

## On the Suitability of Turbulence Models for the Prediction of Velocity and Temperature Distributions in Methane Non-Premixed Flame

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**Abstract**— This study focuses on the investigation of the performance of dissimilar turbulence models on the calculations of flow-field and reactive scalars (temperature and species) of a turbulent non-premixed flame. Turbulence models examined in this study included: the standard  $k-\varepsilon$ , RNG  $k-\varepsilon$ , standard  $k-\omega$ , SST  $k-\omega$  (Shear Stress Transport) and the Reynolds Stress Model (RSM). For the sake of ease and simplicity, Eddy Dissipation combustion model (EDM) was used to calculate the temperature fields and species concentrations in the flame. Predictions generated by different turbulence models are then compared and validated against experimental measurements from a turbulent methane-air flame called flame A. Experimental measurements of flame A provides data on velocity, temperature and species concentrations. Results of the investigation showed that among five turbulence models tested, the standard  $k-\varepsilon$  model provides the predictions that are in closer agreement to the experimental data of flow-field, temperature, and species concentrations. In general, it can be deduced that apart from the standard  $k-\varepsilon$  model, other turbulence models are not capable of capturing the position and the value of peak temperature accurately. On the other hand, the standard  $k-\varepsilon$  turbulence model is able to accurately capture the position and compute the value of peak temperature in the flame. This is attributed due to a better prediction of the flow-field by the standard  $k-\varepsilon$  turbulence model than those of other turbulence models. These findings indicate that the standard  $k-\varepsilon$  turbulence model in combination with Eddy dissipation combustion model is capable of producing accurate predictions of flame flow-field and temperature.

**Keywords**— simulation; non-premixed turbulent flame; turbulence model; combustion.

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### I. INTRODUCTION

Combustion is an exceptionally complicated phenomenon that involves the interaction between physical and chemical processes. Generally, in many combustion systems such as internal combustion engine, rocket engines, industrial combustors and chimney, combustion occurs and is associated with highly turbulent flows, because turbulent mixing increases burning rates, allowing more power to be produced per unit volume. However, since experimental and analytical studies are difficult to perform due to the complexity of the measurement, numerical modelling with the aid of computational fluid dynamics becomes a promising alternative in combustion research. This does not imply that the modelling problem can be solved without any challenge, because basically even for the case of laminar flow, the combustion itself is already complicated process.

Another complexity comes from the turbulence itself due to the presence of length and time scales in the reacting flow which up to present day still cannot be described in detail even with the utilization of a super-fast computer. Another important issue to be considered in the study of combustion modelling is the interaction between turbulence and combustion. In a turbulent flame, the turbulence is influenced by combustion due to an alteration in the acceleration of the front flame because of heat release. On the contrary, the turbulence disturbs the structure of the flame which boosts the chemical reactions.

Various studies have been reported with regard to modelling of non-premixed turbulent flames. Namazian et al. [1] employed the standard  $k-\varepsilon$  turbulence model to study the effect of air velocity on the length of flame, temperature distribution and mole fraction of species in a turbulent methane flame. The results of the simulation show that at a particular flow rate of fuel, increasing the air velocity

