partial U}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\mu_{eff}r\frac{\partial V}{\partial r}\right)-2\mu_{eff}\frac{V}{r^2}+\frac{\rho V_\theta^2}{r}-\frac{\partial P}{\partial r}$
Tangential momentum	rV_θ	μ_{eff}	$-\frac{2}{r}\frac{\partial}{\partial r}(\mu_{eff}V_\theta r)$
Kinetic energy	k	$\frac{\mu_{eff}}{\sigma_k}$	$G_{k_1}-\rho\epsilon$
Dissipation rate	ϵ	$\frac{\mu_{eff}}{\sigma_\epsilon}$	$\frac{\epsilon}{k}(C_1G_{k_1}-C_2\rho\epsilon)$
Stagnation enthalpy	H	$\frac{\mu_{eff}}{\sigma_H}$	0
Mass fraction of fuel	m_{fu}	$\frac{\mu_{eff}}{\sigma_{fu}}$	S_{fu}
Mass fraction of CO	m_{CO}	$\frac{\mu_{eff}}{\sigma_{co}}$	$S_{CO}-r_2S_{fu}$
Mixture fraction	f	$\frac{\mu_{eff}}{\sigma_f}$	0

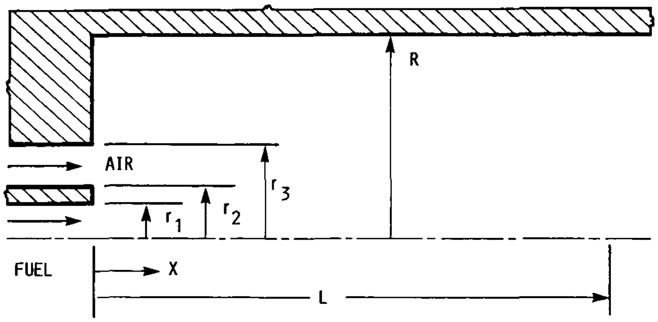
$$G_{k_1}=\mu_{eff}\left[2\left(\left(\frac{\partial U}{\partial x}\right)^2+\left(\frac{\partial V}{\partial r}\right)^2+\left(\frac{V}{r}\right)^2\right)+\left(\frac{\partial V_\theta}{\partial x}\right)^2+\left(r\frac{\partial}{\partial r}\frac{V_\theta}{r}\right)^2+\left(\frac{\partial U}{\partial r}+\frac{\partial V}{\partial x}\right)^2\right]$$

TABLE II. - COMBUSTOR PARAMETERS AND BOUNDARY CONDITIONS

Primary gas: natural gas	
Temperature, K	300
Flow rate, g/s	2.84
Velocity, m/s	21.3
Composition, mol %	
CH_4	83.9
C_2H_6	7.1
N_2	2.4
CO_2	1.3
Ar	5.3
Secondary gas: air	
Temperature, K	589
Flow rate, g/s	36.3
Velocity, m/s	34.3
Composition, mol %	
N_2	79
O_2	21
Pressure, N/m^2	94 000
Wall temperature, K	1140

TABLE III. - VALUES OF UNDERRELAXATION PARAMETERS

Variable	Underrelaxation parameter
U velocity	0.3
V velocity	.3
Primary pressure correction	1.0
Turbulence energy	.4
Dissipation rate	.4
Total enthalpy	.6
Fuel concentration	.6
CO concentration	.6
Mixture fraction	.6
Second pressure correction	.7
Viscosity	1.0
Density	.1



r_1 = 0.008 M
r_2 = 0.0111 M
r_3 = 0.0286 M
R = 0.1016 M
L = 1.524 M

FIGURE 1. - GEOMETRY OF AXISYMMETRIC COMBUSTOR WITH COAXIAL FUEL AND AIR JETS.

