MODELING OF NON-CONFINED TURBULENT FLOW
OF TWO COAXIAL STREAMS
UNDER COMBUSTION CONDITIONS

UDC 621.43.019+52-46

Miroslav Sijerčić, Žarko Stevanović, Srdjan Belošević

Institute of Nuclear Sciences - Vinca, Laboratory for Thermal Engineering and Energy
11001 Belgrade, P.O. Box 522, Yugoslavia

Abstract. The investigation of turbulence and combustion interaction is most conveniently done in simple configurations where the influence of various physical processes can be isolated and studied in details. This paper deals with mathematical modeling of turbulent combustion and complements the experimental research of methane flame occurring in two coaxial streams. The geometry is two coaxial streams, where the inner one is the stoichiometric mixture of the air and methane, and the outer one is the pure air, so the premixed and diffusion combustion mechanisms coexist in the flow field. This flow configuration is interesting for design of efficient combustors that enable pollution reduction and energy savings.

Turbulent model for reactive flow field is based on the second-order closures for Reynolds stresses and fluxes. Closure of the system of Reynolds equations of momentum and continuity equation for stationary axial-symmetric turbulent flow of incompressible fluid has been carried out based on the solution of conservation equations for turbulent stresses and turbulence kinetic energy dissipation rate. The model encompasses conservation equations of gas components participating in the process (CH₄, O₂, N₂, CO₂, H₂O) and energy equation. To deal with chemical reaction, conservation equations of participating species in terms of mass fraction of species are solved. The energy equation is solved in term of mixture enthalpy. The system of equations has been closed by means of conservation equations for Reynolds scalar fluxes scalar variance.

Combustion rate based on the chemical kinetic is obtained by the Arrhenius relation, that is much greater than combustion rate in the real flame. Because the time scale of the turbulence decay is typically much longer than the chemical kinetic time scale, the reaction is controlled by turbulent mixing. Since practically all of the combustion occurs after mixing between the small scale dissipative eddies, we cannot go too far wrong by linking the combustion rate to the turbulence decay rate by “Eddy-Break-Up” model. According to this model, it was assumed that the combustion reactions are

Received June 10, 2001
Presented at 5th YUSNM Niš, 2000, Nonlinear Sciences at the Threshold of the Third Millenium, October 2-5, 2000, Faculty of Mechanical Engineering University of Niš
controlled by the rate of turbulence production destruction, which is characterized by
the turbulence time scale of large eddies. In domain of lower temperatures, the rate is
controlled by the chemical reaction kinetics.

The comparison of the experimentally obtained and calculated parameters of the flame
flow field, such as $U, V, T, \bar{u}', \bar{v}', \bar{w}', \bar{T}'$, has been made. Turbulent mass fluxes are also
calculated but not compared with experimental data.

1. INTRODUCTION

The investigation of turbulence and combustion interaction is most conveniently done
in simple configurations where the influence of various physical processes can be isolated
and studied in detailed. This paper deals with mathematical modeling of turbulent
combustion and complements the experimental research of methane flame occurring in
two coaxial streams [1], [2]. The flow configuration includes two coaxial streams, where
the inner one is the stoichiometric mixture of the air and methane, and the outer one is the
pure air, so the premixed and diffusion combustion mechanisms coexist in the flow field.
This flow configuration is interesting for design of efficient combustors that enables
pollution reduction and energy savings.

In these reactive flows, correlations connected to the density fluctuations appear in the
transport equations ($\rho \bar{u}', \rho \bar{v}', \rho \bar{w}', \rho \bar{T}', \rho \bar{u}_i, \rho \bar{u}_j, \rho \bar{T}_i$, and others). This problem may be overcome
using Favre mass averaging with PDF approach for mean scalar determination, which
eliminates density fluctuation correlation. With Favre averaging, which appears most
appropriate for variable density flows, the solution of mean velocity and mean scalar field
requires the density-weighted turbulent stress and turbulent flux of scalar quantities to be
determined. Formally, there is nothing new in usage approach based on Favre averaging,
but some difficulties arise when comparing calculated to the experimentally obtained flow
characteristics. Furthermore, the choice between Favre and Reynolds averaging is not
easy and straightforward. Modeling of mass averaged conservation equations is partially
taken from the time averaging, that is one more cause of uncertainties. Boundary
conditions for the scalar variables are not the same, so the Crocco’s similarity is not
satisfied. Finally, there is a great difficulty in the joint probability density function
determination for open flame. On the other hand, turbulent models for reactive flow-fields
based on the second-order closures for Reynolds stresses and fluxes give more detailed
information and opportunities for overcoming the above uncertainty.

