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Combustion modeling in a model combustor

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Abstract: The flow-field of a propane air diffusion flame combustor with interior and exterior conjugate heat transfers was numerically studied. Results obtained from four combustion models, combined with the re-normalization group (RNG) $k-\epsilon$ turbulence model, discrete ordinates radiation model and enhanced wall treatment are presented and discussed. The results are compared with a comprehensive database obtained from a series of experimental measurements. The flow patterns and the recirculation zone length in the combustion chamber are accurately predicted, and the mean axial velocities are in fairly good agreement with the experimental data, particularly at downstream sections for all four combustion models. The mean temperature profiles are captured fairly well by the eddy dissipation (EDS), probability density function (PDF), and laminar flamelet combustion models. However, the EDS finite rate combustion model fails to provide an acceptable temperature field. In general, the flamelet model illustrates little superiority over the PDF model, and to some extent the PDF model shows better performance than the EDS model.

Key words: combustion model; flamelet model; diffusion flame combustor; conjugate heat transfer

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Introduction

To provide a benchmark database for the development and evaluation of various physical models, a series of experiments were performed at National Research Council Canada. With advanced techniques, measurements were made in a propane diffusion flame combustor, as shown in Fig. 1. The combustor geometry was relatively simple compared with practical combustion devices, but fundamentally similar and relevant to the modeling of complex combustion systems. The comprehensive database includes mean and fluctuating velocity components, mean temperature, radiation heat flux, as well as species and pollutant concentrations. The detailed experiments and instrumentation will be published separately.

These experimental data have been used extensively to assess various turbulence, combustion and emission models^[1,2]. In many combustor simulations, the computational domain was limited to the combustion chamber only, while in the present study, the entire combustor flow-field, from the fuel and air inlets to the nozzle exit, was numerically modeled. In addition, the internal and external conjugate heat transfers from the combustion products to the flame holder and insulation walls were also simulated.

Presented and discussed in this paper are the numerical results obtained from four combustion models, i. e., the eddy dissipation (EDS), EDS-finite rate, probability density function (PDF) and laminar flamelet combustion models. In all cases, also used are the re-normalization group (RNG) $k-\epsilon$ turbulence model, the discrete ordi-

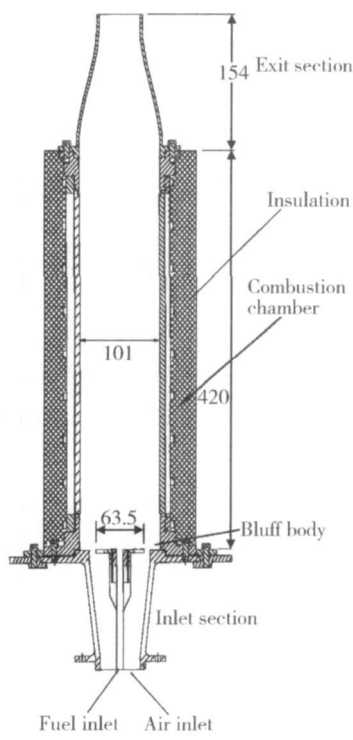


Fig. 1 The model combustor

nates radiation model, and the enhanced wall treatment. The numerical results are compared with the experimental database in detail, and the advantages and shortcomings of these combustion models are revealed.

1 Numerical simulations

Axisymmetric, steady, turbulent, reacting flows were considered, and a commercial software package, Fluent, was used in the present study. The computational domain, selected physical models, boundary conditions, and solution methods are described in the following subsections.

1.1 Computational domain

Figure 1 is a schematic diagram of the model combustor, including the fuel and air inlets, combustion chamber, disk flame holder and contracted exhaust section. Air entered the combustion chamber around a bluff body, while fuel was fed through the center of the disk flame holder.

Since the computational domain is axisymmetric, 2-D quadrilateral meshes were generated over the flow region, and interior and exterior conjugate heat transfer regions. Fine grids were

laid behind the flame holder in the combustion chamber to resolve flow recirculation. Fine grids were also generated in the shear layers between the recirculation region and fuel and air jets, as well as the gap between the flame holder edge and air inlet chamber wall. Coarse grids were used downstream of the combustion chamber and in the solid stainless steel and ceramic regions. A total number of 74 100 elements were used for most of the simulations. The skewness was less than 0.2 in the flow-field domain and the aspect ratio was less than 12 for 99.5% elements. Efforts were made to keep the wall parameter, y^+ in the desired range (30 to 60). However, there were local low-velocity regions where the y^+ values were well below 30. A number of meshes were tested to ensure the mesh independence of the numerical solutions.