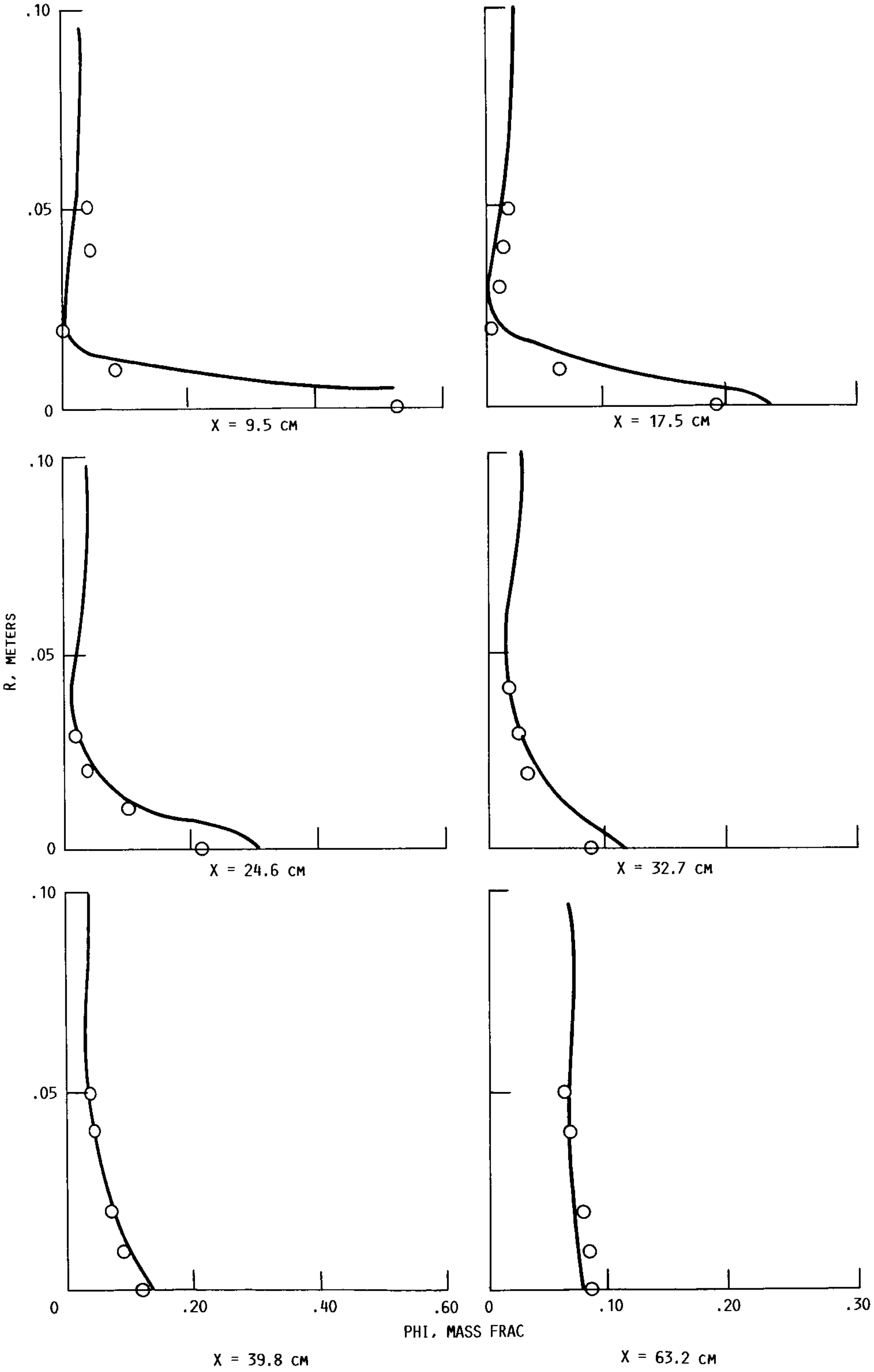


FIGURE 2. - 2-STEP SCHEME, TOTAL FUEL PROFILES.