affected the width and the temperature of the flame; the width of the flame becomes thinner and the maximum temperature turns out to be higher. Roy and Sreedhara [2] employed four different turbulence models comprising standard  $k-\varepsilon$ , modified  $k-\varepsilon$ , RNG  $k-\varepsilon$  and RSM coupled with conditional moment closure combustion (CMC) modelling to simulate methanol and  $H_2/CO$  bluff-body flames. Results of the study demonstrated that simulated mixture fraction profile, obtained employing RSM exhibited an excellent agreement with the experimental measurements. Predicted mean temperature and species mass fraction obtained from the CMC calculation showed improved predictions when coupled with RSM for both the flames. This result suggests that different turbulence models employed may produce different temperature predictions. Meslem et al. [3] utilized seven turbulence models to simulate jet flow from cross-shaped orifice. The seven models include linear (LR and RNG) and nonlinear (quadratic and cubic)  $k-\varepsilon$  turbulence models, the standard  $k-\omega$  and the shear stress transport (SST)  $k-\omega$  turbulence models and a Reynolds stress turbulence model (RSM). Among the seven models being tested, Meslem et al. [3] concluded that none of them is able to predict well all jet characteristics in the same time. However, they recommended that SST  $k-\omega$  turbulence model is the most suitable one to simulate the flow-field in the jet flow issued from cross-shaped orifice. On the basis of the above-mentioned studies, it is clear that no single turbulence model that could solve all reactive and non-reactive flow problems. Therefore, selection of appropriate turbulence model for a particular flow problem becomes important.

Although a number of turbulence models are available, choosing the right turbulence model which suits the flow being investigated would not be easy. Each turbulence model each model has inherent strengths and weaknesses, no model is intrinsically superior to other ones. On this basis, the present work aims at investigating the performance of different turbulence models in predicting the flow-field and reactive scalar in a turbulent non-premixed flame and discussing the suitable model for the flame being investigated.

It has been well known that the turbulence significantly affects the combustion, and vice versa. The development of various turbulence models at present creates difficulties in the selection of appropriate turbulence model for a particular type of flow. Generally, investigators tend to choose established turbulence models such as Reynolds Stress Model (RSM) and standard  $k-\varepsilon$  model without considering possibilities that other turbulence models might be more suitable for the flow being investigated. On this basis, the present research aims at investigating the performance of various turbulence models under RANS category, including standard  $k-\varepsilon$  model, RNG  $k-\varepsilon$ , standard  $k-\omega$ , SST  $k-\omega$  and Reynolds stress model (RSM) in simulating the flow-field of a turbulent non-premixed flame. In conjunction with the Eddy Dissipation model, those turbulence models were tested their performance in simulation the temperature and species concentrations in a methane flame. All predictions by each turbulent model were validated against experimental data called Flame A reported by Meier et al. [4].

### A. Turbulence Models Description and Numerical Simulation

Turbulence theories, simulation and modelling have been always imperative subjects in fluid dynamics and engineering. Descriptions of different turbulence approaches can be found in various computational fluid dynamics textbooks. Any modelling technique involves a number of descriptive equations whose solution needs to be obtained numerically. In general, with respect to turbulence prediction alone, three fundamental classes of numerical simulations are presently being progressed: (i) direct numerical simulation (DNS); (ii) large eddy simulation (LES); and (iii) Reynolds averaged Navier-Stokes (RANS) approaches [5].

The DNS of turbulent flows basically engages a full numerical solution of the time dependent Navier-Stokes equations and accommodates all time and length scales of turbulence. From the conceptual point of view, it is fundamentally the simplest method to implement, since no turbulence modelling is needed. In DNS, all of the turbulent motions are resolved in the computational model from the largest scale to the smallest scale of turbulent eddy. As a consequence, the computational domain will be sufficiently large to cover the largest eddies, and the grid spacing should be fine enough to resolve the smallest eddies. Therefore, it is extremely expensive to simulate even the simplest types of flow (e.g. homogeneous turbulence), primarily due to the refined grid required to resolve the small-scale turbulence structures, as well as the small time-steps required for the time-scales of the smallest eddies. In the Reynolds-averaged Navier-Stokes (RANS) approach, instead of directly solving for the flow-field, solutions are obtained by solving time-averaged transport equations. The approach models all scales and solves the governing time-averaged equations which introduce unknown apparent stresses known as the Reynolds stresses. This produces an additional second-order tensor of unknowns for which various models can provide different levels of closure. Basically, two distinct types of RANS models have been developed: first-moment closure models and second-moment closure models. In the former, the unknown Reynolds stresses are reduced by correlation with the first-moment. The second moment closure models approximate the higher-order moments (i.e. the triple fluctuating velocity correlations) by second-moment terms, and solve transport equations for the Reynolds stresses directly. As a consequence of modelling the unknown terms, RANS turbulence models like, standard  $k-\varepsilon$  model, RNG  $k-\varepsilon$  model, standard  $k-\omega$  model, SST  $k-\omega$  (Shear Stress Transport), and Reynolds Stress Model (RSM) are capable of producing much faster computation in comparison to those of LES and DNS. This is the reason to use such models in the present investigation [5].

