A NUMERICAL ANALYSIS OF COMBUSTION PROCESS IN AN AXISYMMETRIC COMBUSTION CHAMBER

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Abstract: Combustion phenomenon is one of the most important problems involved in different industries, such as gas turbines, combustion chamber, melting of metals, etc. In this paper, combustion process of methane downstream of an axisymmetric sudden expansion in a circular pipe with a constant wall temperature has been studied. The conservation equations of mass, momentum, energy, and species as well as additional equations due to turbulence modeling have been numerically solved. The standard k-\varepsilon model and eddy dissipation combustion model has been used to simulate the turbulence and combustion phenomenon, respectively. Properties of gaseous mixture have been computed using the ideal gas equation of state. The governing equations have been discretized using a finite volume approach and power law scheme and the resulting set of algebraic equations has been solved simultaneously using the SIMPLER algorithm on a non-uniform staggered grid system. The numerical results have been compared with the other’s numerical results and experimental data.

Keywords: combustion chamber, CFD, methane combustion, turbulent flow

1. INTRODUCTION

The design of combustion chambers is of great importance. The geometry of these chambers may change gradually or suddenly. When the fluid path is changed abruptly, flow parameters, flow characteristics and the heat transfer rate are altered consequently. On the other hand, turbulent flows through axisymmetric sudden expansions are influenced by many parameters. Among these are inlet geometry, inlet flow Reynolds number, expansion ratio, step height, inlet turbulence intensity and inlet boundary condition. The interaction between turbulence and combustion is very important in the design of combustion chamber. Combustion phenomenon and the important design parameters are governed by this interaction.

Numerical simulation is becoming a powerful means in understanding combustion process and designing or optimizing combustion systems. The mathematical modeling of turbulent combustion has been outlined by Magnussen et al. [1]. They have developed the eddy dissipation concept for modeling of combustion. Turbulent non-reacting flows have been briefly studied by Ramous [2]. He, later, developed a mathematical model to study turbulent, confined, swirling flows under reacting non-premixed condition [3]. It is observed that the dimensions of the recirculation zone are larger for non-premixed reacting flows than for incompressible conditions. This seems to be caused by the heat released from the chemical reaction, which affects the density, centrifugal forces and radial pressure gradient.
Two fast-chemistry models, the eddy dissipation concept (EDC) and the conserved scalar (CS) approach, have been analyzed [4]. In this work turbulence is simulated by three types of $k - \varepsilon$ models. The equations are discretized using a hybrid scheme and the SIMPLE algorithm is employed to solve the resulting algebraic equations.

Ohtsuka has performed the numerical study of reacting and non-reacting flows using the Reynolds stress differential [5]. He has modeled mixing of air and helium and also the combustion of propane.

In this work, combustion of methane in turbulent flow is studied. It is assumed that the fuel and air enter the cylindrical chamber with abrupt expansion as confined coaxial jets.

2. GOVERNING EQUATIONS

The combustion chamber geometry under study is shown schematically in Fig. 1. This geometry consists of two confined, coaxial jets; the inner jet contains pure fuel (methane) and the outer jet contains air. It is assumed here that the methane and air react by means of a one-step overall and irreversible chemical reaction rather than through a multitude of elementary reaction steps. It is assumed that the flow is statistically stationary and axisymmetric.

![Fig. 1. Schematic of flow geometry and solution domain](image)

The hydrodynamic equations governing the statistical stationary, axisymmetric, turbulent flow field in the geometry shown in Fig.1 can be written as:

- **Continuity**

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

- **Axial momentum component**

$$\frac{\partial}{\partial x} (\rho uu) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho vv) = \frac{\partial}{\partial x} \left( \mu_\text{eff} \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu_\text{eff} \frac{\partial u}{\partial r} \right) + S_u$$  \hspace{1cm} (2)

where,

$$S_u = \frac{\partial \rho}{\partial x} + \frac{\partial}{\partial x} \left( \mu_\text{eff} \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu_\text{eff} \frac{\partial v}{\partial r} \right) - \frac{2}{3} \frac{\partial}{\partial x} \left( \mu_\text{eff} \nabla V + \rho k \right)$$  \hspace{1cm} (3)

- **Radial momentum component**

$$\frac{\partial}{\partial x} (\rho uv) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho vv) = \frac{\partial}{\partial x} \left( \mu_\text{eff} \frac{\partial v}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r \mu_\text{eff} \frac{\partial v}{\partial r} \right) + S_v$$  \hspace{1cm} (4)
where,

\[
S_v = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x}\left(\mu_{\text{eff}} \frac{\partial u}{\partial r}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r \mu_{\text{eff}} \frac{\partial v}{\partial r}\right) - 2 \mu_{\text{eff}} \frac{v}{r^2} - \frac{2}{3} \frac{\partial}{\partial r}\left[r \left(\mu_{\text{eff}} \nabla V + \rho k\right)\right] + \frac{2}{3} \frac{1}{r} \left(\mu_{\text{eff}} \nabla V + \rho k\right)
\]  