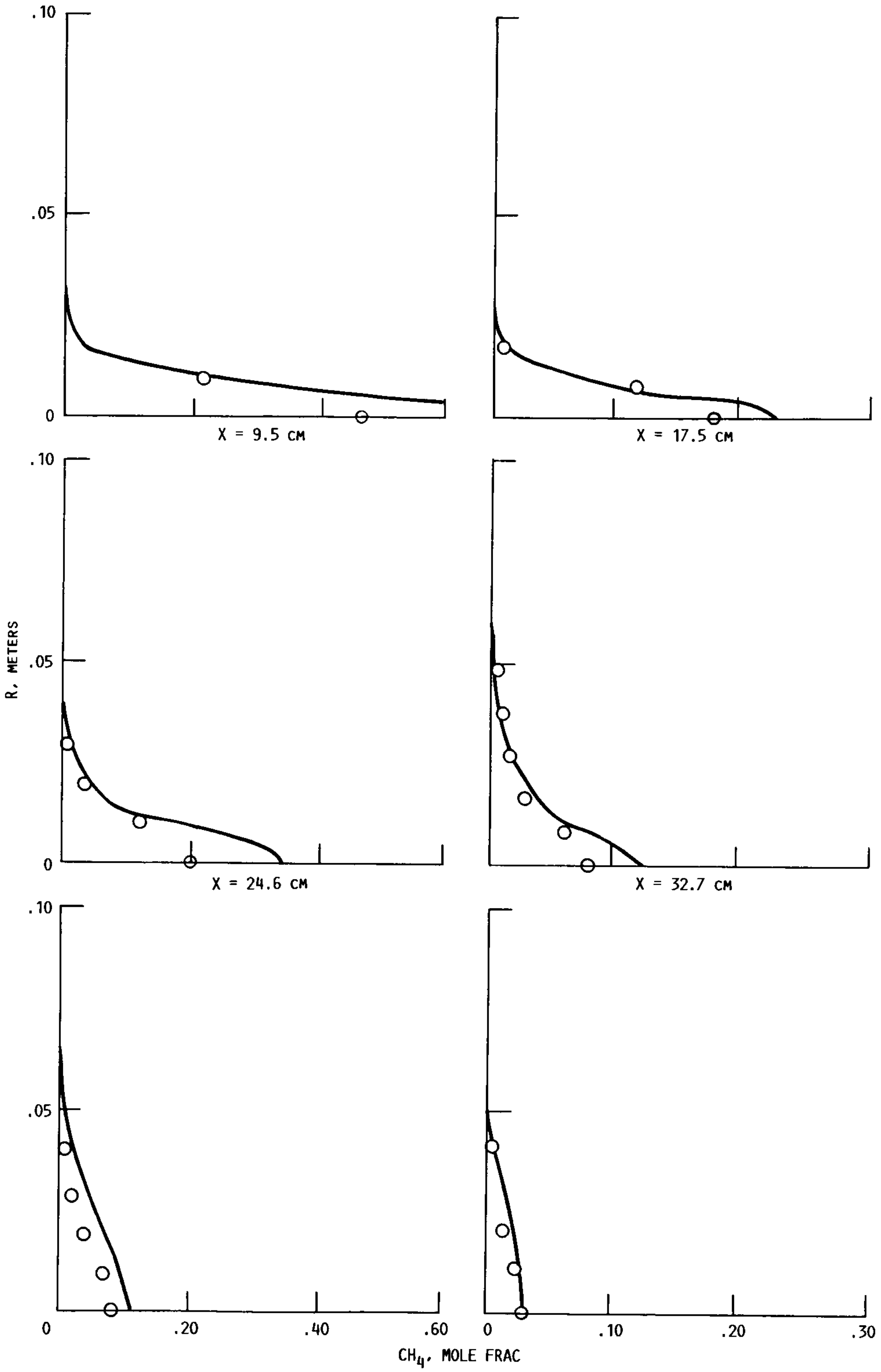