1.2 Turbulence modeling

The governing Favre-averaged conservation equations for mass, species, momentum and energy are not reproduced here. They can be readily found in many classic literatures, such as Reference[3]. For closure of the basic equations, the RNG $k-\epsilon$ turbulence model derived from a renormalization group theory was used to model turbulent transfers in the reacting flow^[4]. This model has shown an excellent agreement between the numerical and experimental results for an isothermal flow over a backward facing step^[5].

According to this model, the turbulent viscosity for high Reynolds number flows is expressed as

$$\mu_t = \rho C_\mu k^2 / \epsilon \tag{1}$$

where $C_\mu = 0.0845$, derived from the RNG theory. It is very close to the empirically determined value of 0.09 used in the standard $k-\epsilon$ model. The quantities of the turbulent kinetic energy, k , and dissipation rate, ϵ , are found from the following pair of equations

$$\begin{aligned} \nabla \cdot (\rho \mathbf{v} k) &= \nabla \cdot (\alpha_k \mu_{\text{eff}} \nabla k) + G_k - \rho \epsilon \tag{2} \\ \nabla \cdot (\rho \mathbf{v} \epsilon) &= \nabla \cdot (\alpha_\epsilon \mu_{\text{eff}} \nabla \epsilon) + C_{1\epsilon} \frac{\epsilon}{k} G_k - C_{2\epsilon}^* \frac{\rho \epsilon^2}{k} \tag{3} \end{aligned}$$

In the above equations, μ_{eff} is the effective viscos-

ity, α_k and α_ε are the inverse Prandtl numbers, and $G_k = \mu_t S^2$ stands for the turbulence production with μ_t the turbulence viscosity and S the modulus of the mean rate of strain tensor, defined as $S \equiv \sqrt{2S_{ij}S_{ij}}$.

The main difference between the RNG and standard $k-\varepsilon$ models is that the coefficient of the destruction term, $C_{2\varepsilon}^*$ in Eq. (3), is no longer a constant, but a function of flow mean strain rate and turbulence field (k and ε). It is defined by the following expression

$$C_{2\varepsilon}^* \equiv C_{2\varepsilon} + \frac{C_\mu \eta^3 (1 - \eta/\eta_b)}{1 + \beta \eta^3} \quad (4)$$

where $\eta \equiv Sk/\varepsilon$, $\eta_b = 4.38$, $\beta = 0.012$. As a result, the RNG model is more responsive to the effects of flow strain rate and thus improves the accuracy for rapidly strained flows. The model constants, $C_{1\varepsilon} = 1.42$ in Eq. (3) and $C_{2\varepsilon} = 1.68$ in Eq. (4).

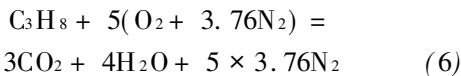
In addition, the RNG model provides an analytical formula to account for variations of turbulent Prandtl and Schmidt numbers in the flow for the energy and species equations^[5,6]

$$\left[\frac{\alpha - 1.3929}{\alpha - 1.3929} \right]^{0.6321} \left[\frac{\alpha + 2.3939}{\alpha + 2.3929} \right]^{0.3679} = \frac{\mu_{mol}}{\mu_{eff}} \quad (5)$$

where μ_{mol} is the laminar viscosity, and $\alpha = 1/Pr_{mol}$ or $1/Sc_{mol}$ (the inverse of the laminar Prandtl or Schmidt number). However, it should be mentioned that the inverse Prandtl numbers, $\alpha = \alpha_\varepsilon = \alpha$, in Eqs. (2) and (3) are determined by simply setting $\alpha = 1$.

