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Comparison of the Numerical Models for the Temperature Distributions of Non-premixed Swirling Methane Flame

Araştırma Makalesi / Research Article

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ABSTRACT

This study aimed to investigate the numerical modelling parameters that are in good agreement with experimental data for the temperature distribution of a non-premixed swirling methane flame. All numerical calculations have been performed with FLUENT, a computational fluid dynamics code. P-1 radiation model has been chosen for all numerical calculations. In addition, the swirl number has been taken 0.4 value to validate the results with respect to reference experimental data. All comparisons have been performed in axial and radial temperature distributions according to experimental data. Firstly, the number of swirls has been defined as a user-defined function. Thus, the effect of defining user-defined functions has been examined in the swirl number. Secondly, the model constant (A) of the eddy dissipation combustion model has been investigated to determine suitable value. After that, the eddy dissipation and PDF mixture fraction combustion models have been compared with each other. Finally, the k-ε standard, realizable and RNG models have been analyzed to determine the proper turbulence model. The results showed that to define the swirl number as a user-defined function in the comparison tests has not been an important effect to obtain good agreement with the experimental temperature distribution data. It has been found that the value of one for the Eddy dissipation model constant is suitable for this model. It has also been found that the experimental results in both combustion models give approximate results, but the PDF model is particularly better at axial temperature distribution. Moreover, it has been seen that the k-ε realizable turbulence model is more suitable for this model.

Keywords: User-defined function, numerical modelling, methane, combustion.

1. INTRODUCTION

Nowadays, the energy demand is ever-increasing with the rise of industrialization and technology. Fossil fuels still play an important role in satisfying this need. Fossil fuels generally come into prominence with their content of the carbon and hydrocarbon. Natural gas is one of the fossil fuels and contains methane, which is a hydrocarbon in its structure. In this regard, methane is an important source of fossil energy. However, the widespread use of fossil fuels is a serious problem for humankind because the resulting emissions are causing global warming. Numerous studies have been conducted to solve this problem. One of these researches is the reduction of emissions by burning fossil fuels in the most efficient way. Reduction of emissions is possible with the complete combustion. For this reason, the swirling of the air inside the combustion chamber is important in terms of achieving the complete combustion. Due to the swirling flow, no unburnt particles remain in the combustion chamber. Swirl flow is an important effect providing flame stability and flame propagation. There are a number of studies that have studied these effects experimentally and numerically. In the literature, many studies have been performed about non-premixed swirling methane flame, up until now. Wilkes et al. have been studied on the measurement of axial and radial temperature distributions in Harwell furnace which is an axisymmetric natural gas-fired swirling furnace [1]. Song et al. have been conducted a numerical study which is about fluid flow and gaseous radiation heat transfer characteristics of the natural gas-fired furnace. It has been shown that the importance of calculations of spectral and narrow-band statistical model enables simplicity for calculations [2]. Chen has been studied the nitrogen dioxide emissions of CH_4 and it's some mixtures. It has been reported that NO_2/NO_x ratio is differently affected CH_4 fuel from H_2. Moreover, it has been concluded that this ratio is increasing with decreasing NO concentration and adiabatic flame temperature [3]. Ma et al. have been performed numerical analysis of the turbulent diffusion flame in a cylindrical combustor by using eddy dissipation and flamelet combustion models. They have been found that the flamelet model has good agreement with experimental data and the eddy dissipation model is useless in the near burner region [4]. Morvan et al. have been numerically investigated a methane/air radiating turbulent diffusion flame. They have been used eddy dissipation concept as a combustion model and both standard k-ε and renormalization group theory (RNG) models for turbulence and finally, they used P1 approximation for the radiation transfer and soot formation. They have reported that the 20-25 percent of released combustion heat comes from the flame. In addition, they have been released that small Froude numbers cause unsteady and unsymmetrical flame behaviour but at the higher Froude numbers, steady and symmetrical behaviour comes back