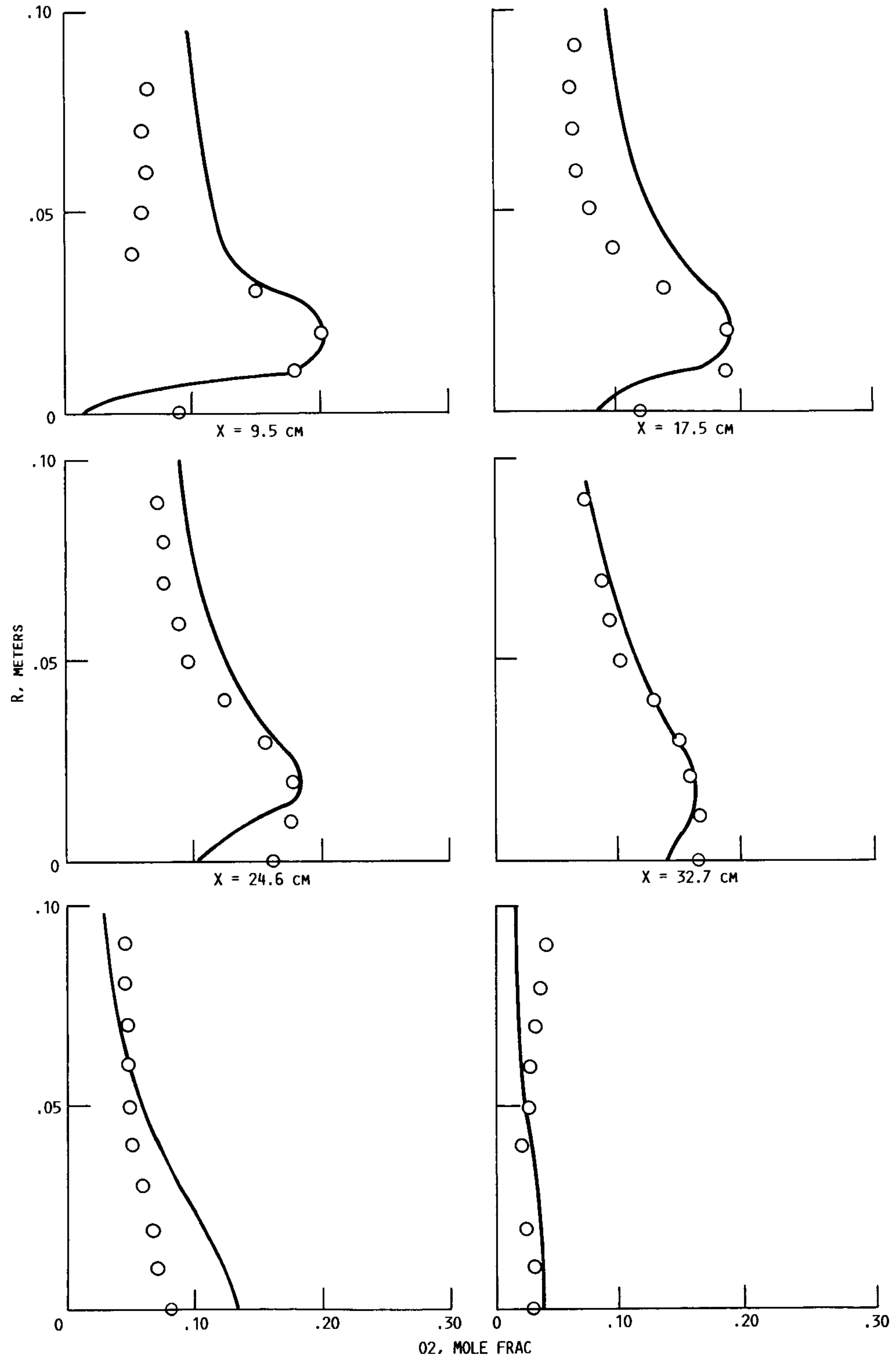