### B. Flame Geometry Configuration and Mesh Generation

Geometry of the flames being investigated is drawn using GAMBIT (Geometry and Mesh Building Intelligent Toolkit) software [6], which functions as a pre-processor designed to draw the system domain and discretise the domain. The procedure of building the geometry is started with drawing a cylinder three dimensional form for the nozzle and domain.

Discretization is performed on the geometry to divide an object into small meshes so the processor could perform the calculation in each node. The boundary condition is set up at this stage in accordance to the experimental data of the flames which include velocity, pressure outlet, wall and interior. The boundary conditions of the flame being investigated follow those stipulated in Meier [4]. Fig. 1 shows the geometry of 3-dimensional domain of Flame A [4] which has been discretised to have a number of nodes of about 105,815.

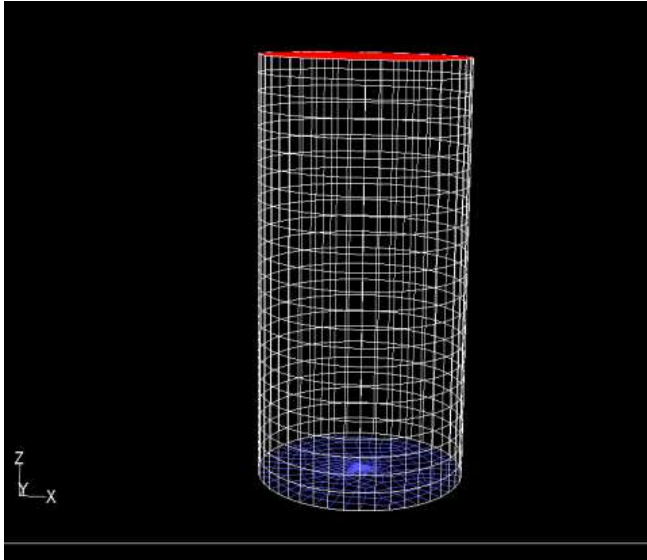


Fig. 1. Three-dimensional geometry of Flame A

### C. Flow-field and Combustion Calculations

The calculations of flow-field and combustion are performed using commercial CFD software FLUENT ver. 6.3 [7] which functions as the processor as well as post processor. A number of five turbulence models under RANS classification were tested for its respective performance in the computation of the flow-field of the flame being investigated, as shown in Table 1. All these turbulence models are embedded in the FLUENT code.

TABLE I  
TURBULENCE MODELS TESTED UNDER THE STUDY

Turbulence Model Classification	Model Derivative	
Reynolds Average Navier Stokes	Two equation model	- Standard $k-\epsilon$ [8] - RNG $k-\epsilon$ [9] - Standard $k-\omega$ [10] - SST $k-\omega$ (Shear Stress Transport) [11]
	Seven equation model	Reynolds Stress Model (RSM) [12]