1.3 Combustion modeling

Four combustion models used in the present study are the eddy-dissipation (EDS), EDS-finite-rate, probability density function (PDF), and laminar flamelet models. The EDS model is based on the work of Magnussen and Hjertager^[7], which has been widely accepted in diffusion flame modeling^[8]. For this model, a one-step global chemical reaction is assumed,



and the reaction rate is governed by turbulent mixing, or the large-eddy mixing time scale, k/ε

The net reaction rate of species “ i ” is given by the smaller of the two following expressions in $\text{kg}/\text{m}^3 \cdot \text{s}$,

$$R_i = \nu_i M_i A \rho \frac{\varepsilon}{k} \min \left[\frac{Y_{\text{C}_3\text{H}_8}}{\nu_{\text{C}_3\text{H}_8} M_{\text{C}_3\text{H}_8}}, \frac{Y_{\text{O}_2}}{\nu_{\text{O}_2} M_{\text{O}_2}} \right] \quad (7)$$

$$R_i = \nu_i M_i A B \rho \frac{\varepsilon}{k} \frac{(Y_{\text{CO}_2} + Y_{\text{H}_2\text{O}})}{(\nu_{\text{CO}_2} M_{\text{CO}_2} + \nu_{\text{H}_2\text{O}} M_{\text{H}_2\text{O}})} \quad (8)$$

where Y is the mass fraction, ν stands for the stoichiometric coefficient, M represents the molecular weight, and the empirical constants, $A = 4.0$ and $B = 0.5$.

For the EDS-finite-rate model, an additional constraint was included to the propane-air combustion, a global chemical reaction rate from Westbrook and Dryer^[9] in $\text{kmole}/\text{m}^3 \cdot \text{s}$,

$$R_{\text{C}_3\text{H}_8} = A \exp(-E/RT) [\text{C}_3\text{H}_8]^{0.1} [\text{O}_2]^{1.65} \quad (9)$$

where the pre-exponential factor, $A = 4.836 \times 10^9$ and the activation energy, $E = 1.256 \times 10^8 \text{ J/kmole}$. The net reaction rate at each point in the flow-field is determined by the smallest one among the three expressions (7), (8) and (9).

The third combustion model is based on the mixture fraction approach with an assumption of fast chemistry^[10]. It offers many advantages over the EDS and EDS-finite-rate models. It allows intermediate (radical) species prediction, dissociation effects, and more rigorous turbulence-chemistry coupling. The mixture fraction can be written in terms of atomic mass fraction as

$$f = \frac{Z_i - Z_{i,ox}}{Z_{i,fuel} - Z_{i,ox}} \quad (10)$$

where Z_i stands for the elemental mass fraction of element, “ i ”, $Z_{i,ox}$ and $Z_{i,fuel}$ denote the elemental mass fraction of “ i ” at the oxidizer and fuel inlets respectively. It is a common practice to assume that all species have the same diffusivity in turbulent flows. As a result, the mixture fraction becomes a conserved quantity, and the transport equations for the mean mixture fraction and its variance may be simplified as

$$\nabla \cdot (\rho \bar{f}) = \nabla \cdot \left(\frac{\mu}{\alpha_i} \nabla \bar{f} \right) \quad (11)$$

and

$$\nabla \cdot (\rho \overline{f'^2}) = \nabla \cdot \left(\frac{\mu}{\alpha_i} \nabla \overline{f'^2} \right) + C_g \mu_i (\nabla^2 \overline{f}) - C_d \rho \frac{\varepsilon}{k} \overline{f'^2} \quad (12)$$

where $f' = f - \overline{f}$, and the constants α_i , C_g and C_d take the values of 0.85, 2.86 and 2.0 respectively.

With the fast chemistry assumption, the chemical equilibrium calculation based on the minimization of Gibbs free energy can be used to determine the combustion system. For a defined combustion system, the instantaneous mole fractions of individual species, density and temperature at each point in the flow-field can be exclusively determined from the instantaneous mixture fraction in the adiabatic condition. When heat loss is concerned, as in the present study, the relationship may be generalized as

$$\phi = \phi(f, H) \quad (13)$$

where ϕ represents the instantaneous species mole fraction, density or temperature, and H is the instantaneous enthalpy.