FIGURE 3. - 2-STEP SCHEME, UNBURNED FUEL PROFILES.



X = 9.5 CM

X = 17.5 CM

X = 24.6 CM

X = 32.7 CM

X = 47.5 CM

X = 63.2 CM

FIGURE 4. - 2-STEP, O_2 PROFILES.

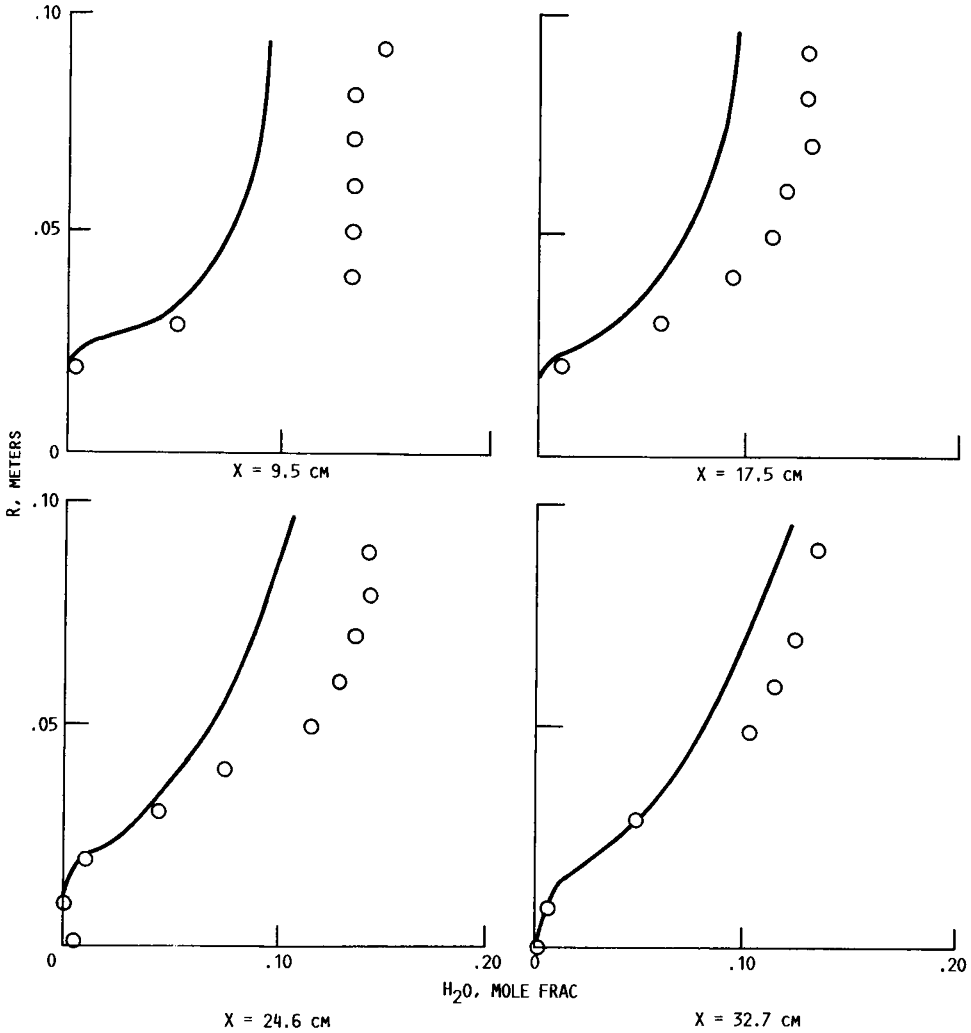
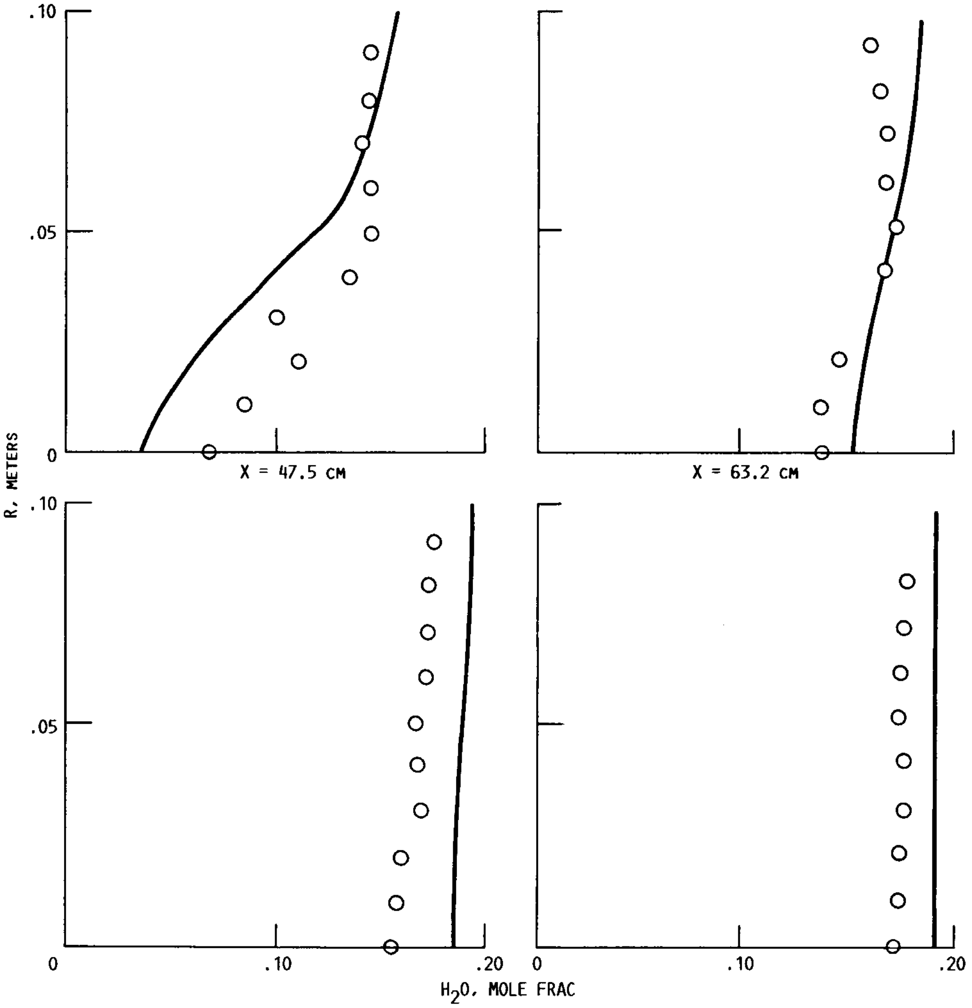