2. MATHEMATICAL MODELING

Closure of the system of Reynolds equations of momentum and continuity Eqn. (1) for
incompressible flow has been carried out based on the solution of conservation equations for
turbulent stresses ($\rho \bar{u}_i, \rho \bar{u}_j$) and turbulent temperature fluxes $\rho \bar{T}_i$. The full differential stress/flux
second-moment closure, including buoyancy effects, can be summarized as follows:

$$\frac{D/Dt(\rho U_i U_j)}{\rho U_i } = -\partial_j P + \partial_j (\mu \partial_j U_i - \rho \bar{u}_i \bar{u}_j) + \rho g \beta (T - T_{ref}) ; \quad \frac{D/Dt(\rho U_i)}{\rho } = 0$$

(1)


\[
\frac{D(pu_iu_j)}{Dt} - D_y = \rho P_{ij} + \rho G_{ij} + \rho \Phi_{ij} - \rho \varepsilon_{ij} \tag{2}
\]

\[
\frac{D(\rho e_{i,j})}{Dt} - D_e = (\rho e/k)(C_{c1}P + C_{c2}G - C_{c4}e) \tag{3}
\]

\[
\frac{D(D(\rho \theta_i))}{Dt} - D_{\theta_i} = -\rho u_i \theta_j \partial_j T - \xi \rho \theta_i \partial_j U_j - \eta p g_i \theta_j - C_{01}(\varepsilon/k) \rho \theta_i - \rho \varepsilon_{ii} \tag{4}
\]

\[
D(D(\rho \varepsilon_{ii}^2)) - D_{\varepsilon_{ii}} = 2\rho P_{\varepsilon_{ii}} - 2\rho \varepsilon_{ii} \tag{5}
\]

\[
D(D(\rho e_{00})) - D_{e_{00}} = C_{c1}^0 P_{e_{00}}(e_{00} / \theta_i^2) + C_{c3}^0 P(e_{00} \varepsilon / k) - C_{c4}^0 P(e_{00}^2 / \theta_i^2) - C_{c4}^0 P(e_{00} \varepsilon / k) \tag{6}
\]

\[
P_{ij} = -(u_i \partial_j U_j + u_j \partial_i U_i), \quad G_{ij} = -\beta (g_i \theta U_j + g_j \theta U_i) \tag{7}
\]

\[
\Phi_{ij} = -C_{c1}(u_i \partial_j U_j - 2 \xi \delta_{ij}) - C_{c2}(P_{ij} - \xi \delta_{ij}) - C_{c3}(G_{ij} - \xi \delta_{ij}) \tag{8}
\]

\[
P = -\rho u_i \partial_j U_j, \quad G = -\beta g_i \theta U_i, \quad P_{\varepsilon_{ii}} = -\delta_{ij} \partial_j T \tag{9}
\]

\[
D_\theta = \delta_{ij} (\mu \partial_j \phi + C_{\varepsilon} \rho u_i \partial_j \phi) \tag{10}
\]

where \( k = (u_i u_i) / 2 \) is the turbulence kinetic energy, \( \tau = \varepsilon/k \) is the dissipative time scale, and \( D/Dt = \partial_0 + U_i \partial_i \) is the substantial derivative. Model coefficients introduced in above equations are listed in Table 1.

<table>
<thead>
<tr>
<th>Table 1. Specification of coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{01} )</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>( C_{c5} )</td>
</tr>
<tr>
<td>0.8</td>
</tr>
</tbody>
</table>

\( P_{ij} \) and \( G_{ij} \) represent Reynolds stress production by strain and buoyancy, respectively. The pressure strain term \( \Phi_{ij} \) is modeled as the sum of slow-term, rapid-term, and buoyancy-pressure term. \( P \) and \( G \) represent the turbulence energy production by strain and buoyancy, respectively. \( P_{\varepsilon_{ii}} \) is the production of temperature variance. \( D_\theta \) denotes the total general diffusion term, in which the turbulent part is modeled by the simple gradient hypothesis. For homogeneous turbulence, the dissipation rate \( \varepsilon_{00} \) is negligible.

