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An Explicit Runge-Kutta Method for Tubulent Reacting Flow Calculations

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REACTING FLOW CALCULATIONS

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SUMMARY

The paper presents a numerical method for the solution of the conservation equations governing steady, reacting, turbulent viscous flow in two dimensional geometries, in both Cartesian and axisymmetric coordinates. These equations are written in Favre-averaged form and closed with a first order model. A two-equation K-ε model, where low Reynolds number and compressibility effects are included, and a modified eddy-breakup model are used to simulate fluid mechanics turbulence, chemistry, and turbulence-combustion interaction. The solution is obtained by using a pseudo-unsteady method with improved perturbation propagation properties. The equations are discretized in space by using a finite volume formulation. An explicit multi-stage dissipative Runge-Kutta algorithm is then used to advance the flow equations in the pseudo-time. The method is applied to the computation of both diffusion and premix turbulent reacting flows. The computed temperature distributions compare favorably with experimental data.

INTRODUCTION

The design of future combustion concepts requires accurate numerical methods for the simulation of liquid or gaseous fuels in a highly turbulent airstream (ref. 1). These chemical reacting turbulent flows involve fluid mechanics, chemistry, and turbulence-combustion interaction. The present approach is devoted to the solution of the full turbulent reacting flow problem within an engineering accuracy, i.e., looking for a solution for averaged quantities and describing the reactive gas as a mixture of three species, fuel, oxidizer, and products, with combustion supposed to be controlled by a single step irreversible chemical reaction.

The reliability of a numerical method is a function of both the mathematical modeling of the physical process and the solution algorithm. The governing equations are written here in Favre-averaged form. No simplification is used in deriving the energy conservation equation, as usually performed (ref. 8). The closure is achieved by using a first order model. The K-ε turbulence model adopted here includes low Reynolds number terms, so that the equations are valid all over the laminar, transition, and turbulent region, as described

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in reference 2. Furthermore, the model includes a density gradient term to better simulate variable density effects. The modified eddy break up mixing controlled reaction rate expression adopted here, introduces a concentration gradient dependence other than the classical concentration dependence (ref. 8). This model has been developed for imperfectly premixed flow (ref. 2), but it is useful in cases where the combustion is neither fully pre-mixed nor entirely diffusion controlled, as it is likely to occur under many circumstances even if the fuel and the oxidizer enter the combustion chamber in separate streams. These two models allow one to simulate fluid mechanics turbulence, chemistry, and turbulence-combustion interaction.

The solution is then obtained by using a pseudo-unsteady method with improved perturbation propagation properties (ref. 3). Pseudo-unsteady methods with artificial equations are quite common in turbomachinery applications (refs. 9 and 10), but up to now they have received little use in computing reacting flows, despite the fact that they are faster and simpler than classi-cal pressure iteration methods. At low speeds, the maximum allowable time step for the proposed artificial equations is indeed (ref. 12) very close to the one obtained in the pressure iteration method of reference 11 even by using the simple Lax-Wendroff algorithm. The equations are discretized in space by using a finite volume formulation, and integrated in the pseudo-time with an explicit multistage dissipative Runge-Kutta algorithm. Multi-stage schemes for the numerical solution of ordinary differential equations are usually designed to give a high order of accuracy, but in a pseudo-unsteady solution these schemes are selected only for their properties of stability and damping. The four stage adopted here allows a CFL number of about 2.6 with only negligible changes with reference to the simple Lax-Wendroff algorithm but with a minimum of artificial viscosity introduced for stability purposes.