FIGURE 5. - 2-STEP SCHEME, H_2O PROFILES.



X = 47.5 CM

X = 63.2 CM

X = 78.5 CM

X = 137.5 CM

FIGURE 6.- 2-STEP SCHEME, H_2O PROFILES.

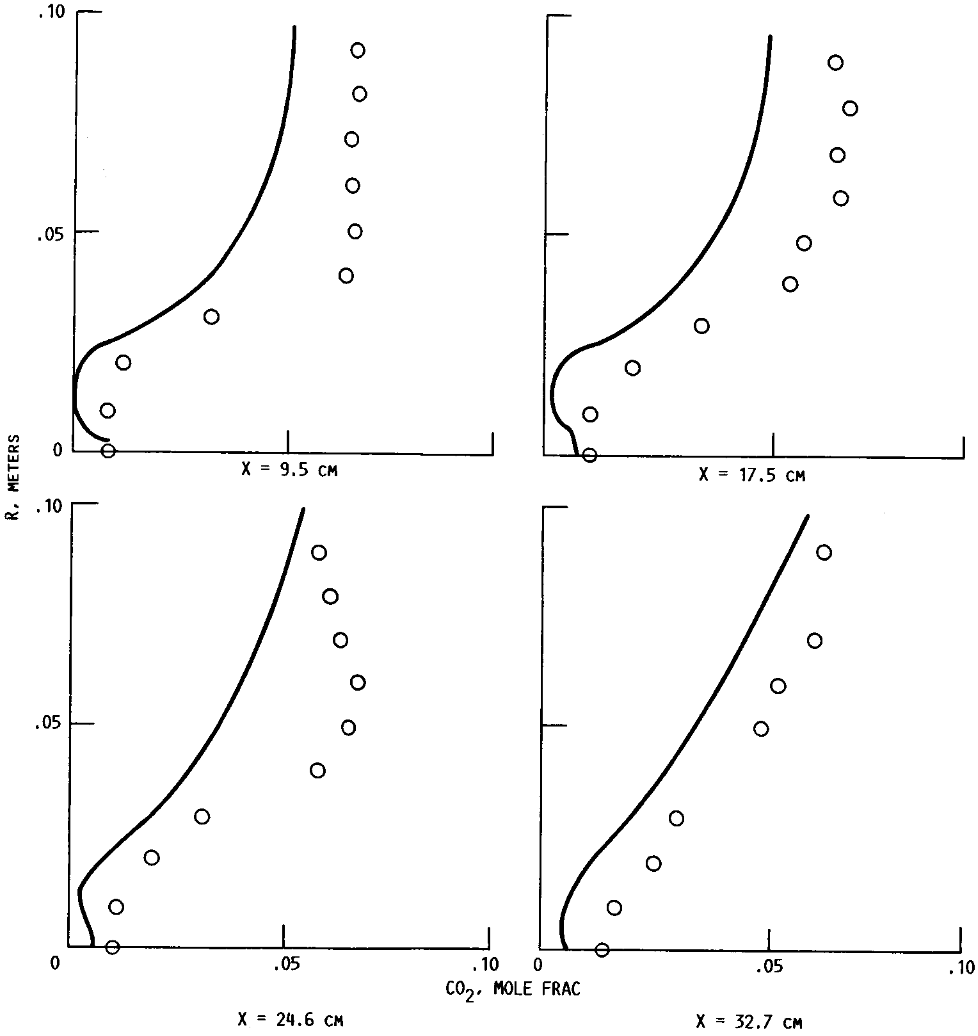


FIGURE 7. - 2-STEP SCHEME, CO$_2$ PROFILES.

