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

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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 (CH_4, O_2, N_2, CO_2, H_2O) 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

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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, $\overline{u^2}, \overline{v^2}, \overline{uv}, \overline{\theta^2}$, *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 ($\overline{\rho' u_i}, \overline{\rho' \theta}, \overline{\rho' y_k}, \overline{\rho' u_i u_j}$, 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 ($\rho \overline{u_i u_j}$) and turbulent temperature fluxes $\rho \overline{\theta u_i}$. The full differential stress/flux second-moment closure, including buoyancy effects, can be summarized as follows:

$$\mathrm{D}/\mathrm{D}t(\rho U_i U_j) = -\partial_i P + \partial_j(\mu \partial_j U_i - \rho \overline{u_i u_j}) + \rho g_i \beta (T - T_{ref}) \; ; \; \mathrm{D}/\mathrm{D}t(\rho U_i) = 0 \qquad (1)$$

$$\frac{\mathrm{D}(\rho\overline{u_i u_j})}{\mathrm{D}t} - \mathsf{D}_{ij} = \rho P_{ij} + \rho G_{ij} + \rho\Phi_{ij} - \rho\varepsilon_{ij} \tag{2}$$

$$\mathrm{D}/\mathrm{D}t(\rho\varepsilon) - \mathsf{D}_{\varepsilon} = (\rho\varepsilon/k)(C_{\varepsilon 1}P + C_{\varepsilon 3}G - C_{\varepsilon 2}\varepsilon) \tag{3}$$

$$\mathrm{D}/\mathrm{D}t(\rho\overline{\theta u_i}) - \mathsf{D}_{\theta i} = -\rho\overline{u_i u_j}\partial_j T - \xi\rho\overline{\theta u_j}\partial_j U_i - \eta\rho g_i\beta\overline{\theta^2} - C_{\theta 1}(\varepsilon/k)\rho\overline{\theta u_i} - \rho\varepsilon_{\theta i} \tag{4}$$

$$\mathrm{D}/\mathrm{D}t(\rho\overline{\theta^2}) - \mathsf{D}_{\theta\theta} = 2\rho P_{\theta\theta} - 2\rho\varepsilon_{\theta\theta} \tag{5}$$

$$\mathrm{D}/\mathrm{D}t(\rho\varepsilon_{\theta\theta}) - \mathsf{D}_{\varepsilon\theta\theta} = C_{\varepsilon 1}^{\theta\theta}\rho P_{\theta\theta}(\varepsilon_{\theta\theta}/\overline{\theta^2}) + C_{\varepsilon 3}^{\theta\theta}\rho P(\varepsilon_{\theta\theta}/k) - C_{\varepsilon 4}^{\theta\theta}\rho(\varepsilon_{\theta\theta}^2/\overline{\theta^2}) - C_{\varepsilon 5}^{\theta\theta}\rho(\varepsilon_{\theta\theta}\varepsilon/k) \tag{6}$$

$$P_{ij} = -(\overline{u_i u_k}\partial_k U_j + \overline{u_j u_k}\partial_k U_i), \quad G_{ij} = -\beta(g_i\overline{\theta u_j} + g_j\overline{\theta u_i}) \tag{7}$$

$$\Phi_{ij} = -C_1\tau(\overline{u_i u_j} - \tfrac{2}{3}k\delta_{ij}) - C_2\tau(P_{ij} - \tfrac{2}{3}P\delta_{ij}) - C_3(G_{ij} - \tfrac{2}{3}G\delta_{ij}) \tag{8}$$

$$P = -\overline{u_i u_j}\partial_j U_i, \quad G = -\beta g_i\overline{\theta u_i}, \quad P_{\theta\theta} = -\overline{\theta u_j}\partial_j T \tag{9}$$

$$\mathsf{D}_{\phi} = \partial_j(\mu\partial_j\phi + C_{\phi}\rho\overline{u_i u_j}\partial_i\phi) \tag{10}$$