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[5]. Keramida et al. have been examined that discrete transfer radiation model for a swirling natural gas diffusion flame in the axisymmetric furnace. They have emphasized that the importance of the radiation effects in a furnace and the success of the discrete transfer model for accurate calculations [6]. İlbas et al. have been studied the laminar burning velocities of the hydrogen, air, methane mixtures, experimentally. They have used different equivalence ratios to measure the temperatures. They have reported that to adding hydrogen in the mixture cause the increase of burning velocity. They have also asserted that 30 % hydrogen and 70 % methane mixture is the most appropriate choice [7]. Park et al. have been investigated the flame structure and emission characteristics of the methane-air diffusion flame when the adding H_2 and H_2O. They have shown that the maximum flame temperature increases due to the effect of H_2O and when the H_2O added, CO_2 emission increases while the emission of CO reduces [8]. Khelil et al. have been studied the emission characteristics of high swirling non-premixed natural gas diffusion flame, numerically. They have used PDF and Reynolds stress model for calculation. They have concluded that the results of these models agree with experimental results [9]. Hu et al. have been analyzed the No emission and velocity of the premixed methane, hydrogen and air flames. They have pointed out that the increase of hydrogen fraction causes the increment in laminar burning velocity. They have also shown that in the rich flames hydrogen, addition causes the decrease of NO emission but in the stoichiometric flames, it does not affect NO emission [10]. Lui et al. have been investigated the premixed methane-air combustion. They have performed the calculations numerically in the porous media using the user-defined function. They have demonstrated that the change in the temperature and velocity is significant at the near wall and interface of the porous media [11]. Bhadraiah et al have been investigated the effect of chemical kinetic mechanisms in laminar methane-oxygen diffusion flames. It has been demonstrated that the 2-steps mechanism is the more suitable solution for oxygen-rich methane flames [12]. Saqr et al. have been studied that the NO_x and soot formation of the CH_4-air flames under the free stream turbulence. They have shown that the increase in free steam turbulence causes an important reduction in NO formation [13]. Khanafer et al. have been computed NO_x and fluid dynamics parameters in swirl burners. They have concluded that the increasing effect of swirl causes the reduction in CO and unburned particles [14]. Monaghan et al. have been analyzed the formation of pollutant in methane flame using the CFD-CRN method. They have stated that the method successfully predicts velocity, mixture fraction, temperature, CO and NO mass fractions according to experimental data [15]. Ilbas et al. have been studied the hydrogen addition effects on methane, experimentally. It is concluded that the addition of hydrogen is positively affecting CO emission and the efficiency of combustion [16]. Yılmaz has been studied the effect of swirling flown a natural gas flame. The results have revealed that the swirling affects the flame temperature and the gas concentrations as well as radial and axial velocities [17]. Abdul-Sater et al have been examined radiation modelling in oxy-methane and diffusion flames using the user-defined function [18]. Yılmaz et al. have been investigated different turbulence and radiation models in propane-hydrogen diffusion flames. It is concluded that the results of numerical models commonly agree with experimental data and the increase of hydrogen concentration causes the decrease in CO_2 emission and an increase in H_2O concentration [19]. İlbas et al. have been studied the effect of swirl flow in hydrogen-containing fuels. They have suggested that the change in swirling flow causes the high NO_x regions [20]. Yılmaz et al. have been analyzed hydrogen-air flames under the different turbulence models. They have shown that the k-ε model gives the best result according to experimental data [21]. Karyeyen et al. have been performed that the experimental study on low calorific syngas mixtures in a new type burner. They have pointed out that the transform of CO to CO_2 is highly affected by hydrogen supply [22]. Ilbas et al. have been determined the characteristics of low calorific syngas under the different turbulator angles. The results have demonstrated that the increase in turbulator angle expediting the syngas reaction [23]. Rashwan has been determined the effect of swirl flow and oxidizer composition in non-premixed methane flames. It is concluded that the increase in swirl flow reduces the thermal NO_x [24].

This study is purposed to determine more suitable numerical model parameters to obtain good agreement with experimental results. All of the numerical calculations of modellings have been performed using the ANSYS FLUENT [25]. Thereafter, the obtained results which from numerical calculations have been used for comparisons of models. Initially, the effect of the define swirl number as a user-defined function has been investigated. A swirling flow has been created with the tangential velocity as an internal boundary condition that is created by using the user-defined function. In the next section, the eddy dissipation model constant (A) has been determined to evaluate the effect of numerical calculations. The comparison of eddy dissipation and PDF mixture fraction combustion models have been performed after these calculations. Finally, k-ε turbulence models have been compared to obtain the experimental results.

2. DETAILS OF MODELLING

2.1. Details of the Combustor and Boundary Conditions

In order to validate our numerical calculations with experimental data, the model of the combustion chamber has been taken from Wilkes et al. [1]. It consists of one outlet and two inlets for air and fuel, separately. Thus, the model is non-premixed, axisymmetric and 2-D. The dimensions of the combustion chamber are shown in Figure-1. The parameters of the boundary and operation conditions for the combustion chamber has been shown in Table-1. As shown in Table-1 as an important parameter, swirling flow is only effective on the air stream. Swirl flow provides that the flame spreads over a larger area so unburnt particles burn in this way. Swirl number (S) is the ratio between the tangential momentum flux and axial momentum flux [17]. It also defined as Eq.-1 where the swirl generator hub diameter and the outer diameter is d_h and d, respectively. In addition, β is the exit angle of the swirl generator [26].

$$S = \frac{2}{3}\left(\frac{1-\left(\frac{d_h}{d}\right)^3}{1-\left(\frac{d_h}{d}\right)^2}\right)\tan\beta \tag{1}$$