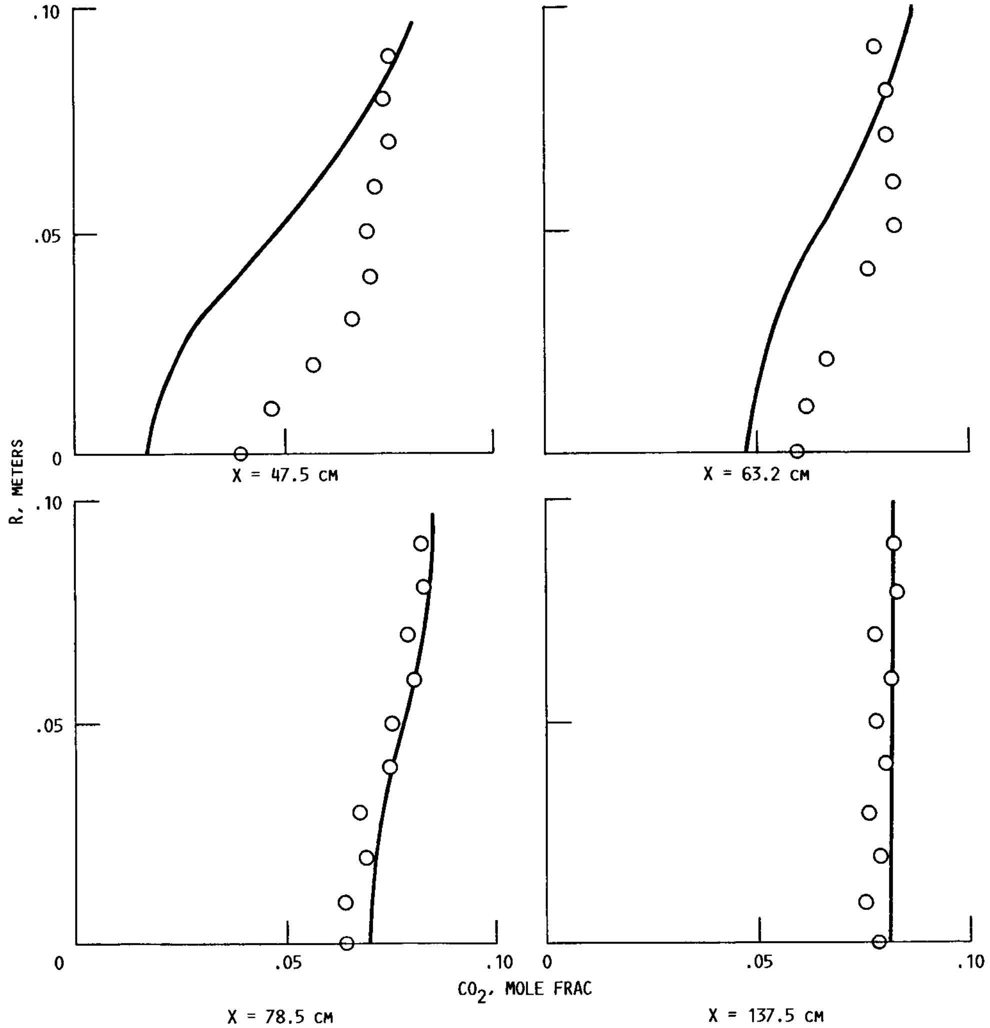


FIGURE 8. - 2-STEP SCHEME, CO_2 PROFILES.