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

Table 1. Specification of coefficients

$C_{\theta 1}$	$\xi=\eta$	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	$C_{\varepsilon 3}$	$C_{\varepsilon 1}^{\theta\theta}$	$C_{\varepsilon 3}^{\theta\theta}$	$C_{\varepsilon 4}^{\theta\theta}$
5	0.5	1.44	1.92	1.44	1.3	0.72	2.2
$C_{\varepsilon 5}^{\theta\theta}$	C_1	C_2	C_3	C_s	C_{ε}	$C_{\theta\theta}$	$C_{\varepsilon\theta\theta}$
0.8	1.8	0.6	0.6	0.22	0.07	0.09	0.09

P_{ij} and G_{ij} represent Reynolds stress production by strain and buoyancy, respectively. The pressure strain term Φ_{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. $P_{\theta\theta}$ is the production of temperature variance. D_{Φ} denotes the total general diffusion term, in which the turbulent part is modeled by the simple gradient hypothesis. For homogeneous turbulence, the dissipation rate $\varepsilon_{\theta i}$ is negligible.

Additionally, the model encompasses conservation equations of gas components participating in the process (CH_4, O_2, N_2, CO_2, H_2O) 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:

$$\mathrm{D}/\mathrm{D}t(\rho Y_A) = -\partial_j\rho\overline{y_A u_j} + \partial_j[\Gamma_A\partial_j(\rho Y_A)] + \dot{\Omega}_A \tag{11}$$

The equations have been closed by means of conservation equations for Reynolds fluxes $\rho\overline{y_A u_i}$ that are of the modeled form:

$$\begin{aligned} \mathrm{D}/\mathrm{D}t(\overline{y_A u_i}) = -(\rho\overline{u_j u_i}\partial_j Y_A + \rho\overline{y_A u_j}\partial U_i) - C_{y1}\rho\overline{y_A u_j}\partial_j U_i - \\ - C_{y2}\rho\frac{k^2}{\varepsilon}(\partial_j\overline{y_A u_i} + \partial_i\overline{y_A u_j}) + S_Y \end{aligned} \tag{12}$$

where: $S_y = \rho\overline{u_i\dot{\omega}} = -C_\omega\frac{k}{\varepsilon}\rho\overline{u_i u_j}\frac{\partial\dot{\Omega}_A}{\partial x_j}$, and $C_{y1} = 3.3$, $C_{y2} = 0.4$, $C_\omega = 0.15$.

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: $CH_4 + 2O_2 = CO_2 + 2H_2O + h_{cr}$, where h_{cr} is the heat effect of chemical reaction. Heat transfer in the flame was considered through the equation of sensitive enthalpy $h_s = \Sigma_l Y_l c_{p,l} T$. Enthalpy equation has the same form as equation (11), but with different source term:

$$\mathrm{D}/\mathrm{D}t(\rho h_s) = U_j\partial_j P - \partial_j\rho\overline{\theta u_j} + \partial_j[\Gamma_h\partial_j(\rho h_s)] + q_{rad} + \dot{\Omega}_{\mathrm{CH_4}}h_{cr} \tag{13}$$

where terms $\dot{\Omega}_{\mathrm{CH_4}}h_{cr}$ 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:

$$\partial_x[(1/k_a)\partial_x R_x] = K_a R_x - \frac{1}{3}K_a I_b \qquad \frac{1}{r}\partial_r[(r/k_a)\partial_r R_r] = K_a R_r - \frac{1}{3}K_a I_b. \tag{14}$$

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

$$q_r = div\,\vec{Q}_r = K_a\left(R_x + R_r - \frac{2}{3}I_b\right) \tag{15}$$

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 $\dot{\Omega}_{ch} = A\rho Y_{CH4}Y_{O2}\exp(-E/RT)$, 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, $\tau = k/\varepsilon$. Fuel and oxidant concentrations appear as the limiting factors, and thus:

$$\dot{\Omega}_{ct} = A_{CH4} \min\left[\rho Y_{CH4} \frac{\varepsilon}{k}, \rho \frac{Y_{O_2}}{s} \frac{\varepsilon}{k}\right] \tag{16}$$

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

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_N/min] and 127.49 [l_N/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 35×37 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*, $\sqrt{\overline{u^2}}, \sqrt{\overline{v^2}}, \overline{uv}, \sqrt{\overline{\theta^2}}$, has been made. Also, in the present study, the turbulent mass fluxes $\overline{y_A u_i}$ 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, $\sqrt{\overline{u^2}}$ and $\sqrt{\overline{\theta^2}}$ 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.