LIST OF SYMBOLS

AE   Arrhenius activation energy

C   constant

c   concentrations fluctuations parameter

CFL   Courant number

D   diffusion vector

E   total specific energy

e   specific internal energy

F   flux tensor

f   unknown vector

f function

H   total enthalpy

Hp   optimization matrix

I   identity matrix

j   index of the spatial discretization

K   turbulence kinetic energy

k   index of the multistage algorithm

L   length scale of turbulent motions

M   Mach number

m   index of the temporal discretization

N   unit outward normal

NV   updating rate

P   production of turbulence kinetic energy

p   pressure

PF   Arrhenius prefactor

Pr   Prandtl number

Q   work due to turbulence

q   heat flux vector

R   low Reynolds number term

Re   Reynolds number

S   source vector

s   stoichiometric ratio

Sc   Schmidt number

T   residual

t   time

tu   turbulence intensity

V   velocity

v   volume

x   axial coordinate

Y	mass fraction
y	radial coordinate
β	perturbation speed
Γ	diffusion coefficient
γ	specific heat ratio
ΔH	chemical heat release
δr	characteristic volume dimension
δt	time step
$\delta\Sigma$	surface area
ε	turbulence kinetic energy dissipation rate
θ	multistage scheme coefficient
κ	thermal conductivity
μ	viscosity coefficient
ρ	density
Σ	boundary of the fixed volume
τ	viscous stress tensor
Φ	reaction rate
ϕ	Schwab-Zeldovich function
Ω	artificial viscosity coefficient

Subscripts

i	inviscid
fu	fuel
l	laminar
ox	oxidizer
t	turbulent
v	viscous

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Governing Equations

The unknown vector f is the solution of a system of conservation equations. This system is written in Favre-averaged, dimensionless, vector, integral form as follows

$$\int_{\Sigma} \int N \cdot (F_i + F_v) d\Sigma = \int \int_V \int S \, dv$$

The basic dependent variables are density, velocity and energy. Their conservation equations read as follows

$$f = \begin{pmatrix} \rho \\ \rho \cdot V \\ \rho \cdot E \end{pmatrix}$$

$$F_i = \begin{pmatrix} \rho \cdot V \\ \rho \cdot V \, V + p \cdot I \\ \rho \cdot E \cdot V + p \cdot I \cdot V \end{pmatrix}$$

$$F_v = \begin{pmatrix} 0 \\ -\tau \\ -\tau \cdot V + q \end{pmatrix}$$

$$S = \begin{pmatrix} 0 \\ 0 \\ \rho \cdot \varepsilon - P + Q + \Delta H \cdot \phi_{fu} \end{pmatrix}$$

where from the equation of state of a perfect gas

$$p = (\gamma - 1) \cdot \rho \cdot e$$

with

$$e = (E - V^2/2) = H - V^2/2)/\gamma$$

The reactive variables are the fuel mass fraction and a Schwab-Zeldovich function

$$\phi = Y_{fu} - Y_{ox}/s$$

Their conservation equations are written as follows

$$f = \begin{pmatrix} \rho \cdot Y_{fu} \\ \rho \cdot \phi \end{pmatrix}$$

$$F_i = \begin{pmatrix} \rho \cdot V \cdot Y_{fu} \\ \rho \cdot V \cdot \phi \end{pmatrix}$$

$$F_v = \begin{pmatrix} D_{fu} \\ D_{\phi} \end{pmatrix}$$

$$S = \begin{pmatrix} -\phi f u \\ 0 \end{pmatrix}$$

The stress tensor τ is the sum of a laminar and a turbulent part, where the latter is expressed according to a classical eddy viscosity concept, i.e.,

$$\tau = -\frac{2}{3} \cdot (\mu/Re \cdot div(V) + \rho \cdot K) \cdot I + 2 \cdot \mu/Re \cdot (def(V))$$

where

$$\mu = \mu_\ell + \mu_t$$

Similarly, the heat flux vector is given by

$$q = -\gamma \cdot \kappa \cdot grad(e)/(Re \cdot Pr)$$

while the diffusion vector is given by

$$D_Y = -\Gamma_Y \cdot grad(Y)/(Re \cdot Sc_Y)$$

where

$$\kappa = \kappa_\ell + \kappa_t$$

$$\Gamma = \Gamma_\ell + \Gamma_t$$

The turbulent viscosity coefficient is expressed accordingly with the Prandtl-Kolmogorov formulation