The combustion calculation was performed using Eddy Dissipation Model [8]. This model has been chosen due to its simplicity without the need to supply complex combustion kinetics scheme. As a consequence, the computer resource required is very reasonable. The results

of combustion calculation, such as temperature of the flame in axial and radial position shall be compared with experimental data of Meier [4]. Meier et al. [4] experimentally studied a simple jet diffusion flame of  $\text{CH}_4$ ,  $\text{H}_2$ , and  $\text{N}_2$  in a low velocity air co-flow. The flame is an axis-symmetric jet flame stabilized without a pilot. The fuel stream consists of 22.1%  $\text{CH}_4$ , 33.2%  $\text{H}_2$ , and 44.7%  $\text{N}_2$  in volumetric parts and is introduced into the flow-field through a straight stainless-steel tube of length 350 mm with a nozzle of an inner diameter of 8.0 mm. The cold jet exit velocity was fixed to 42.15 m/s resulting in a Reynolds number of 15,200. The jet was mounted concentrically to the exit nozzle of a wind tunnel with a diameter of 140 mm providing co-flowing air of 0.3 m/s. Velocity distributions for these flames were measured using laser Doppler anemometry. Temperature and major species concentrations were measured using Raman scattering.

## III. RESULTS AND DISCUSSION

### A. Flow-field Predictions

Fig. 2 shows the contour of velocity profile generated by the simulation using FLUENT software. On the right side of Fig. 2 (a), it displayed the jet profile while on the left it shows values of the velocity based on the colour on profile. Fig. 2 (b) illustrated the real flame performed by Meier [4]. Comparing the prediction and the real flame, it is clear that with the use of  $k-\epsilon$  turbulence model, the results of prediction are in excellent agreement with the real flame. The highest velocity is observed in the zone just above the surface of the nozzle. Moving towards further downstream, the velocity decreases until reaching the lowest at the top of the flame.

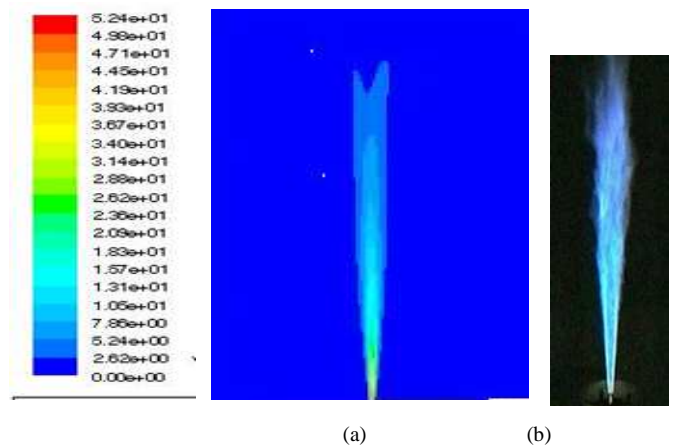


Fig. 2. Flow-field contours of standard  $k-\epsilon$  turbulence model

Fig. 3 shows the results of axial velocity prediction by various turbulence models compared with experimental data. The symbol in Fig. 3 represents the experimental data of velocity, while the lines display predicted results by various turbulence models. Inspecting the centreline of the flame, it is clear that each turbulence model produces different predictions in terms of axial velocity in the core of the flame. Although, all turbulence models produce similar results up to 40 mm above the nozzle, each model started to deviate from one to another above the position. Qualitatively, the

velocity evolution resulted from all turbulence models follow the trend of experimental data, where the velocity decreases with the increasing of height of flame. However quantitatively, the results of axial velocity in the core of the flame presented by the standard  $k-\varepsilon$  turbulence model are in closer agreement with experimental data. Although predictions are not exactly close to each experimental data point, the standard  $k-\varepsilon$  model is able to predict well the velocities in regions close to the surface of the nozzle and further downstream 300 mm above the nozzle. Among five turbulence models being tested, the SST  $k-\omega$  model quantitatively gives the worst predictions compared with results from other turbulence models. On the contrary, the standard  $k-\varepsilon$  model qualitatively and quantitatively produced better predictions in axial velocity than those generated by SST  $k-\omega$  model. It should be noted that the SST  $k-\omega$  model was developed by combining the original Wilcox  $k-\omega$  model for use near walls and the standard  $k-\varepsilon$  model away from walls using a blending function, and the eddy viscosity formulation is modified to account for the transport effects of the principle turbulent shear stress. Therefore, the SST  $k-\omega$  will give accurate prediction for boundary layer simulation. As it depends on wall distance makes this model less suitable for free shear flows, as the case of the flame being investigated, compared to standard  $k-\omega$ .