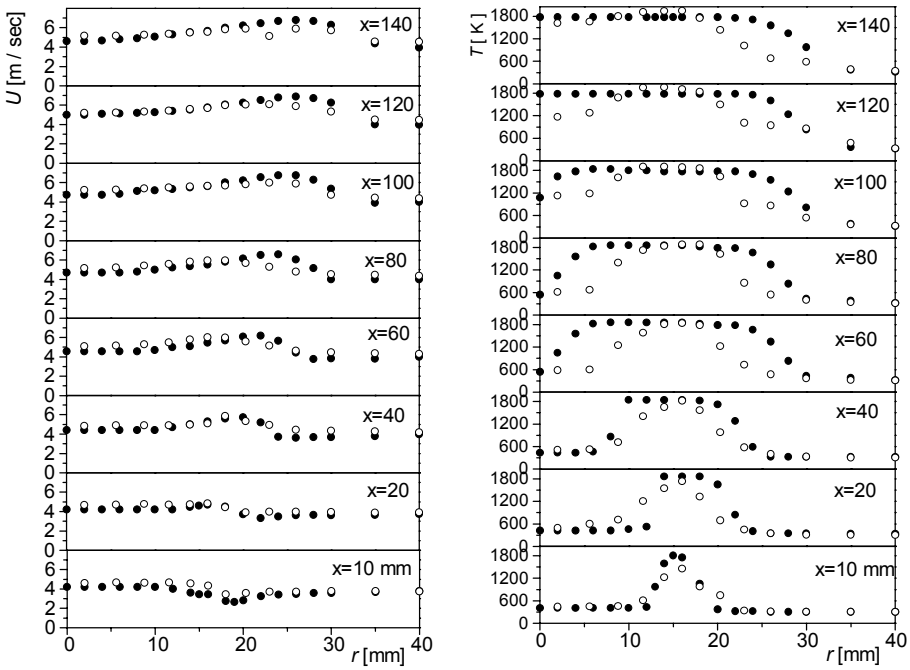

Fig. 1. Average axial velocity (U) and temperature (T) comparison (● - experimental data [1,2], ○ - numerical results)

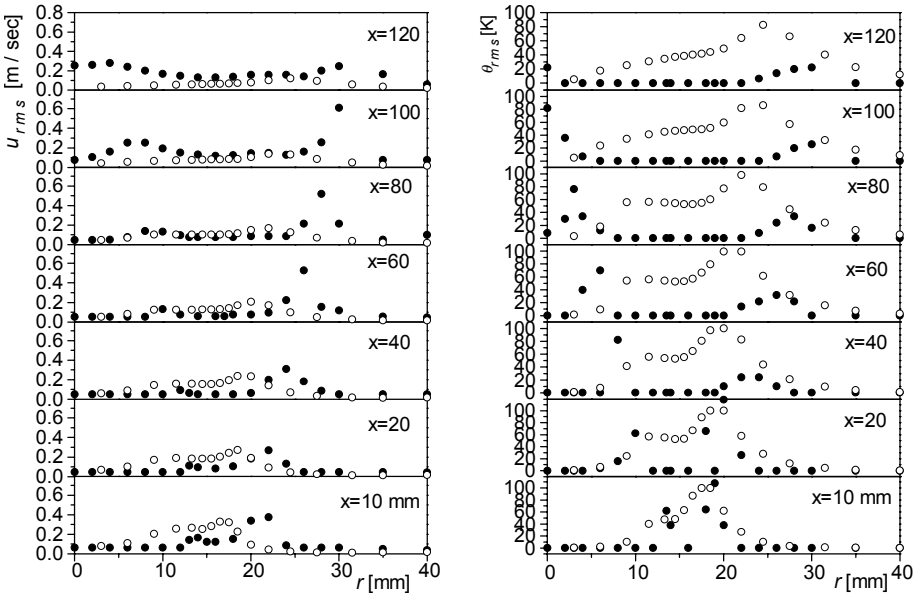

Fig. 2. Intensity of turbulence for axial velocity ($u_{rms} = \sqrt{\overline{u^2}}$) and temperature ($\theta_{rms} = \sqrt{\overline{\theta^2}}$) comparison (● - experimental data [1,2], ○ - numerical results)