$$\mu_t = C_\mu \cdot f_\mu \cdot \rho \cdot Re \cdot K^2/\epsilon$$

while

$$\Gamma \approx \kappa \approx \mu$$

The turbulence variables are the turbulence kinetic energy and its dissipation rate. Their conservation equations are written in the following low Reynolds number and compressible form

$$f = \begin{pmatrix} \rho \cdot K \\ \rho \cdot \epsilon \end{pmatrix}$$

$$F_i = \begin{pmatrix} \rho \cdot V \cdot K \\ \rho \cdot V \cdot \epsilon \end{pmatrix}$$

$$F_v = \begin{pmatrix} D_K \\ D_\epsilon \end{pmatrix}$$

$$S = \begin{pmatrix} P - Q - \rho \cdot \varepsilon + R_K \\ (P - Q) \cdot C_{\varepsilon 1} \cdot f_{\varepsilon 1} \cdot \varepsilon/K - C_{\varepsilon 2} \cdot f_{\varepsilon 2} \cdot \rho \cdot \varepsilon^2/K + R_\varepsilon \end{pmatrix}$$

where the production of turbulent energy from the mean flow energy P and the work due to turbulence Q are given by

$$P = \mu_t \cdot (def(V) : def(V))/Re$$

$$Q = C_\rho \cdot \mu_t \cdot \left(grad(\rho) \cdot grad(p)/\rho^2\right)/Re$$

the low Reynolds number functions are given by reference 2

$$f_\mu = exp(-3.4/(1 + Re_t/50))$$

$$f_{\varepsilon 1} = 1.0$$

$$f_{\varepsilon 2} = 1.0 - 0.33 \cdot exp\left(-Re_t^2\right)$$

$$R_\varepsilon = -2 \cdot \mu_\ell \cdot (grad(\varepsilon))^2/Re$$

$$R_K = -2 \cdot \mu_\ell \cdot (grad(K))^2/Re$$

where

$$Re_t = \rho \cdot K^2 \cdot Re/(\mu_\ell \cdot \varepsilon)$$

and the model constant are assumed as

$$C_{\varepsilon 1} = 1.43 \qquad C_{\varepsilon 2} = 1.92 \qquad Sc_\varepsilon = 1.3 \qquad Sc_K = 1.0$$

$$C_\mu = 0.09 \qquad C_\rho = 1.0$$

The above two equation models do not take into account the preferential damping of velocity fluctuations in the direction normal to the wall, but it is quite general and it is useful in laminar, transition and turbulent regions. Furthermore, the model adopts the assumptions and approximations which are normally used for constant density flows, by retaining the gradient diffusion model to be rewritten in the density weighted form without any explicit account being taken of density fluctuations. However, the introduction of the compressibility term Q allows a partial consideration of variable density effects.

The reaction rate is finally expressed according to a modified eddy-breakup model. The mixing controlled reaction rate is given as follows

$$\phi_{fu,mix} = C_{\phi 1} \cdot \rho \cdot c^{1/2} \cdot K/\varepsilon$$

where for imperfect premixing we may suppose

$$c = c(Y_{fu}, \phi, grad(Y_{fu}), grad(\phi))$$

We use here (ref. 2)

$$c = min\left(Y_{fu}^2, (Y_{ox}/s)^2, K^3/\varepsilon^2 \cdot grad(Y_{fu})^2 \cdot C_{\phi 2}\right)$$

The kinetics controlled reaction rate is then evaluated as follows

$$\phi_{fu,kin} = \rho^2 \cdot Y_{fu} \cdot Y_{ox} \cdot PF \cdot exp(-AE/e)$$

Finally, the actual reaction rate is taken to be the smaller of the values from the previous expressions.