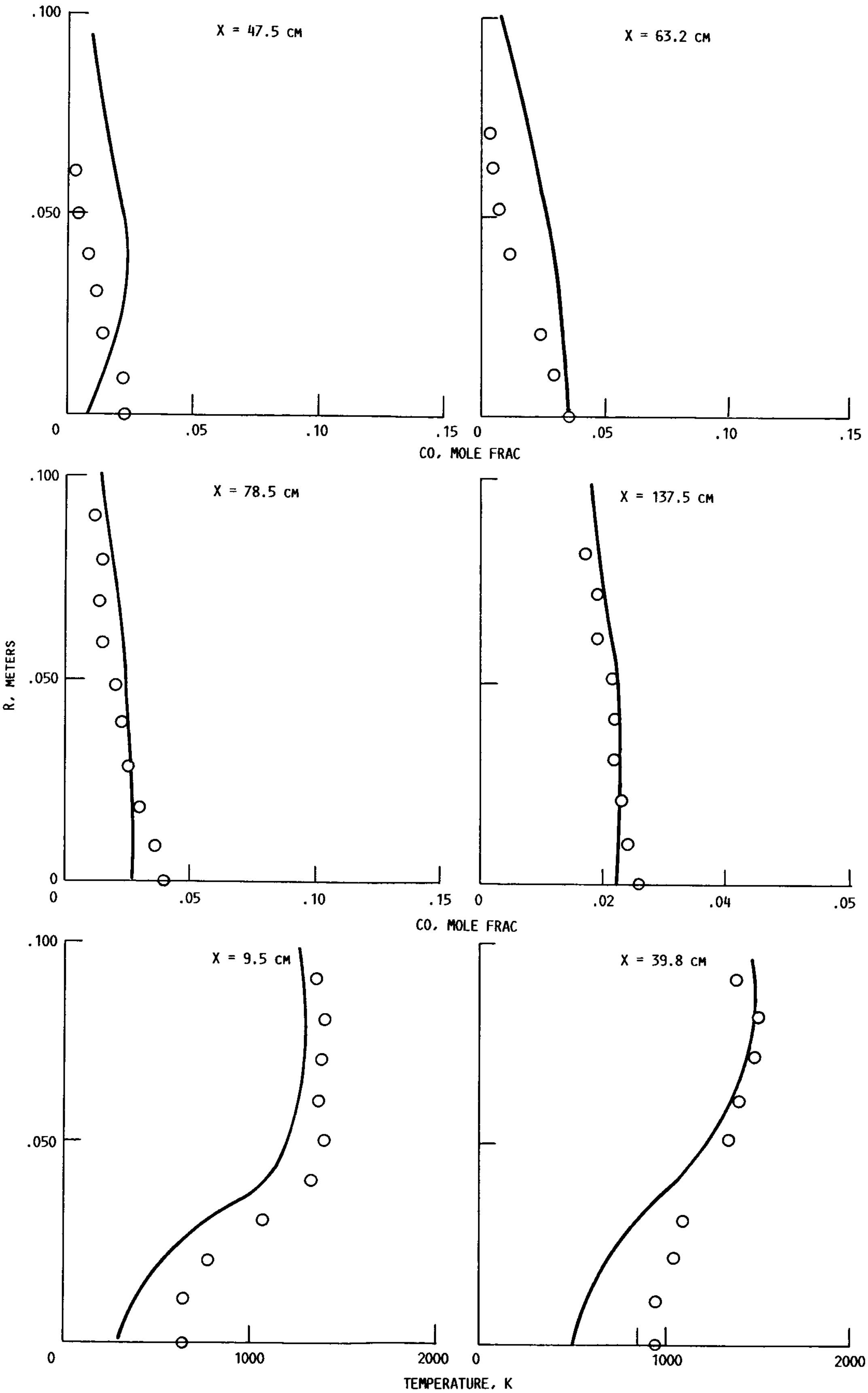


FIGURE 9. - 2-STEP SCHEME, CO AND TEMPERTURE PROFILES.

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16. Abstract

A numerical study for confined, axisymmetrical, turbulent diffusion flames is presented. Local mean gas properties are predicted by solving the appropriate conservation equations in the finite-difference form with the corresponding boundary conditions. The $k-\varepsilon$ two-equation turbulence model is employed to describe the turbulent nature of the flow. A two-step kinetic model is assumed to govern the reaction mechanism. The finite reaction rate is the smaller of an Arrhenius type of reaction rate and a modified version of eddy-breakup model. Reasonable agreement is observed between calculations and measurements, but to obtain better agreement, more work is needed on improvements of the above mathematical models. However, the present numerical study offers an improvement in the analysis and design of the gas turbine combustors.

17. Key Words (Suggested by Author(s))

Gas-turbine combustor; Turbulent reacting flow; Two-equation turbulence model; Chemical reaction model; Two-step kinetics mechanism

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