The exit angle of the swirl generator has been obtained from Eq.-1. This angle has been used with the axial velocity of air (U_x) in Eq-2 to obtain the tangential velocity component of the air (U_θ).

$$U_\theta = U_x \times \tan\beta \tag{2}$$

The user-defined function that obtained from Ref.26 has been used to calculate the Eq-2. The value of the swirl angle has been calculated using Eq.-2 to obtain the swirl number is 0.4. Finally, the calculated tangential velocity value and other necessary values have been applied to the tangential momentum equation as a boundary condition. The tangential momentum equation can be seen in Eq.-3 for the 2-D swirling flow in the cylindrical coordinates [26].

$$\frac{\partial(\rho U_\theta)}{\partial t} + \frac{1}{r}\frac{\partial(r\rho U_\theta U_x)}{\partial x} + \frac{1}{r}\frac{\partial(r\rho U_\theta U_r)}{\partial r} = \frac{1}{r}\frac{\partial\left[r\mu\frac{\partial U_\theta}{\partial x}\right]}{\partial x} + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^3\mu\frac{\partial(\frac{U_\theta}{r})}{\partial r}\right] - \rho\frac{U_\theta U_r}{r} \tag{3}$$

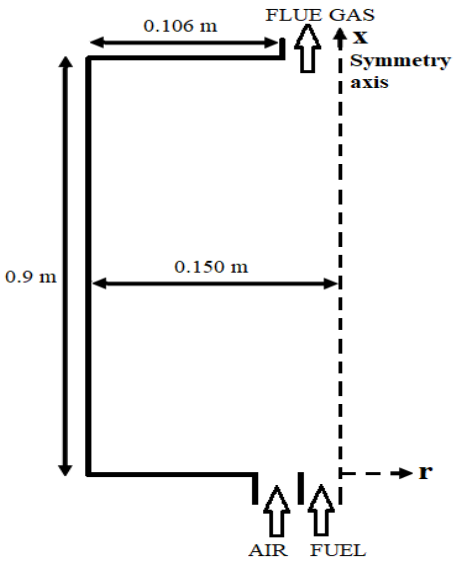

Figure 1. The geometric model of the combustor

Table 1. Boundary and operation conditions

Boundary Conditions	Fuel	Air	Operation Conditions	
CH_4 (mass fraction)	1.0	-	Temperature (K)	295
N_2 (mass fraction)	-	0.77	Pressure	1 Atm
O_2 (mass fraction)	-	0.23	Reynolds number	10909 (fuel)
Axial Velocity (m/s)	15.0	12.8	Thermal Power	60 kW
Radial Velocity (m/s)	-	-	Equivalence ratio	0.83
Turbulent kinetic energy (m^2/s^2)	2.26	1.63	Swirl Number	0.4 (air)
Turbulence dissipation rate (m^2/s^2)	1131.8	692		

2.2. Details of the Mathematical Models

In this work, two combustion models have been chosen for calculations and comparisons. One of them is the Eddy Dissipation model and the other is PDF mixture fraction model. In the Eddy dissipation model, it is assumed that the chemical reactions in the turbulent flow occur very quickly and the reaction rate is determined in this way. The reaction rate could be calculated using Eq.-4 considering to the minimum value [26].

$$R_f = A\rho\frac{\varepsilon}{K}\min\left(\overline{Y_f}, \frac{1}{v}\overline{Y_o}, B\frac{1}{1+v}\overline{Y_p}\right) \tag{4}$$

In Eq.-4, the local mass fractions of fuel, oxidizer, products are $\overline{Y_f}$, $\overline{Y_o}$, $\overline{Y_p}$ and v is the oxidizer to fuel stoichiometric mass ratio. In addition, A and B are constant that equals to 4.0 and 0.5 respectively.

Another model that has been used in this study is the Mixture Fraction/PDF Model. Instead of solving the transport equation for each chemical species, the PDF model solves the transport equation for a single conserved scalar (the mixture fraction). The general form of the transport equation is seen Eq.-5 [23].

$$\frac{\partial(\rho\phi)}{\partial x} + div(\rho\phi u) = div(\Gamma grad\phi) + S_\phi \tag{5}$$

Where Γ is the transport coefficient for dependent variables (ϕ) and the source term (S_ϕ). The equation of the local mixture fraction (f) could be seen in Eq.-6 where the mass fraction of the fuel is m_f and the mass fraction of oxidant is m_o [23].

$$f = \frac{m_f}{m_f + m_o} \tag{6}$$

Mixture fraction distribution provides the approximate thermochemical state of the fluid. One could be obtaining the mean mixture fraction ($\bar{f}$) and its variance ($\bar{f'}^2$) from Eq.-7 and 8.