Along the inflow boundary, all the flow variables except the static pressure are specified. Along the outflow boundary, only the static pressure is specified. Along the solid boundaries, the no-slip condition requires the vanishing of velocity, turbulence kinetic energy, and turbulence kinetic energy dissipation rate, the latter being obviously intended as the modified quantity used in the conservation equations. The specific internal energy is then set equal to the value following from the wall temperature for constant temperature walls, or the energy gradient normal to the wall is set equal to zero for adiabatic walls. Furthermore, the species concentration gradient normal to the wall is set equal to zero. Along a symmetry plane (axis) the normal derivatives of all the flow parameters vanish, with the exception of the normal velocity component, to be set equal to zero.

NUMERICAL SOLUTION

The proposed equations are solved in two-dimensional geometries. The derivation of the two-dimensional equations from the previous general form is straightforward and not presented here. The equations are written in a form useful in both Cartesian and axisymmetric geometries by introducing a switch parameter distinguishing between these two coordinates (ref. 2).

The discretization adopted is a pseudo unsteady, finite volume, dissipative, explicit one. In the proposed pseudo unsteady, the solution of the steady equations is obtained as the asymptotic solution of the following artificial unsteady equations

$$\int \int_V \int \left(\frac{\partial f}{\partial t}\right) \cdot H_p^{-1} dV + \int_\Sigma \int N \cdot (F_i + F_v) d\Sigma = \int \int_V \int S \, dv$$

These unsteady equations are generally constructed in order to obtain the better convergence rate, obviously providing that the steady state solution is not altered.

From the identity between the convergence process and the elimination process of the initial perturbations to the steady solution, the convergence

parameters are determined in order to improve the perturbation propagation or damping. We use (ref. 3)

$$H_p = \delta r / \beta_{max} \cdot$$

$$
\begin{vmatrix}
1 & 0 & 0 & 0 & \ldots & 0 \\
0 & 1 & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & \ldots & 0 \\
f_1 \cdot V^2/2 & -f_1 \cdot V_x & -f_1 \cdot V_y & f_2 & \ldots & 0 \\
\cdot & \cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & & \cdot \\
0 & 0 & 0 & 0 & \ldots & 1
\end{vmatrix}
$$

where

$$f_1 = min(M^2 - 1, 0)$$

$$f_2 = max(f_1 + 1, C_p)$$

with

$$M = V \cdot (\gamma \cdot p/\rho)^{-1/2}$$

Cp is a small positive number, and

$$\beta_{max} = min(\beta_1, \beta_2)$$

$$\beta_1 = V \cdot \{(1 + M^2)/2 + [((1 - M^2)/2)^2 + 1]^{1/2}\}$$

$$\beta_2 = V \cdot (1 + 1/M)$$

This produces an improved propagation, but only for subsonic flows.

These equations are then discretized in space by using a finite volume discretization. The mesh is nonorthogonal and curvilinear, conforming to the boundaries of the domain, with lines intersecting at arbitrary angles, properly refined where high gradients are expected to occur. The discretization nodes, located at the intersection of these lines, are the centers of hexagonal control volumes, obtained by connecting the six surrounding nodes. A sample computational domain and the hexagonal control volume are shown in figure 1.

The discretized equations are written as follow (ref. 2 and 4)

$$\frac{\partial f}{\partial t} = H_p \cdot \left[-\sum_{j=1}^{6} (F_{i,j} + F_{v,j}) \cdot N_j \cdot \delta \Sigma_j \right] v + S$$

where the subscript j refers to every face of the finite volume.

The equations are finally discretized in time by using an explicit, dissipative discretization. Let the previous equation be rewritten with the addition of a dissipative term as follows

$$\frac{\partial f}{\partial t} = T(f) + D(f)$$

where T represents the residual and D is the dissipative term. The explicit k-stage Runge-Kutta algorithm is written as follows (δt = CFL)

$$f^{(0)} = f^m$$

$$f^{(1)} = f^{(0)} - \theta_1 \cdot \delta t \cdot \left[T_i(f^{(0)}) + T_v(f^{m^*}) + D(f^{(0)}) - \Omega \cdot D(f^{m^*}) \right]$$

$$f^{(k-1)} = f^{(0)} - \theta_{k-1} \cdot \delta t \cdot \left[T_i(f^{(k-2)}) + T_v(f^{m^*}) + D(f^{(0)}) - \Omega \cdot D(f^{m^*}) \right]$$