In the same figure, it is also observed that the RNG  $k-\varepsilon$  turbulence model, a variant model of the standard  $k-\varepsilon$ , qualitatively and quantitatively could not also produce better predictions in terms of axial velocity than its original model, standard  $k-\varepsilon$ . Basically the RNG  $k-\varepsilon$  has similar formulation as the standard  $k-\varepsilon$ ; however, the former includes some modifications to cover effects of low Reynolds number, strained and swirling flows. The most probable reason of poor prediction by RNG  $k-\varepsilon$  is because the Flame A in concern is a simple jet in nature which does not require complex model to represent its flow-field.

Among all turbulence models being tested, the RSM model is the most complex compared to the others, because this model was developed to cover the deficiencies contained in the two-equation models such as standard  $k-\varepsilon$ . However, the predicted results presented by RSM model are not better than those of standard  $k-\varepsilon$ . These results indicate that a more complex turbulence model does not always produce better predictions.

Fig. 3 also presented comparison of predicted axial velocity by various turbulence models with experimental data in radial direction of the flame at various axial positions. Again similar findings as obtained in axial direction are observed in radial profile, where the prediction by the standard  $k-\varepsilon$  is in excellent agreement with the data. Compared with predictions produced by other turbulence models, those by the standard  $k-\varepsilon$  are the best which gave the most suitable turbulence model for modelling the flow-field of methane jet flame. Contrary to this study, Balabel et al [13] reported that the SST  $k-\omega$  turbulence model performed better than standard  $k-\varepsilon$ , extended  $k-\varepsilon$ , and  $v^2-f$  turbulence models, when they modelled the dynamics of turbulent gas flow through a rocket nozzle. However, it was found out that there is little difference between results derived on the basis of standard  $k-\varepsilon$  and Reynolds stress turbulence models

(RSM) for the majority of flow parameters considered on the modelling of several non-premixed methane flames [14].