$$\frac{\partial(\rho\bar{f})}{\partial t} + \frac{\partial(\rho u_i \bar{f})}{\partial x_i} = \frac{\partial}{\partial t}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \bar{f}}{\partial x_i}\right) + S_m \tag{7}$$

Where S_m is the source term.

$$\frac{\partial(\rho\bar{f'}^2)}{\partial t} + \frac{\partial(\rho u_i \bar{f'}^2)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_t}\frac{\partial}{\partial x_i}\bar{f'}^2\right) + C_g \mu_t \left(\frac{\partial \bar{f'}^2}{\partial x_i}\right)^2 - C_d \rho \frac{\varepsilon}{k}\bar{f'}^2 \tag{8}$$

In Eq.-8, C_g, C_d and σ_t are the constants.

The time-averaged values of the mixture fraction and its variance are related to probability density function (PDF). The PDF mixture model supplies the knowledge about the formation of the intermediate species not using the detailed chemical kinetics [26].

k-ε models have been selected for the modelling the turbulent flow to obtain good agreement with experimental data. Standard, realizable and RNG k-ε models have been compared to each other. These models are well-known and mostly used models for turbulent flows. In this calculations, Eddy dissipation model has been used for combustion modelling.

The radiation heat transfer is another important phenomenon in the combustion process. In this study, P-1 radiation model has been chosen for the modelling radiative heat transfer. P-1 model is the simpler case of the P-N radiation model and it's very commonly used in combustion modelling. This model accounts for the radiation heat transfer between gas and particulates.

The SIMPLE algorithm has been chosen for Pressure-velocity coupling. In addition, second order upwind has been selected for all interpolation in the spatial discretization except pressure. Second order spatial discretization has been chosen for pressure interpolation. The convergence criteria have been determined below 10^{-6} for all scaled residuals. Numerical solutions have been performed using ANSYS FLUENT that uses the finite volume method to solve governing equations.

3. GRID INDEPENDENCY

In numerical studies, the solution depends on the mesh size. As the mesh increases, the solution can converge after some point. In order to investigate this effect, four different mesh size has been selected for in this study. These are mesh sizes are 14350, 24600, 63250, 121200. Comparisons of these mesh sizes have been performed on the axial temperature distribution of the combustion chamber. This comparison could be seen in Figure-2. Experimental results that were taken by Wilkes et. al. [1] have been used to determine the mesh size that has good agreement values. According to Figure-2, 63250 and 121200 mesh sizes are more compatible with experimental data. In addition, there is no significant difference between the results of 63250 mesh size and 121200 mesh size. Therefore, 63250 mesh size has been found to be sufficient for numerical solutions, and all numerical analyzes were performed on this mesh size, in this study. The numerical calculation time has been decreased in this way.

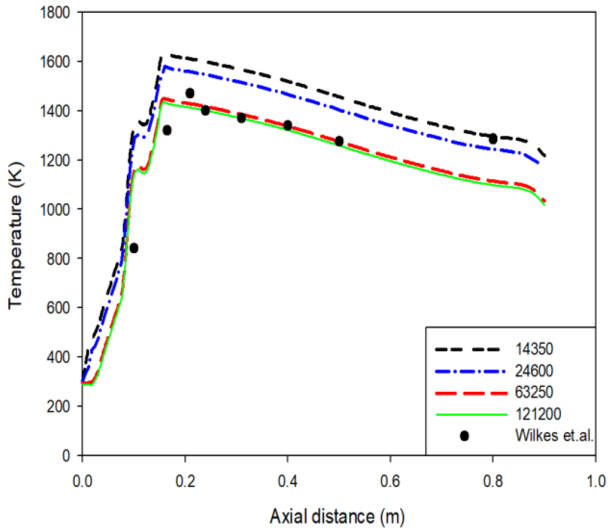

Figure 2. The comparison of grid independency at axial temperature distribution

4. RESULTS AND DISCUSSIONS

4.1. The Effect of User Defined Function

One of the main purposes of this study is to determine the effect of user-defined function in the relation between experimental results and numerical results. For this purpose, a user-defined function has been used to define the swirling velocity and integrated into the boundary conditions of the swirling velocity in the computational fluid dynamics code. According to the conclusions from the next section, the mixture ratio (A) has been taken as 1 in Eddy-dissipation concept. The effect of user-defined function on the predicted axial and radial temperature profiles is presented in Figure 3 and Figure 4. When Figure 3 and Figure 4 are examined together in detail, it has been demonstrated that there is no considerable change for the temperature profiles of the methane flame except the flame region when the programmed user-defined function is used. In particular, however, the predicted radial temperature profiles under conditions in which user-defined function has been used are more coherent with the measured data in terms of trends and values. Therefore, it has been determined that the programmed user-defined function is used for boundary conditions of swirling velocity.