$$f^{(k)} = f^{(0)} - \delta t \cdot \left[T_i(f^{(k-1)}) + T_v(f^{m^*}) + D(f^{(0)}) - \Omega \cdot D(f^{m^*}) \right]$$

$$f^{m+1} = f^{(k)}$$

The dissipative terms are given as follows (ref. 2)

$$D^m = 1/(6 \cdot \delta t) \cdot \sum_{j=1}^{6} \left(f_j^m - f^m \right)$$

and

$$\Omega = C_{\Omega 1} \cdot \left| 1 - C_{\Omega 2} \cdot \frac{1}{6} \cdot \sum_{j=1}^{6} \left(\rho_j^m - \rho^m \right) \right|$$

$C\Omega 1$ and $C\Omega 2$ are vectors of coefficients of the order of unity (ref. 2).

The subscript j refers now to every surrounding node involved in the definite volume approximation, and the superscript m refers to local time $m \cdot \delta t$. The terms referring to time $m^* \cdot \delta t$ are updated only at specific iterations and assumed constant between two updatings. The updating rate is taken equal to NV iterations, to be determined accordingly with a numerical optimization.

A four-stage scheme, with the standard coefficients

$$\theta_1 = \frac{1}{4} \qquad \theta_2 = \frac{1}{3} \qquad \theta_3 = \frac{1}{2}$$

has a Courant limit of about CFL = 2.6.

The time step is evaluated according to the classical CFL stability limit all over the computational domain. It is taken slightly smaller than the local CFL number in order to take into account the neglected stability limit due to the viscous terms.

Thanks to the efficient pseudo unsteady solution, the method appears to be rather fast, while the explicit finite volume discretization allows ease of understanding and computer programming.

RESULTS

First calculations were performed for a partially premixed turbulent reacting flow. Figure 2 shows schematically the flow domain. Experimental and theoretical results are presented in reference 13. In this configuration, mixing of two parallel streams, one of hot gases and the other of a fresh mixture of air and methane, in a constant area duct is considered. The hot jet causes a flame to be ignited and stabilized in the duct. The inlet duct, with a cross section of 100 by 100 mm^2, is split into two parts. The upper section (80 by 100 mm^2) is assigned to the fresh air and methane mixture, with a velocity of 65 m/s, a temperature of 580 K, and a mixture ratio of 0.8; the lower one (20 by 100 mm^2) is assigned to the pilot flame made up of hot gases, with a velocity of 130 m/s and a temperature of 2000 K; the walls are insulated.

Calculations were performed on a 35 by 45 computational grid, nonuniform but orthogonal. Conventional steady solutions were obtained in about 2x10^3 iterations with a total CPU time of about 1-1/2 hr on a VAX 8800. Figures 3 and 4 show a comparison of predicted /method 2/ and measured transverse temperature profiles at x = 42 mm and at x = 122 mm. The agreement in both sections lies within engineering accuracy. The introduction of the influence of kinetics in the evaluation of the reaction rate and a better calibration of the model constants leads to a better accuracy than the one obtained in reference 2 /method 1/, even if at x = 122 mm the temperatures in the mixing layer are still underestimated.

The method has then been applied to a turbulent diffusion reacting flow. Figure 5 shows schematically the flow domain. Experimental and theoretical results are presented in reference 8. In this configuration, there is a central jet of fuel, substantially methane, with a velocity of 21.3 m/s and a temperature of 300 K, and a concentric jet of oxidizer, with a velocity of 34.3 m/s and a temperature of 589 K. The outer radius of the fuel jet is 8 mm, the inner and outer radius of the air jet are respectively 11.1 and 28.6 mm. The radius of the combustor is 101.6 mm. The wall temperature is 1140 K.