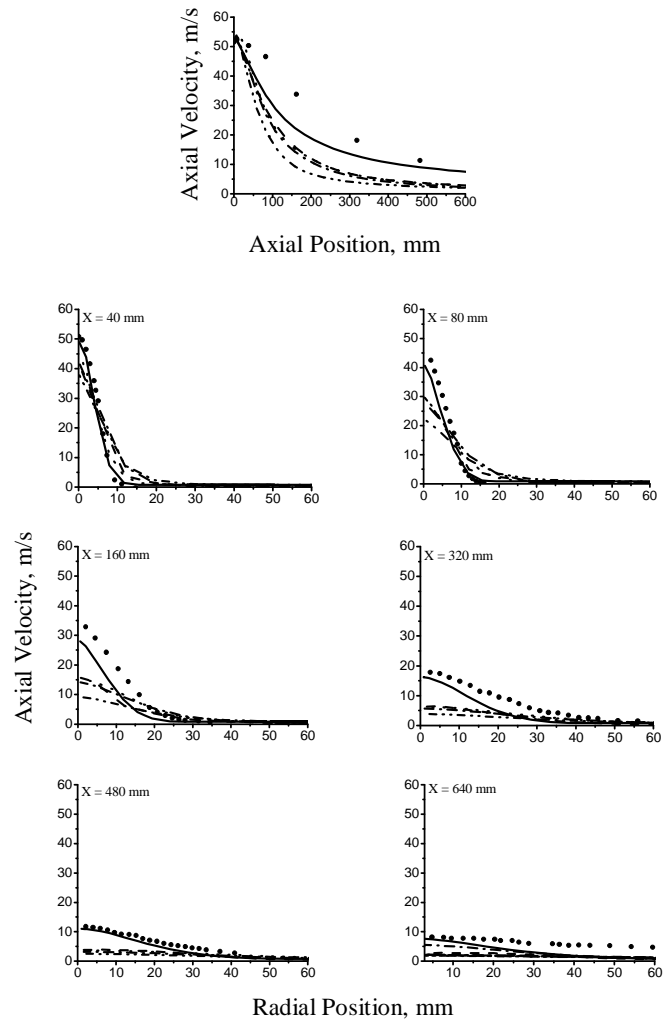


Fig. 3. Comparison of the flow-field predicted results and experimental data on axial and radial profiles at  $X = 40, 80, 160, 320, 480,$  and  $640$  mm, (symbol = experimental data; Line = prediction results; solid line — standard  $k-\varepsilon$ ; dash line --- RSM; dash dot line -•- RNG  $k-\varepsilon$ ; dot line ••• SST  $k-\omega$ ; dash dot-dot line -••- Standard  $k-\omega$ ).

The results of this study were in agreement with those reported by Sanders and Lamers [15] Castineira [16] found out that predictions of flow-field turbulent jet flames with the use of standard  $k-\varepsilon$  turbulence model are in excellent agreement with the experimental data. A recent simulation study on free jet flow also supports this result [17]. Among seven turbulence models being tested to model slightly swirling turbulent free jets, Miltner et al [17] found out that a simple and inexpensive standard  $k-\varepsilon$  turbulence model is capable of serving very well for the representation of most effects in the turbulent jets being considered.

### B. Flame Temperature Predictions

Fig. 4 on the right side shows the temperature contours of flame A generated by standard  $k-\varepsilon$  model recorded after the combustion reached steady state condition. On the left side is shown the relationship of the contour colour with values of temperature, where the redder the colour of the flame

contour the higher the temperature. The blue colour indicates room temperature at 300 K. It can be noted that the vertical flame continuously burning with no sign of the influence of cross wind effect on the flame, since the flame is released into a co-flow air of low velocity. From the temperature profile, it shows that the highest temperature inside the flame is at 1760 K, and occurs at about 50% of the height of the flame. At this position the air and the fuel fraction of methane is in a stoichiometric state. Temperature contour gives the temperature value at every point in the flame. The temperature of the fuel is still same as room temperature when the fuel was just issued out of the nozzle. Soon after burning, the temperature rises until it reaches the stoichiometric position and above this position the temperature decreases in the direction to the flow until reaching the tip of the flame.

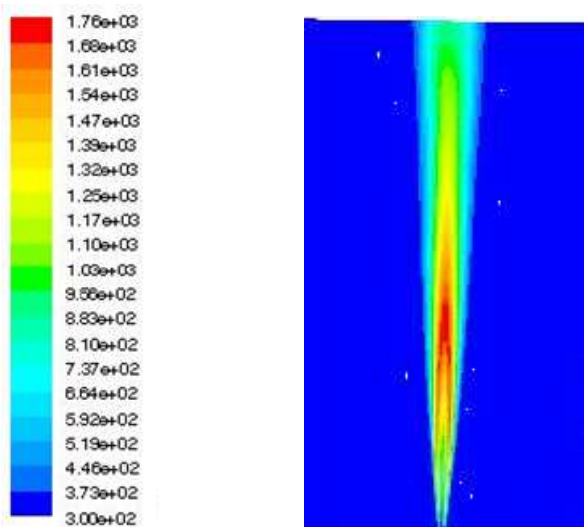


Fig. 4. Temperature contours resulted from the use of standard  $k-\epsilon$  turbulence model

Comparison of temperature predictions produced by different turbulence models with experimental data is shown in Fig. 5. The trend obtained here is similar to that obtained in the flow-field profile. The graph on the top shows the temperature predictions along the axial direction of the flame compared to experimental data. Experimental data show that the stoichiometric position, where the highest temperature in the flame, occurred at a position about 510 mm above the nozzle with a temperature of 1760 K. Standard  $k-\epsilon$  prediction is able to capture this stoichiometric position quite well, both quantitatively and qualitatively. The excellent performance shown by standard  $k-\epsilon$  turbulence model is much due to its capability to accurately predict the flow-field in which other turbulence models were unable to do so. As a result, the axial temperature predictions by other turbulence models qualitatively were far below the performance of those of the standard  $k-\epsilon$ .