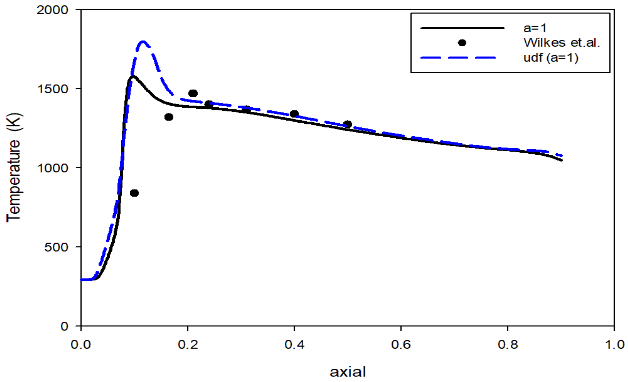

Figure 3. The comparison between Eddy dissipation models using user-defined function (UDF) and not using UDF at axial temperature distribution

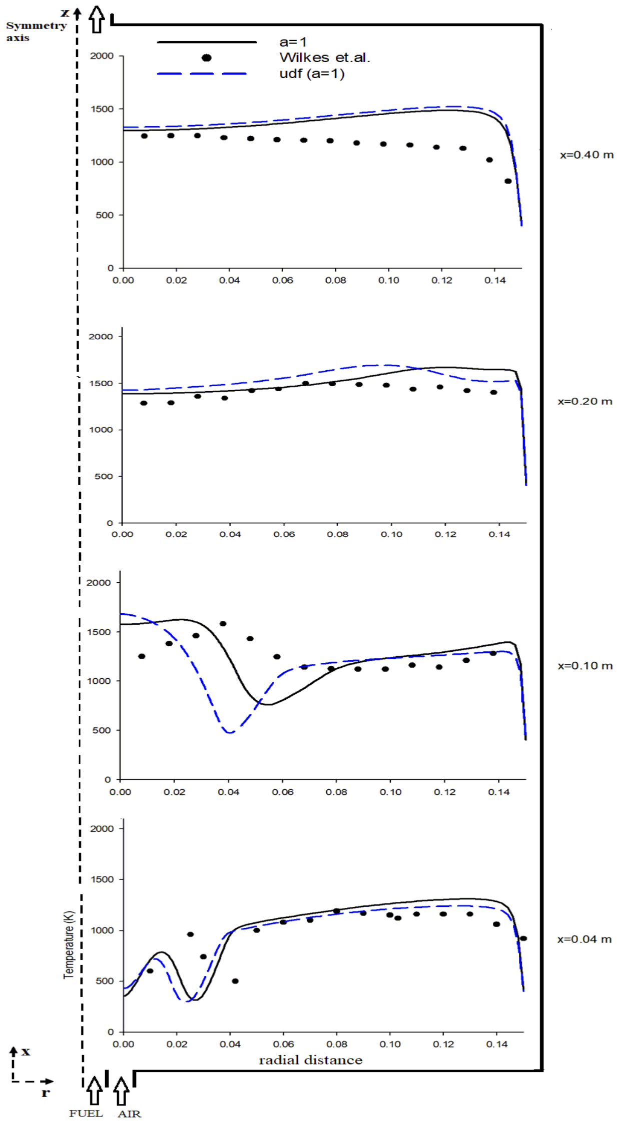

Figure 4. The comparison between Eddy dissipation models using user-defined function (UDF) and not using UDF at radial temperature distributions

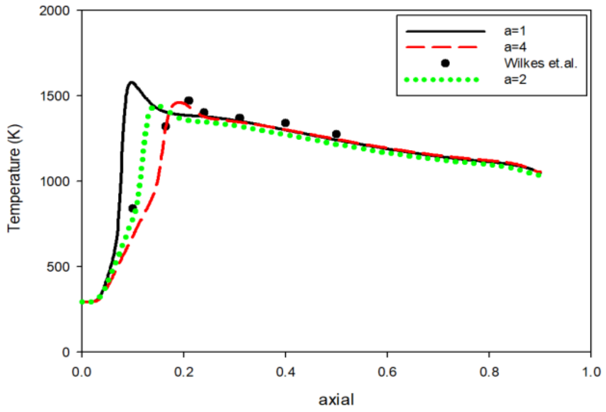

Figure 5. The effect of the change of the model constant (A) in the Eddy dissipation combustion model on the axial temperature distribution