Calculations were performed on a 45 by 45 computational grid, nonuniform but orthogonal. Conventional steady solutions were obtained in less than 3x10^3 iterations with a total CPU time of about 3 hr on a VAX 8800. Figures 6 and 7 show a comparison of predicted /method 2/ and measured radial temperature profiles at x = 95 mm and x = 398 mm.

Even if the accuracy appears to be not optimal, the proposed method allows a better accuracy than the method presented in reference 8 /method 1/, despite the single step chemical reaction adopted here. This is substantially due to a better modeling of the reaction rate. The mixing controlled reaction rate of reference 8 is simply taken proportional to the smaller value of the fuel and the oxidizer concentration. The present mixing controlled reaction rate is taken proportional to the fuel concentration gradients with limitations arising from the availability of fuel and oxidizer.

In a laminar diffusion flame, little oxidizer is detectable within the reaction zone envelope, and little fuel is detectable outside of it. The reaction zone is a very thin envelope, and fuel and oxidizer concentrations show a small overlapping. In a turbulent diffusion flame, the reaction zone is thicker, and the averaged values of fuel and oxidizer overlap significantly. The reaction zone is now a finite volume, even if always relatively small. The introduction of the gradient concentration dependence other than the concentration dependence appears to lead to a better simulation of the thickness of the reaction zone.

CONCLUSIONS

The paper has presented a numerical method for the study of steady, reacting turbulent viscous flow in two-dimensional geometries, both Cartesian and axisymmetric.

The proposed two-equation $K-\varepsilon$ model, where low Reynolds number and compressibility effects are included, and a modified eddy-breakup model give a satisfactory description of fluid mechanics turbulence, chemistry, and turbulence-combustion interaction within an engineering accuracy.

The pseudo-unsteady method with improved perturbation propagation properties and the explicit multi-stage dissipative Runge-Kutta algorithm appear to be fast and reliable.

The application of the method to the computation of the temperature distributions for a diffusion and a premixed turbulent reacting flow shows a satisfactory agreement between experimental and computational results.

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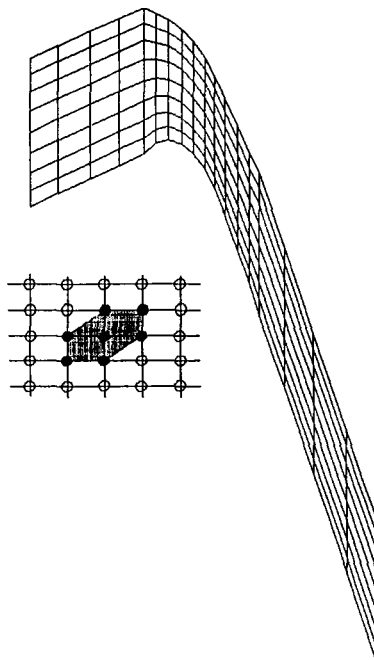
FIGURE 1. - SAMPLE COMPUTATIONAL DOMAIN AND HEXAGONAL CONTROL VOLUME.
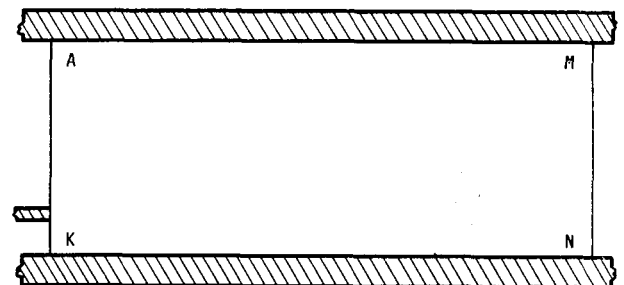