Additionally, the model encompasses conservation equations of gas components participating in the process (CH\(_4\), O\(_2\), N\(_2\), CO\(_2\), H\(_2\)O) and energy equation. To deal with chemical reactions we have solved conservation equations of participating species that, with mass fraction of species "\( A \)", \( Y_A \) having a general form:

\[
\frac{D(D(p Y_A))}{Dt} = -\partial_j (\rho Y_A u_j) + \partial_j (\Gamma_j \partial_j (p Y_A)) + \Omega_A \tag{11}
\]
The equations have been closed by means of conservation equations for Reynolds fluxes $\rho \dot{y}_j \mu_i$ that are of the modeled form:

$$\frac{D}{Dt}(\dot{y}_j \mu_i) = -(\rho \mu_i \mu_j \mu_i \cdot y_j U_j + \rho \dot{y}_j \mu_i \mu_j U_j) - C_{yj} \rho \dot{y}_j \mu_i \mu_j U_j -$$

$$- C_{y2} \frac{k^2}{\epsilon} \left( \partial_j \dot{y}_j \mu_i + \partial_i \dot{y}_j \mu_j \right) + S_y$$

(12)

where: $S_y = \rho u_t u_j = -C_{aw} \frac{k}{\epsilon} \frac{\partial \Omega_4}{\partial y_j}$, and $C_{y1} = 3.3$, $C_{y2} = 0.4$, $C_{aw} = 0.15$.

Production and destruction of particular components in the mixture are shown as a part of the source terms of the equations, through the kinetic relations and corresponding stoichiometric ratios. Basic chemical equation of methane combustion is as follows: $\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O} + h_{cr}$, where $h_{cr}$ is the heat effect of chemical reaction. Heat transfer in the flame was considered through the equation of sensitive enthalpy $h_s = \sum l Y_l c_p T_l$. Enthalpy equation has the same form as equation (11), but with different source term:

$$\frac{D}{Dt}(h_s) = U_j \partial_j P - \partial_j \rho \dot{u}_j + \partial_j [\Gamma_{\delta} \partial_j (\rho h_s)] + q_{rad} + \dot{\Omega}_{\text{rad}} h_{cr}$$

(13)

where terms $\dot{\Omega}_{\text{rad}} h_{cr}$ describe the heat effect of the chemical reaction in the flame. The term $q_{rad}$ on the right hand side of the Eqn. (13) represents the heat source due to the radiation.

For the radiation heat transfer, six flux model was reduced for axial-symmetric case of purely emission-absorption radiation to the two-equation model. The diffusion type for radiation fluxes, in axial ($R_x = I_x + J_x$) and radial ($R_r = I_r + J_r$) directions, was used:

$$\partial_x \left[ (1/K_a) \partial_x R_x \right] = K_a R_x - \frac{1}{3} K_a I_b$$

$$\partial_r \left[ (r/k_a) \partial_r R_r \right] = K_a R_r - \frac{1}{3} K_a I_b$$

(14)

where $I_b$ is the emission power of the black body, and $K_a = -(1/L)\ln(1-c_a)$ is the absorption coefficient of the medium. In the energy equation, the heat source due to the radiation is described by the term:

$$q_r = \text{div} \ \hat{Q}_r = K_a \left( R_x + R_r - \frac{2}{3} I_b \right)$$

(15)

Determination of adequate term for the average combustion rate is the basic problem concerning the free turbulent flame. Combustion rate based on the chemical kinetic is obtained by the Arrhenius relation $\Omega_{\text{ch}} = A \rho Y_{\text{CH}} Y_{\text{O}_2} \exp(-E/RT)$, that is much greater than combustion rate in the real flame. Because the time scale of the turbulence decay is typically much longer than the chemical kinetic time scale, the reaction is controlled by turbulent mixing. Since practically all of the combustion occurs after mixing between the small scale dissipative eddies, we cannot go too far wrong by linking the combustion rate to the turbulence decay rate by "Eddy-Break-Up" model. According to this model, it has been assumed that the combustion reactions are controlled by the rate of turbulence production destruction, which is characterized by the turbulence time scale of large eddies, $\tau = k/\epsilon$. Fuel and oxidant concentrations appear as the limiting factors, and thus:
\[ \dot{\Omega}_{ct} = A_{\text{ct},i} \min \left( \rho Y_{\text{ct},i} \frac{\epsilon}{k} , \rho \frac{Y_{\text{ct},i} \epsilon}{s} \right) \] (16)

In domain of lower temperatures, the rate is controlled by the chemical reaction kinetics, so the combustion rate has been determined by relation \( \dot{\Omega}_{c} = \min(\dot{\Omega}_{b}, \dot{\Omega}_{ct}) \).