As pointed by Bilger^[8], full chemical equilibrium gives considerable errors in temperature on the rich side of hydrocarbon flames. To avoid this, a partial equilibrium approach was applied in the rich flame region. When the instantaneous equivalence ratio exceeded 1.75, the combustion reaction was considered extinguished and unburned fuel coexisted with reacted products.

The turbulence-chemistry interaction is accounted for by the β function probability density function (PDF), $p(\overline{f}, \overline{f'^2})$, which is determined solely by the mean and variance of mixture fraction. The time-averaged values of species mole fractions and temperature are computed as

$$\overline{\phi} = \int_0^1 p(\overline{f}, \overline{f'^2}) \phi(f, H) df \quad (14)$$

Eighteen species were considered for the PDF model, including C_3H_8 , CO_2 , H_2O , O_2 , N_2 , CO , HO , H , O , H_2 , C_3H_6 , C_2H_6 , C_2H_4 , CH_4 , CH_3 , CH_2 , CH , and $C(s)$. The selection of these species was based on the propane-air chemical kinetics^[11] and the requirements for emission modeling.

The last combustion model is a laminar flamelet combustion model. This model views

the turbulent flame as an ensemble of laminar flamelets. For diffusion flames, it approximates the unsteady distorted turbulent diffusion flame using a steady laminar counter-flow diffusion flame^[12]. With this approach, a coordinate-free formation of the flamelet structure can be derived. The species fractions, density and temperature in the flamelet can be uniquely determined by two parameters, namely the mixture fraction, f and the scalar dissipation rate, χ in the adiabatic case. The later parameter is equivalent to the strain rate, which quantifies the departure of flame from chemical equilibrium.

A major advantage of the flamelet model over other combustion models is that detailed, realistic, chemical kinetics can be incorporated into turbulent reacting flows. In the present study, the chemical reaction mechanism for propane-air flames used by Stahl and Warnatz^[13] was employed. It consists of 228 chemical reactions and 31 species. Four chemical reactions (86, 87, 177 and 178) in the mechanism were replaced by the corresponding ones from the GRI-Mech 3.0 mechanism because their pre-exponential factors are too large.

The coupling between nonequilibrium chemistry and turbulence is accounted for by the probability density function, $p(f, \chi)$, as in the PDF model case. The mean flow parameters are computed according to the following expression

$$\overline{\phi} = \iint p(f, \chi) \phi(f, \chi, H) df d\chi \quad (15)$$

where ϕ represents the instantaneous species fraction, density or temperature, and H is the instantaneous enthalpy. The flamelet library is preprocessed and tabulated, which offers tremendous computational savings.

To account for the radiation heat transfer between the gas mixture and combustion chamber walls, the discrete ordinates radiation model^[14] was employed. The absorption coefficient of gaseous mixture was determined from the local species mass fractions in the mixture. An enhanced wall boundary treatment was applied at the walls. In this approach, an enhanced two-layer

er model is combined with enhanced wall functions, and the viscous and fully turbulent regions are smoothly blended.

Polynomials were used to calculate the specific heat of species as a function of temperature. These polynomials were determined from the JANNAF tables. In the case of the EDS and EDS-finite rate models, the polynomials from Reference [15] were used, where the chemical dissociation was considered. For other thermal properties such as molecular viscosity, thermal conductivity, diffusivity and absorption coefficient, the values at 900 K were used.

1.4 Boundary conditions

The fuel mass flow rate was 16.2 g/s, the air flow rate was 550 g/s, and the corresponding global equivalence ratio was 0.46. A turbulence intensity of 10% and hydraulic diameters were used at the fuel and air inlets to estimate inlet turbulence kinetic energy and dissipation rate. An inlet temperature of 293 K was used for both flows.

The boundary temperatures were defined based on the experimental measurements. A room temperature of 293 K was assigned to the inlet section walls, and the upstream edges of the combustion chamber and ceramic insulation walls. A linear temperature profile from 293 K to 405 K was specified at the outer boundary of the ceramic insulation in the axial direction. The temperature of the outer boundary of the exit nozzle was set to 823 K. The same temperature was assigned to the downstream edge of the combustion chamber wall since its heat resistance was much smaller than the ceramic insulation (the thermal conductivity is 25 W/m·K for the stainless steel, while only 0.10 W/m·K for the ceramic insulation). A linear temperature profile from 823 K to 405 K was assigned to the downstream edge of the insulation wall. The pressure at the combustor exit was set to the atmospheric value.