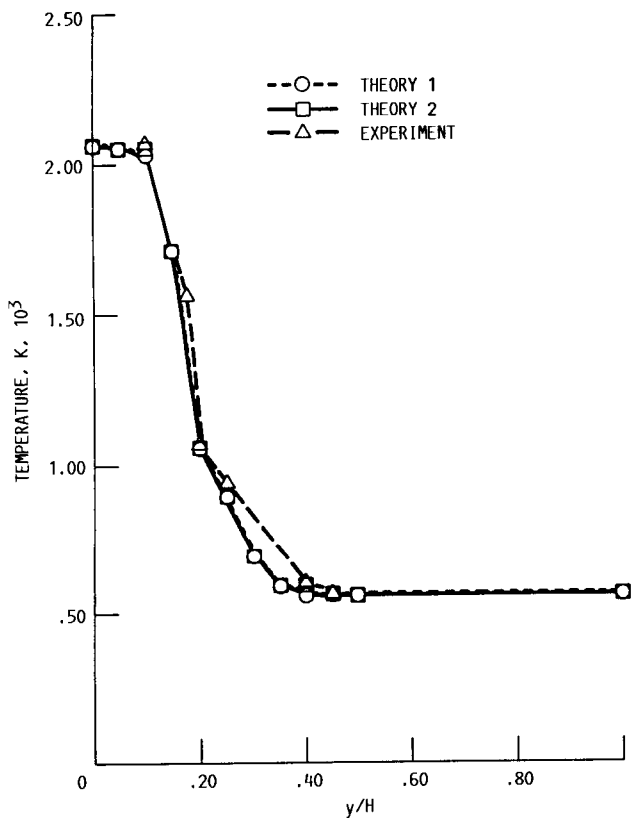FIGURE 2. - PREMIXED TURBULENT REACTING FLOW: PHYSICAL DOMAIN.

FIGURE 3. - PREMIXED TURBULENT REACTING FLOW: COMPARISON
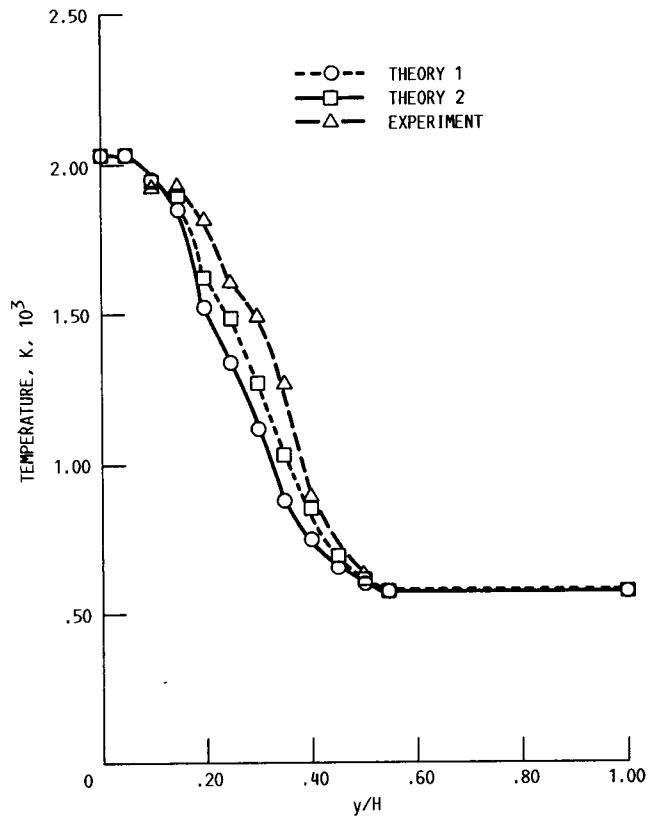OF PREDICTED AND MEASURED TEMPERATURE DISTRIBUTIONS.

FIGURE 4. - PREMIXED TURBULENT REACTING FLOW: COMPARISON
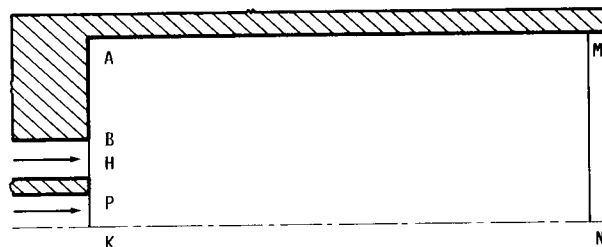OF PREDICTED AND MEASURED TEMPERATURE DISTRIBUTIONS.