(5)

\cdot Scalar equation

The scalar variables \(k\) (turbulent kinetic energy), \(\varepsilon\) (turbulent dissipation rate), \(H\) (specific total enthalpy), \(Y_f\) (mass fraction of fuel) and \(Y_m\) (mass fraction of species \(m\)) satisfy the following equation (substitute generic variable \(\phi\)):

\[
\frac{\partial}{\partial x}\left(\rho u \phi\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r \rho v \phi\right) = \frac{\partial}{\partial x}\left(\Gamma_{\text{eff}} \frac{\partial \phi}{\partial x}\right) + \frac{1}{r} \frac{\partial}{\partial r}\left(r \Gamma_{\text{eff}} \frac{\partial \phi}{\partial r}\right) + S_\phi
\]

where, the source term, \(S_\phi\) for \(Y_m\) and \(H\) is zero and for \(Y_f\) [1], \(k\), \(\varepsilon\), are as follows:

\[
S_{Y_f} = -\rho \varepsilon k_{\min} \left(A \cdot Y_f + A \cdot \frac{Y_{O2}}{S} + A \cdot B \cdot \frac{Y_{Pr}}{S+1} \right),
\]

\[S_k = P - \rho \varepsilon, \quad S_\varepsilon = \left(C_1 P - C_2 \rho \varepsilon\right) \frac{\varepsilon}{k}
\]

(6)

where,

\[
P = 2 \mu_{\text{eff}} \left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial r}\right)^2 + \left(\frac{v}{r}\right)^2\right] + \mu_{\text{eff}} \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial r}\right)^2
\]

(8)

\[
\mu_t = C_\mu \rho \varepsilon k^{1/2}, \quad \mu_{\text{eff}} = \mu + \mu_t, \quad \Gamma_{\text{eff}} = \frac{\mu_{\text{eff}}}{\sigma_\phi}
\]

(9)

\[
\nabla \cdot V = \frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r}\left(r v\right)
\]

(10)

and the constants for the turbulence model [6] and combustion model [1] are:

\[
C_1 = 1.44, \quad C_2 = 1.92, \quad C_\mu = 0.09, \quad \sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3, \quad \sigma_T = 1.0, \quad A = 4.0, \quad B = 0.5, \quad S = 4.0
\]

(11)

\textit{Remark:} \(A\) and \(B\) are model constants [1] which depend on both the structure of the flame and the reaction between the fuel and oxygen; \(Y_f\), \(Y_{O2}\) and \(Y_{Pr}\) are the mass fraction of fuel, oxygen and products; \(S\) is the stoichiometric mass ratio of oxygen to fuel.

\cdot Chemical reaction equation:

The overall reaction can be written as:

\[
CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 2 \times 3.76N_2
\]

(12)

The mean density of mixture is calculated from the ideal gas equation of state:
\[ \rho = \rho_0 \exp\left(-\frac{RT\sum_{i=1}^{N_s} \frac{Y_i}{M_i}}{\sum_{i=1}^{N_s} Y_i}ight) \]  

(13)

where, \( R \), \( N_s \), and \( M_i \) are the universal gas constant, the number of species and the molecular mass of specie \( i \), respectively.

The specific heat at constant pressure for the mixture is computed as:

\[ CP_m = \sum_{i=1}^{N_s} Y_iCP_i, \quad CP_i = \frac{R}{M_i}\left(a_i + b_iT + c_iT^2 + d_iT^3 + e_iT^4\right) \]  

(14)

in which, \( CP_i \) is the specific heat of the specie \( i \) and \( a_i, b_i, c_i, d_i, e_i \) are constants for each specie that can be determined from tabulated data [7].

The temperature of gas, \( T \), is obtained from:

\[ T = \left(\frac{H - Y_fH_R}{CP_m}\right) \]  

(15)

where, \( H_R \) is the enthalpy of combustion.

### 3. BOUNDARY CONDITIONS

To solve the governing equations, boundary conditions must be applied to the inlet, outlet, solid walls and centerline of the solution domain.

A brief description of these boundary conditions is as follows.

Two flows were assumed to have zero radial velocities at the inlet and enter the combustion chamber with uniform but different axial velocities and temperatures. The inlet turbulence kinetic energy and its dissipation are taken as \( k = I^2u^2 \) and \( \varepsilon = C_{\mu}k^{1.5}/0.03l \), respectively, in which \( I \) is the inlet turbulence intensity and \( l \) is either the radius of the fuel inlet flow, or annular height of the air inlet flow. The flow is assumed to leave the combustion chamber with zero axial gradients of flow quantities. At the solid walls, the no slip condition for normal velocity component was applied while the wall function [6, 8] was employed to calculate the tangential velocity near the wall and heat transfer rates. At the combustion chamber centerline, radial velocity component is zero, and the radial gradients of other flow quantities are zero because of symmetry.