1.5 Solution method

A segregated solver with a second-order accurate scheme was used to resolve the flow-field.

At convergence, the normalized residuals of flow variables were less than or approximately equal to 10^{-5} for all test cases. Monitored axial velocities at two points in the shear layer downstream of the flame holder remained unchanged at least for the first four digits. A LINUX PC server with two Pentium 2.8 GHz CPUs and 4 GB RAM was used to perform all simulations.

2 Results and discussion

2.1 Velocity distributions

The axial velocity contours and flow path lines obtained from the flamelet model are shown in the upper half in Fig. 2, while the experimental data are presented in the lower half, with the zero axial velocity lines specified. The contour plot provides an overall picture of comparison between the numerical and experimental results. The flow patterns in the combustion chamber are well captured by the numerical simulation. Two recirculation zones are formed behind the flame holder although, in the experimental case, the central recirculation zone is not completely resolved and no flow path-lines are drawn due to the limited data points. The central recirculation zone created by the fuel jet is completely confined within the annular recirculation zone created by the annular air jet. This implies that the transportation of fuel into the flow-field, via the annular recirculation zone, is realized by diffusion only.

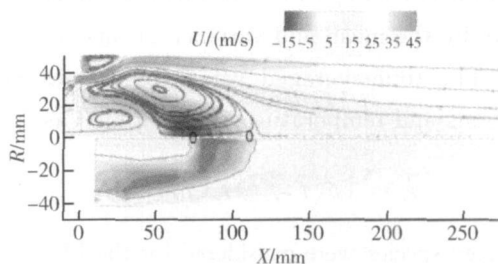


Fig. 2 Axial velocity contours and flow path lines

More remarkably, the reattachment point or the length of the recirculation region is accurately predicted by the numerical results. It is about 110 mm long. As expected, another separated flow zone is observed at the upper left corner in

the combustion chamber.

The axial velocity contours and flow path lines for the PDF and EDS models are similar to those for the flamelet model. This is also true for the case of the EDS-finite-rate combustion model, except that the annular recirculation zone is a little larger than the other three cases. Due to the limited space, contour plots for the PDF, EDS and EDS-finite-rate models are not illustrated here.

Figure 3 presents the axial velocity profiles along the combustor centerline for the four combustion models and compared with the experimental results. From $x \approx 80$ mm, where the negative axial velocity is close to its peak value (about -10 m/s), up to $x = 360$ mm, the predicted axial velocities agree well with the experimental data. Discrepancies are observed at $x \approx 55$ mm. The predicted axial velocities are lower than the measured values, and the velocity deficit region is wider than the experimental observation. This is consistent with the observation in Fig. 2, where the central recirculation region is under-predicted. In general, the EDS-finite-rate model has less agreement than the other three.

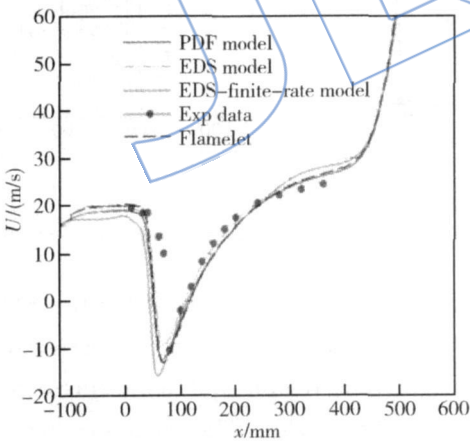


Fig. 3 Axial velocities along the centerline

Figures 4 and 5 give the axial velocity profiles at cross-sections from $x = 30$ mm to 360 mm. Again, the trend and magnitude are fairly well captured, except for the upstream section $x = 60$ mm. The axial velocity magnitudes downstream of the recirculation region ($x \geq 120$ mm) are in good agreement with the experimental data.

The flamelet and PDF results are close to each other, and show little improvement over the other two models. Considerable discrepancies at sections $x = 30$ mm and 60 mm are attributed to the disagreement between the predictions and measurements near the entrainment recirculation zone.