FIGURE 5. - DIFFUSION TURBULENT REACTING FLOW: PHYSICAL DOMAIN.
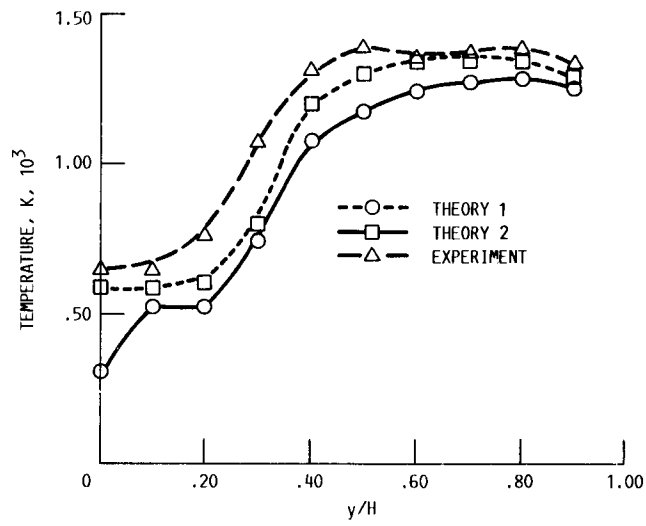
FIGURE 6. - DIFFUSION TURBULENT REACTING FLOW: COMPARISON
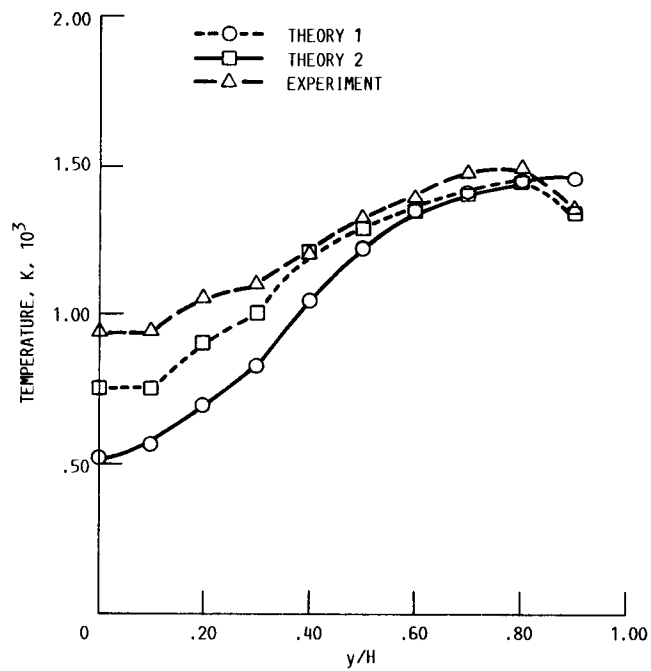OF PREDICTED AND MEASURED TEMPERATURE DISTRIBUTION.

FIGURE 7. - DIFFUSION TURBULENT REACTING FLOW: COMPARISON
OF PREDICTED AND MEASURED TEMPERATURE DISTRIBUTIONS.

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16. Abstract

The paper presents a numerical method for the solution of the conservation equations governing steady, reacting, turbulent viscous flow in two dimensional geometries, in both Cartesian and axisymmetric coordinates. These equations are written in Favre-averaged form and closed with a first order model. A two-equation K-ϵ model, where low Reynolds number and compressibility effects are included, and a modified eddy-break up model are used to simulate fluid mechanics turbulence, chemistry and turbulence-combustion interaction. The solution is obtained by using a pseudo-unsteady method with improved perturbation propagation properties. The equations are discretized in space by using a finite volume formulation. An explicit multi-stage dissipative Runge-Kutta algorithm is then used to advance the flow equations in the pseudo-time. The method is applied to the computation of both diffusion and premixed turbulent reacting flows. The computed temperature distributions compare favorably with experimental data.

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