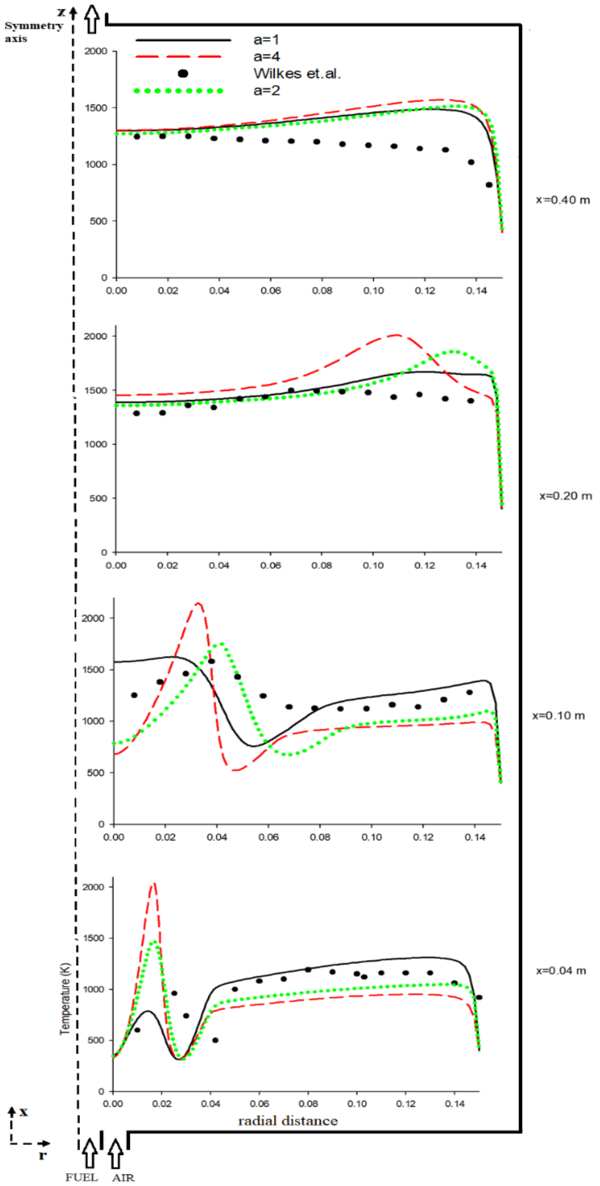

Figure 6. The effect of the change of the model constant (A) in the Eddy dissipation combustion model on the radial temperature distribution

4.2. The Effect of Model Constant (A) in Eddy Dissipation Model

In this part of the present study, the effect of the model constant (A) on the predicted temperature profiles is presented. The model constant (A) has been taken as 4 (the default value), 2 and 1. The predicted and the radial temperature distributions for different cases are given in Figure 5 and Figure 6. As can be seen in Figure 5, it can firstly be said that the predicted axial temperature profiles for A=4 are in good agreement with the measured data. However, predicted axial temperature profiles for the other values of A are not satisfactorily good agreement with the measured data. In particular, the predicted temperature values are not good in the flame region. This conclusion can be explained that the model constant (A) is directly related to the reaction rate. Therefore, it is revealed that the reaction rate is reduced as the model constant (A) is decreased. In other words, the predicted temperature values are consistency after the middle of the combustor when the model constant (A) is reduced. This conclusion can be supported when Figure 6 is examined in detail. It can be readily said that the predicted radial temperature profiles for case of A=1 are in good agreement with the measured data. In particular, after the middle of the combustor, it can be seen that there is a consistency between the predicted radial temperature profiles for case of A=1 and the measured data. It can be consequently concluded that there is a considerable consistency between predictions and measurements due to decreasing of the reaction rate when the model constant (A) is reduced in the modellings.

4.3. The Comparison of Combustion Models

Two combustion models, Eddy dissipation and PDF mixture fraction models, has been selected to compare the numerical results. Both combustion models have standard k-ε turbulence model and P1 radiation model. Moreover, user-defined function has been used for swirl velocity in the calculations of both models. The comparisons can be seen in Fig.7 and 8. Figure-7 shows the axial temperature distribution throughout the combustion chamber. In the Fig.-7, Eddy dissipation model has been shown worse results compared to the PDF model, especially at the initial axial distances. The reason of this problem is the structure of Eddy dissipation model. Eddy model is the known as "mixed is burned" and this is causing more combustion products emergence than expected. Therefore, this situation has been causing more high-temperature lines than experimental data in the graph. Both models have good agreement with experimental results at the after 0.2 m axial distance. In addition, it can be seen that PDF mixture model could be predicted finely the experimental values throughout all of the axial distance. In the Figure-8, it can be seen radial temperature distribution of the combustion models. The Eddy dissipation model have been given better results than PDF model at the radial temperature distribution at