The RNG  $k-\epsilon$  and the SST  $k-\omega$  turbulence models produce adequate peak temperature quantitatively. However, from qualitative wise, the predictions are quite poor as the peaks took place at lower positions at 125 and 200 mm above the nozzle, far away from the peak point of experimental data. On the other hand, the axial temperature predictions resulted

from standard  $k-\omega$  turbulence model and RSM model deviate much from the overall experimental data. Both models are unable to catch the position and the value of peak temperature. However, both models are able to predict well the temperature in the region close to the nozzle.

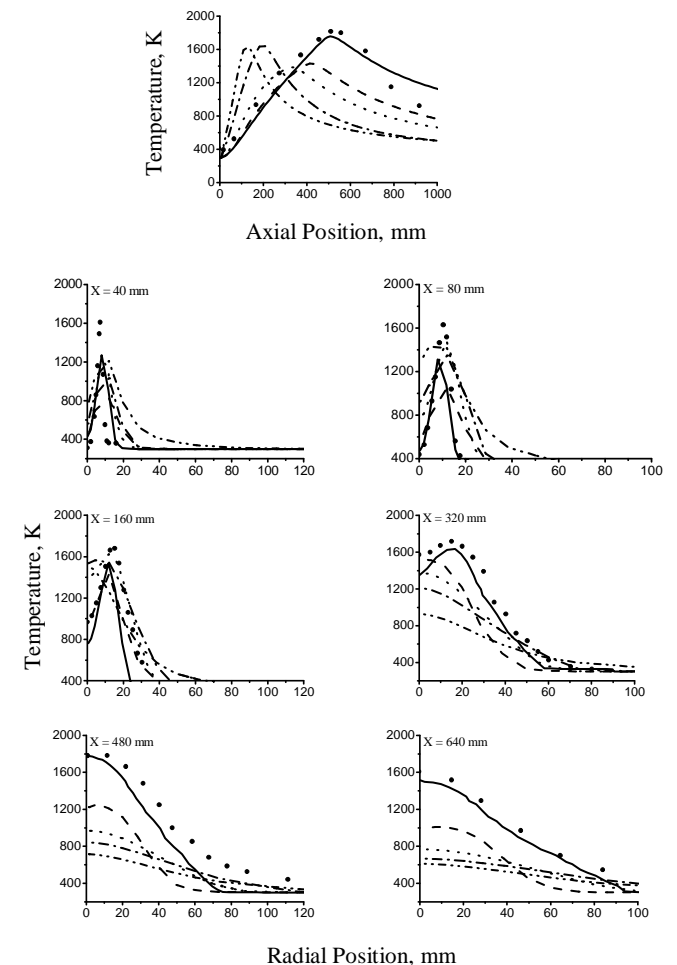


Fig. 5. Comparison of temperatures prediction results and experimental data on axial and radial profiles at  $X = 40, 80, 160, 320, 480,$  and  $640$  mm, (symbol = experimental data; Line = prediction results; solid line — standard  $k-\epsilon$ ; dash line --- RSM; dash dot line - • - RNG  $k-\epsilon$ ; dot line ••• SST  $k-\omega$ ; dash dot-dot line - •• - Standard  $k-\omega$ ).