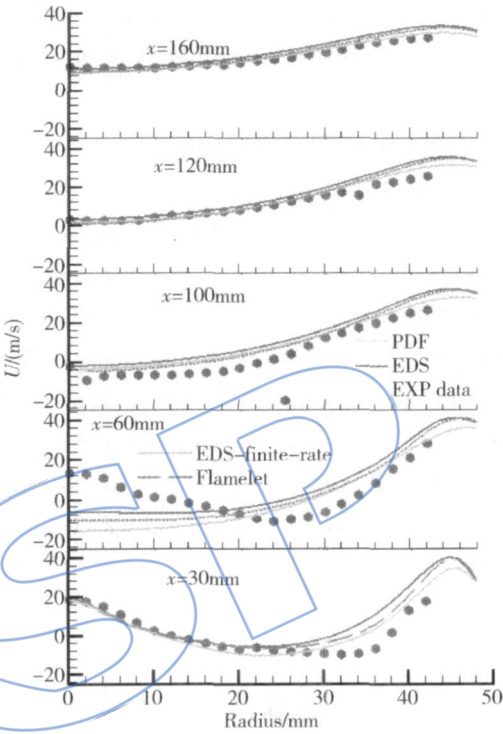


Fig. 4 Axial velocity profiles, $x = 30 \sim 160$ mm

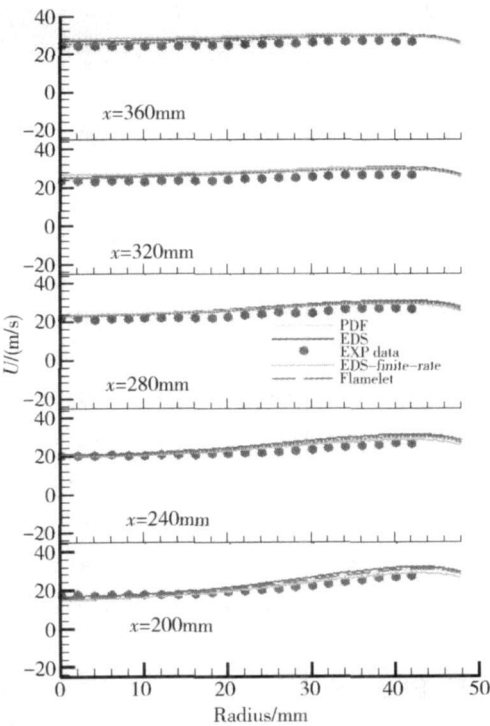


Fig. 5 Axial velocity profiles, $x = 200 \sim 360$ mm

The fairly good agreement between the numerical results and experimental data suggests that the RNG turbulence model, combined with the enhanced wall treatment, is capable of predicting the flow separation and recirculation behind the axisymmetric bluff body. Moreover, the momentum mixing between the central wake and annular air can also be adequately predicted for similar practical combustion systems.

2.2 Temperature distributions

The temperature contours behind the flame holder obtained from the flamelet model (top) are compared with the experimental data (bottom) in Fig. 6. As an overall picture, the predicted temperature distributions are fairly well correlated to the experimental data, except for the downstream portion in the annular recirculation zone. In this region, the predicted temperatures are higher than the measured values. This is a gain due to the fact that the size of the central recirculation zone is under-predicted.

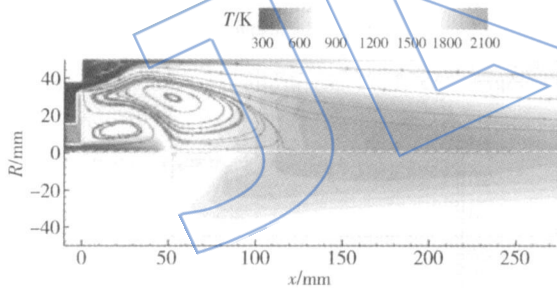


Fig. 6 Temperature contours behind the flame holder

Similar temperature distributions are observed for the PDF and EDS models. However, the results from the EDS-finite-rate model substantially weaker than the other three models (not shown here). The high temperature region is shifted about 125 mm upstream and the thermal wake region becomes shorter and narrower in comparison with the experimental results and the other three cases. It should be mentioned that the EDS-finite-rate results were verified by switching the combustion model from the EDS to the EDS-finite-rate and iterating based on the

converged EDS solution with the fuel mass fraction patched in the flow-field, and vice versa.