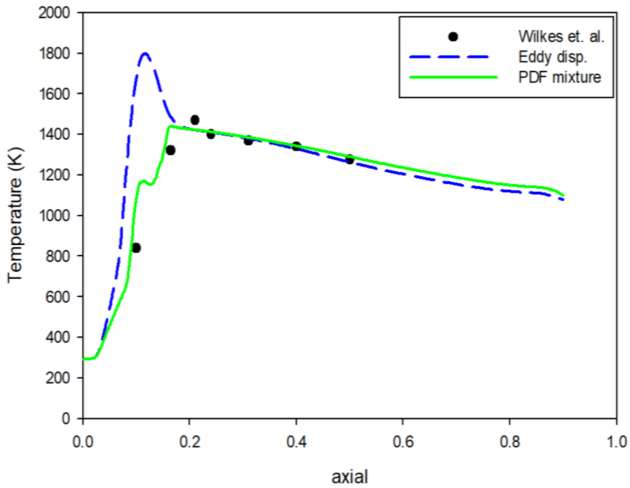

Figure 7. The comparison between Eddy dissipation models and PDF mixture model at axial temperature distribution

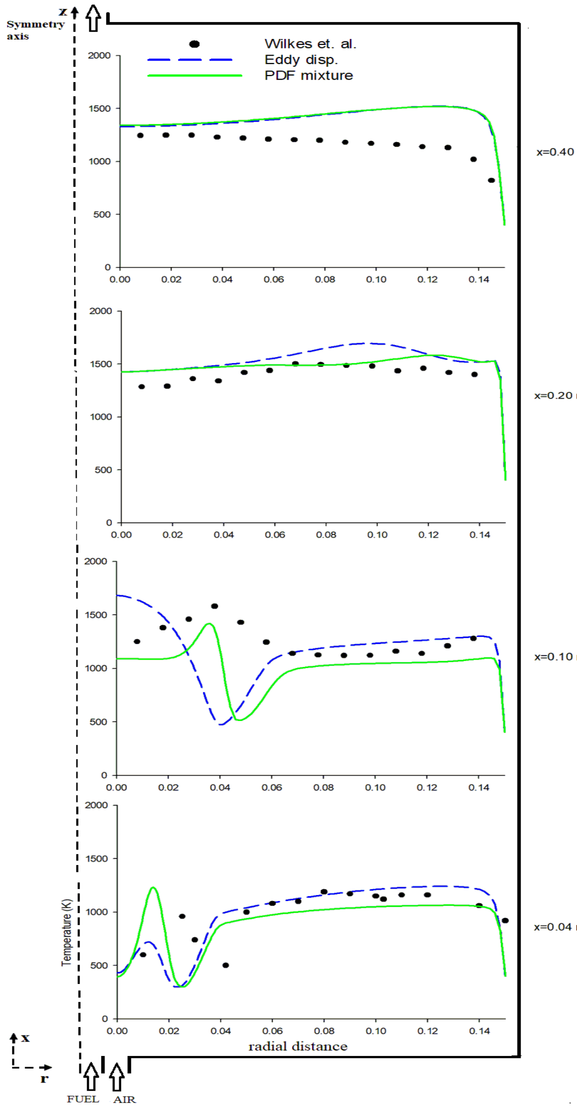

Figure 8. The comparison between Eddy dissipation models and PDF mixture model at radial temperature distribution

0.04 m, the closest distance to the start of the combustion chamber. Both combustion model gives better results at between 0.06 and 0.14m radial distance where the axial distances are 0.04m and 0.10m, respectively. However, both models have not been reached appropriate results in near the flame zone. The PDF model is more approximate than Eddy model in the near the swirl flow. On the other hand, eddy model can give better results than PDF mixture at the near of the fuel and air entrance region. At x=0.20 m, there is no difference between both models, except the distance between 0.06 and 0.12m radial distances. Because Eddy models more predict the formation of combustion product and cause to obtain high-temperature values. The eddy and PDF models have the same trends and approximate values in the middle of the combustion chambers.

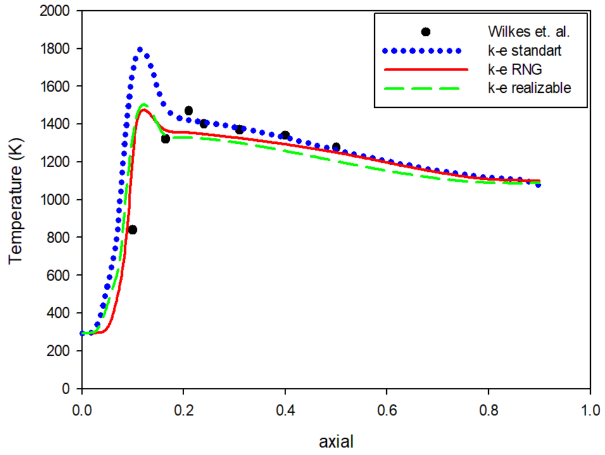

Figure 9. The comparison of k-ε turbulence models at axial temperature distribution using Eddy dissipation combustion model