3. COMPUTATIONAL DETAILS

Two coaxial free streams were considered, where the inner one is the stoichiometric mixture of the air and methane, and the outer one is the pure air, so the premixed and diffusion combustion mechanisms coexist in the flow field. The settings of the inner flow were: mass flow rate of methane and air were 13.39 [l/min] and 127.49 [l/min], respectively. These settings result in a mean inner stream velocity of 3.63 [m/s] and a Reynolds number of about 7500. The energy release rate of the flame was 8 [kW]. The outer flow velocity was set to 3.6 [m/s], before ignition, at the radial position 30 [mm] and axial position 10 [mm] after the nozzle exit. Inner nozzle diameter was 30 [mm] and outer one was 160 [mm]. Thicker walls of the inner nozzle was 2 [mm]. The ambient temperature was 20°C. The calculation was performed in 35x37 non-uniform grid cells in radial and axial directions, respectively.

The flow and gas mixture characteristics were changed from rich flame to a stoichiometric flame. The case of a rich flame is very complicated from the numerical point of view, because premixed and diffusion combustion mechanisms coexist in the same area. This makes the numerical prediction complicated and there is no possibility to test the parameters of the used models; it was the reason of stoichiometric flame calculation, only.

4. COMputation RESULTS

The comparison of the experimentally obtained and calculated parameters of the flame flow field, such as \( U, T, \sqrt{u'^2}, \sqrt{\nu'^2}, \sqrt{\theta'^2} \), has been made. Also, in the present study, the turbulent mass fluxes \( \overline{Y_{i} \mu_{i}} \) are calculated but not compared to experimental data. For illustration, the average axial velocity and temperature are shown on Fig. 1., and the root-mean-square values, \( \sqrt{u'^2} \) and \( \sqrt{\theta'^2} \) are shown on Fig. 2.

5. CONCLUSIONS

In the paper we have considered mathematical modeling of non-confined turbulent flow under combustion conditions. These numerical simulations complement the experimental investigations of methane flame and could have importance in designing of the efficient combustors with reduction of pollution.
Fig. 1. Average axial velocity (U) and temperature (T) comparison
(● - experimental data [1,2], ○ - numerical results)

Fig. 2. Intensity of turbulence for axial velocity ($u_{rms} = \sqrt{u'^2}$) and temperature
($\theta_{rms} = \sqrt{\theta'^2}$) comparison (● - experimental data [1,2], ○ - numerical results)
Model for reactive turbulent flow field is based on the second-order closures for Reynolds stresses and fluxes. The combustion reactions are assumed to be controlled by the rate of turbulence production destruction, and in domain of lower temperatures, by the chemical reaction kinetics. Comparisons between obtained numerical results and corresponding experimental data have shown mostly a good agreement, for average as well as fluctuating velocity and temperature. The model is a good basis for further improvements, needed in prediction of temperature field and fluctuating characteristics for both velocity and temperature.

REFERENCES
sagorevanja sa brzinom odumiranja turbulencije pomoću modela drobogenja vrtloga. Prema ovom modelu, pretpostavlja se da su reakcije sagorevanja kontrolisane brzinom destrukcije produkcije turbulencije, koju karakteriše vremenski razmer turbulencije velikih vrtloga. U oblasti nizih temperaturi, ova brzina je kontrolisana kinetikom hemijske reakcije.

Izvedeno je poređenje eksperimentalno dobijenih i proračunatih parametara strujnog poja plamena, kao što su $U, V, T, \overline{u}, \overline{v}, \overline{w}, \overline{\theta}$, $\overline{\rho u}$. Takode su u ovom radu proračunati i turbulentni maseni fluksevi $\overline{\rho u}$. 