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

1. D. Trimis, F. Durst and A. Melling., "Study of Turbulent Transport Phenomena in Combustion", 4th periodic report of JOULE R&D Program, Lehrstuhl für Strömungsmechanik, Universität Erlangen-Nürnberg, 1994.
2. D. Trimis, "Verbrennungsvorgänge in porösen inert Medien", ESYTEC Energie - und Systemtechnik GmbH, Erlangen, 1995.

MODELIRANJE SLOBODNOG TURBULENTNOG TOKA DVE KOAKSIJALNE STRUJE U USLOVIMA SAGOREVANJA

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Istraživanje interakcije turbulencije i sagorevanja se najčešće izvodi u jednostavnim konfiguracijama gde se uticaj različitih fizičkih procesa može izolovati i detaqno proučiti. Ovaj rad se bavi matematičkim modeliranjem turbulentnog sagorevanja i dopunjuje eksperimentalno istraživanje metanskog plamena koji nastaje pri strujanju dve koaksijalne struje fluida. Geometrija obuhvata dve koaksijalne struje, gde unutrašnja predstavqa stehiometrijsku mešavinu vazduha i metana, a spoqašnju čini samo vazduh, tako da u strujnom poqu istovremeno postoje pojave karakteristične za sagorevanje u predmešanom i difuzionom plamenu. Ovakva konfiguracija strujanja je interesantna za projektovanje efikasnih gorionika, koji omogućavaju smanjenje zagađenja i uštedu energije.

Primenjeni model turbulencije za strujno poqe sa hemijskim reakcijama se zasniva na modelima drugog reda za Rejnoldsove napone i flukseve. Zatvaranje sistema Rejnoldsovih jednačina količine kretanja i jednačine kontinuiteta za stacionarno osnosimetrično turbulentno strujanje nekompresibilnog fluida izvedeno je na bazi rešavanja jednačina održanja za turbulentne napone ($\rho\overline{u_i u_j}$) *i disipaciju kinetičke energije turbulencije* (ε). *Model obuhvata i jednačine održanja gasovitih komponenti koje učestvuju u procesu (metan, kiseonik, azot, ugqen-dioksid, vodena para) i jednačinu energije. Radi uvođenja hemijskih reakcija u model, jednačine održanja učestvujućih hemijskih komponenti se rešavaju u funkciji njihovih masenih udela. Jednačina energije se rešava u funkciji entalpije smeše. Sistem jednačina se zatvara pomoću jednačina održanja za Rejnoldsove skalarne flukseve* ($\rho\overline{\varphi u_i}$) *i skalarnu varijansu* ($\overline{\varphi^2}$).

Brzina sagorevanja bazirana na hemijskoj kinetici, dobija se iz Arenijusove relacije i kao takva je mnogo veća od brzine sagorevanja u realnom plamenu. Zbog toga što je vremenski razmer odumiranja turbulencije obično mnogo duži od vremenskog razmera hemijske kinetike, reakcija je kontrolisana turbulentnim mešanjem. Pošto se praktično celokupno sagorevanje odigrava nakon mešanja između disipativnih vrtloga malih razmera, ne možemo mnogo pogrešiti povezujući brzinu

sagorevanja sa brzinom odumiranja turbulencije pomoću modela drobqenja vrtloga. Prema ovom modelu, pretpostavqa se da su reakcije sagorevanja kontrolisane brzinom destrukcije produkcije turbulencije, koju karakteriše vremenski razmer turbulencije velikih vrtloga. U oblasti nižih temperatura, ova brzina je kontrolisana kinetikom hemijske reakcije.

Izvedeno je poređenje eksperimentalno dobijenih i proračunatih parametara strujnog poqa plamena, kao što su U, V, T, $\overline{u^2}, \overline{v^2}, \overline{uv}, \overline{\theta^2}$. *Takođe su u ovom radu proračunati i turbulentni maseni fluksevi* $\overline{\varphi u_i}$.