The detailed comparisons of temperature distributions are given in Figs. 7 ~ 9. Figure 7 shows temperature profiles along the centerline of the combustor. In the range of measurements (50 mm to 350 mm), the predicted temperatures from the flamelet, PDF and EDS models agree fairly well with the experimental data, although the predictions do show peaks in the middle, while the measurements tend to be flat. Among the three models, the flamelet case is slightly superior to the PDF case, and the PDF profile displays better agreement than the EDS profile. The maximum temperature reaches 2 098 K for the flamelet model, 2 120 K for the PDF model, and 2 147 K for the EDS model, while the experimental value is 1 950 K.

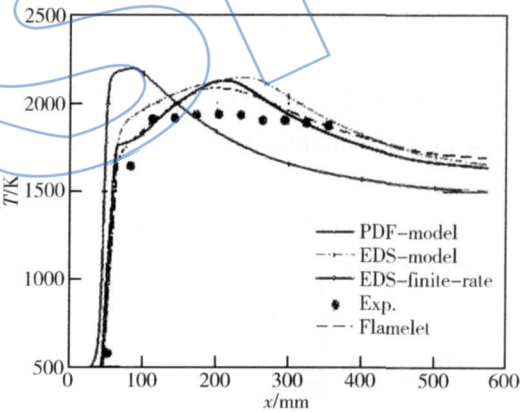


Fig. 7 Temperature along the combustor centerline

Poor agreement is observed for the EDS-finite-rate case. The temperature is over-predicted in the upstream region and under-predicted in the downstream region. The maximum temperature reaches 2 201 K.

Figures 8 and 9 present the temperature profiles at cross sections from $x = 52$ mm to 353 mm. Again, the results from the flamelet, PDF and EDS models agree fairly well with the experimental data, except for the most upstream section and the region near the combustor wall. Poor agreement of the EDS-finite-rate model is also observed, particularly at two upstream sec-

tions.

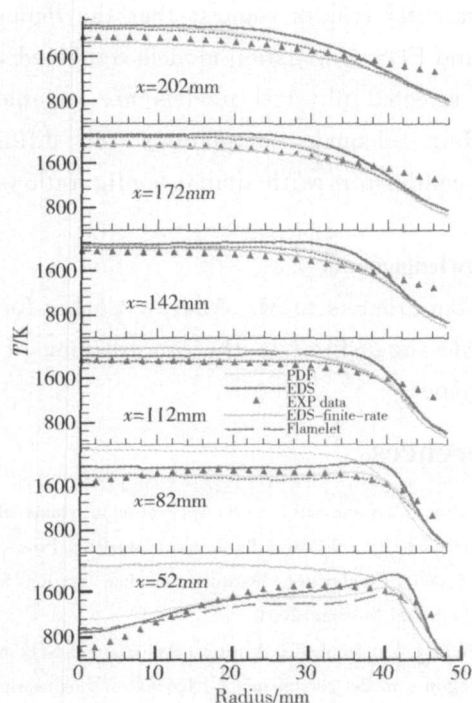


Fig. 8 Temperature profiles, $x = 52 \sim 202$ mm

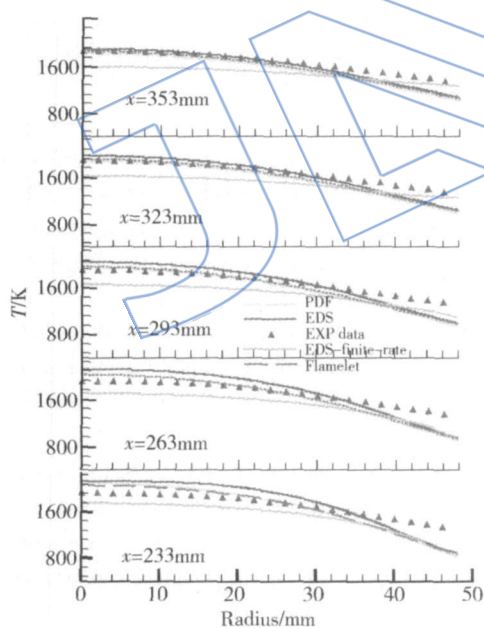


Fig. 9 Temperature profiles, $x = 233 \sim 353$ mm

At upstream sections ($x = 52 \sim 142$ mm) where chemical reactions are intense, the flamelet and PDF results illustrate slightly better overall performance than the EDS results. The EDS-finite-rate model excessively overpredicts the temperature at sections $x = 52$ and 82 mm. At