### 4. NUMERICAL PROCEDURE

The conservation equations for mass, axial and radial momentum, energy, species, kinetic energy of turbulence and its dissipation rate, are discretized using the finite volume method and the power law scheme [9]. For this purpose, the computational domain is considered as a non-uniform staggered grid, which covers the whole solution domain.

The grid has a higher node concentration at the annulus-mixing layer between the fuel and the air stream, in the recirculation zone near the inlet and near the wall where steep gradients of the flow variables are expected. The values of scalar variables are calculated at the grid nodes, while the axial and radial velocity components are calculated at the grid midpoints in order to have a conservative finite-difference algorithm.
The resulting algebraic equations are coupled and are simultaneously solved by Tri-Diagonal Matrices Algorithm (TDMA). The SIMPLER algorithm is used to introduce pressure gradient in the momentum equations. In order to prevent the divergence of non-linear equations, the suitable under relaxation factors are used. Because of intensive influence of temperature and pressure changes on density, the density is assumed to be constant at the first 500 iterations to prevent divergence. Then the resulting flow variables are taken as initial quantities to solve equations simultaneously. Therefore the equations are solved iteratively until a prescribed convergence criterion is achieved.

The criterion for convergence of numerical solution was that the total normalized residual is less than $10^{-3}$. This convergence was achieved in about 1800 iterations.

5. RESULTS AND DISCUSSIONS

The geometrical and dynamical parameters of the combustion chamber and the flows have been chosen as to be comparable with those in [10]. The length, $L$, of the combustion chamber is 1.7 m, and the radius, $R_c$, is 0.06115 m. The inner radii of the fuel, $R_i$, and air, $R_o$, inlets are 0.0295 m and 0.0465 m, respectively. The fuel and air mass flow rates are 7.2 gr/s and 137.0 gr/s, which yield an air/fuel velocity ratio of approximately 20:1. The temperatures of combustion chamber walls, $T_w$, fuel inlet, $T_i$, and air inlet, $T_o$, are 500K, 300K and 600K, respectively.

To ensure the precision of computations, the numerical procedure has been thoroughly checked. First, the sensitivity analysis has been done. The proper choice of grid size has been examined in [11]; solutions have been performed with different grid densities and grid points to ensure a grid-independent solution. The axial velocity at the centerline of combustion chamber (central velocity) for two different grid points (80×60, 200×120) has been compared. It has been observed that the difference between them is less than 5%. Then, it was found that a grid consisting of 200×120 points is sufficient in providing a grid-independent solution.

Typical fluid flow and streamlines are shown in Fig. 2a, b. Two recirculation zones are observed; one, appears at the centerline immediately downstream of the fuel inlet which was produced due to high momentum flux ratio of the air and fuel flows and resulting in flame stabilization, the other, appears near the outer wall because of the sudden expansion. Figure 3 shows the results for a grid with 1700 x 140 nodes (l=7%) using Fluent solver.

![FIG. 2. (a) Fluid flow near the inlet of combustion chamber; (b) Streamlines near the inlet of combustion chamber](image-url)
Moreover the published experimental and numerical results [4, 10] have been used to verify the correctness of the numerical procedure. In Fig. 4, the temperature profiles at different sections of combustion chamber are compared with EDC model results [4] and experimental results [10]. It is observed that the results of this study are in good agreement with experimental data.
Also it is observed that, increasing turbulence intensity decreases the dimensions of recirculating zone. The central velocity at different conditions are compared with each other in Fig. 5:

1. using the existing model and $I=7\%$,
2. using the existing model and $I=17\%$,
3. using the existing model without combustion (cold flow),
4. using the EDC model
5. using the FLUENT model EDC, and
6. using experimental data.

It is observed that, the existing model is more effective in prediction of recirculation zone than the EDC model. Also the axial velocity profiles for cold flow (without combustion) and hot flow (with combustion) at different axial sections of combustion chamber are compared with experimental data (Figure 6). It is observed that the flow is expanded due to high temperature caused by combustion reaction. Numerical results are in good agreement with experimental data especially at downstream of recirculation zone.
CONCLUSIONS

The model can predict the velocity, pressure, temperature, fuel mass fraction, mixing mass fraction and combustion products mass fraction distributions. Using these distributions, one can estimate the critical values of the above properties. As an example, using the pre-mentioned conditions, the maximum temperature of the combustion products turns out to be approx. 2000K. Because of high temperatures caused by combustion reaction, fluid flow is expanded. Increasing the turbulence intensity decreases the dimensions of recirculation zone.

REFERENCES