4.4. The Comparison of Turbulence Models

The comparison of turbulence models can be seen in Fig.9 and 10. Figure-9 shows the axial temperature distribution, at this figure, the k-ε RNG model has good agreement with experimental data. Also, the k-ε realizable model has approximate prediction compared to the k-ε standard model. The k-ε RNG model contains the additional rate of strain term in the ε equation. In addition, it involves the turbulent viscosity modification to obtain the best numerical results in swirling flows. Thus, our numerical results showed that k-ε RNG model provides a good approximation to experimental data throughout the axial temperature distribution. The k-ε realizable model has some improvements with respect to other the k-ε models. It is also known that this model is suitable for strong rotation, vortices. While investigating the radial temperature distribution, it is observed that the k-ε realizable and RNG models give the better results than the standard model in the close to the flame region. Especially, as we approach the walls of the combustion chamber, it appears that the k-ε realizable model gives results that are closer to experimental values. This may be due to the fact that the k-ε realizable model contains a different turbulent viscosity formulation than the other models. All the models have given the same results towards the exit of the combustion chamber in the radial direction.

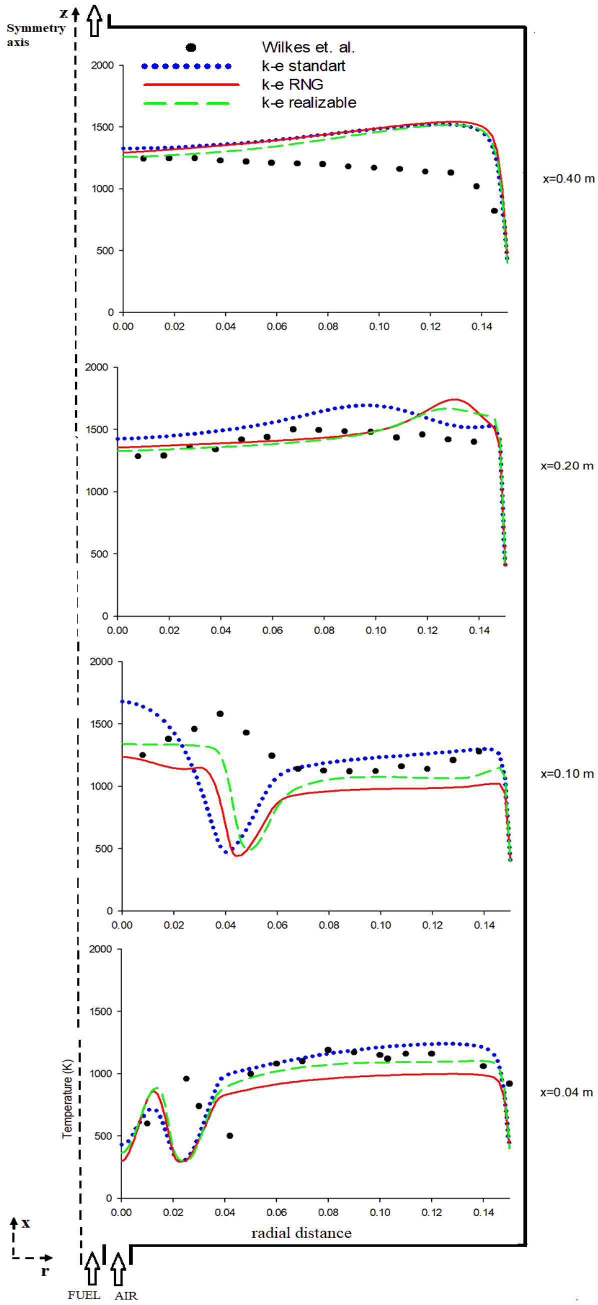

Figure 10. The comparison of k-ε turbulence models at radial temperature distributions using Eddy dissipation combustion model

5. CONCLUSIONS

The results have been showed that the definition of swirl velocity using the UDF may not significantly affect the results. However, it is seen that the using of UDF has a little bit of contribution to the coherence between the experimental data and numerical results. It is clearly seen that the determination of model constant (A) in the Eddy dissipation model calculations have a significant effect on the obtain more accurate temperature distribution. According to the results, it is seen that taking this value as one and closer values of one is an important effect in obtaining experimental results. As the combustion models are considered, it has been seen that, in the flame zone, the PDF mixture model gives good agreement with experimental results at the axial temperature distribution. On the radial direction, it has been obtained that both of the models give appropriate results especially, in the close regions of the wall of the combustion chamber. As for considering the turbulence models, the closest results to the experimental data have been obtained using k-ε RNG and realizable models. Particularly, one can observe from the results that the k-ε realizable model is more suitable to obtain experimental results than other models.

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