downstream sections ($x \geq 172$ mm), the results from the flamelet and PDF models are close to each other, and the maximum difference is about 40 K at section $x = 202$ mm and $R \approx 13$ mm. At these downstream sections, the EDS results are higher than the results from the flamelet and PDF models. The maximum difference reaches ~ 160 K at section $x = 172$ mm and $R \approx 30$ mm. The difference decreases gradually downstream and moves towards the combustor centre. In the EDS-finite-rate case, the predicted temperature profile is lower than the measured values from section $x = 172$ mm. The deviation increases further downstream, exceeding 230 K at the centre of section $x = 293$ mm.

From Figs. 6~9, it is found that the predicted temperatures from the flamelet, PDF and EDS models are higher than the measured values in the centre region from $x \approx 140$ mm to 250 mm. The maximum difference is about 140 K in the flamelet model case and a little larger for the PDF and EDS cases. The reasons for this are two-fold. First, the temperature was measured by a 0.25 mm thermocouple. Owing to the radiation and conduction losses from the thermocouple, the measurement error could exceed 100 K over regions where the gas temperature is high and the flow velocity is low^[16]. The second reason is that the predicted thermal spreading is somewhat less than the experimental observations. This leads to the temperature near the combustor wall being under-predicted, as observed in Figs. 8~9. The results suggest that different turbulent Prandtl and Schmidt numbers should be used in order to more accurately predict the thermal mixing.

In general, the flamelet model proves to be the best among the four tested. This is due to the flamelet model taking into account the effects of the detailed, relatively realistic, nonequilibrium chemistry. As mentioned earlier, the PDF model offers intermediate species prediction, dissociation effects, and statistical turbulence chemistry coupling. Consequently, it offers a better performance than the EDS model that assumes the

combustion process being controlled by turbulent mixing only. However, these improvements are limited since most diffusion flames are mainly controlled by the turbulent mixing^[8]. Moreover, for the PDF model, the potential errors in temperature on the rich side of the flame are minimized with the chemical partial-equilibrium approach. In the case of the EDS model, the well-known problem of temperature overshoot is alleviated using the specific heats where the chemical dissociation is considered. For the EDS-finite-rate model case, the turbulent mixing control mechanism is combined with a global finite chemical reaction rate that is calibrated by laminar flame speeds^[9]. The present study indicates that this combination is not suitable to predict diffusion flames where complicated turbulence-chemistry interactions are involved.

The comparisons between the numerical and experimental temperature fields indicate that the flamelet, PDF and EDS combustion models, in conjunction with other selected physical models, can provide adequate simulations for diffusion flame combustors stabilized by a bluff body flame-holder. This provides a reliable base to evaluate NO_x emission models in the near future.

3 Conclusions

A propane diffusion flame combustor with the interior and exterior conjugate heat transfers was numerically studied with four combustion models, i. e., the laminar flamelet model, the PDF model, the EDS model and the EDS-finite-rate model. Also used were the RNG $k\text{-}\epsilon$ turbulence model, the discrete ordinates radiation model and the enhanced wall treatment.

In comparison with the comprehensive experimental measurements, it is found that the flow patterns and the recirculation length are accurately determined. The mean velocity profiles are fairly well captured by all four combustion models. For the temperature field, the results obtained from the flamelet, PDF and EDS models show fairly good agreement with the experimental results. However, the EDS-finite-rate model

fails to provide an acceptable temperature field.

The comparisons between the numerical and experimental results suggest that the flamelet, PDF and EDS combustion models combined with other selected physical models are capable of providing adequate simulations for diffusion flame combustors with similar configurations.

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