Fig. 5 also presents predictions of temperature by all turbulence models on radial profile of the flame. It is observed that only at the position of  $x = 160$  mm that the RSM turbulence model is capable of superior predicting the radial temperature than the standard  $k-\epsilon$  turbulence model. At this position predicted temperature by the standard  $k-\epsilon$  model is slightly lower than the experimental data. However, at other axial position, the radial temperature predictions begin to approach the experimental data as shown in the position of  $x = 320$  to  $x=640$  mm. Although at the position of  $x = 480$  mm predicted temperatures by the standard  $k-\epsilon$  model is lower than the experimental data, its performance is better than other models. Although Woolley [14] found out that temperature predictions were found in better agreement with the use of RSM, from these results it can be concluded that the predictions of axial and radial temperature of the methane non pre-mixed turbulent flame is more appropriate with the use of standard  $k-\epsilon$  turbulence model.

### C. Mass Fraction Predictions

Fig. 6 shows a comparison of CH<sub>4</sub> and CO<sub>2</sub> mass fraction predictions with experimental data. Experimental data show that the mass fraction of CH<sub>4</sub> continues to decrease along the flame during the combustion process. Predictions generated by standard *k-ε* can accurately estimate the change of methane mass fraction along the flame. However, the prediction of CO<sub>2</sub> fraction generated by this model is not as good as predictions of methane. The standard *k-ε* model is not able to follow the inclination data up to a height of 600 mm above the nozzle, but it recovers to approach experimental data from both qualitative and quantitative point of view above the said height.

With regard to the oxygen mass fraction, it demonstrated that above the nozzle its mass fraction in the fuel is too low, because the fuel is just issued from the surface of the nozzle and the region is fuel rich and the flow is significantly turbulence. As the air starts to diffuse, air mass fraction starts to increase along the flame. Each model produces different positions for the onset of the air to diffuse into the flame. As the CH<sub>4</sub> and O<sub>2</sub> start to decrease and increase respectively, the CO<sub>2</sub> and H<sub>2</sub>O start to increase until reaching the stoichiometric position and decrease thereafter.

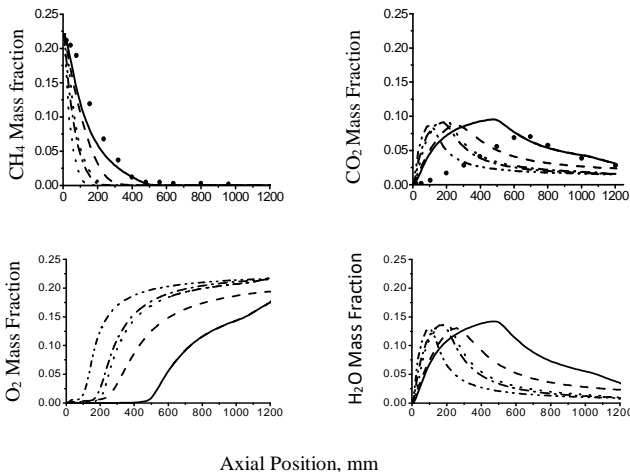


Fig. 6. Comparison of species mass fraction and experimental data on axial profile, (symbol = experimental data; Line = prediction results; solid line — standard *k-ε*; dash line --- RSM; dash dot line -•- RNG *k-ε*; dot line ••• SST *k-ω*; dash dot-dot line -••- Standard *k-ω*).

### IV. CONCLUSIONS

The numerical investigation on the performance of various turbulence models for prediction of flow-field and reactive scalars when they were coupled with the Eddy Dissipation Model has been performed to give the following conclusions: Among five turbulence models tested, it shows that each model produced predictions that are different from one to another. Therefore, the selection of an appropriate turbulence model becomes important in order to be able to accurately predict the flow-field and reactive scalars in a turbulent non pre-mixed flame; Among five turbulence models investigated in this study, the standard *k-ε* turbulence model provided reasonable predictions both in terms of flow and reactive scalar fields. Predictions resulted from the application of the standard *k-ε* model are in closer agreement

with experimental data than those of produced by other turbulence models, RNG *k-ε*, standard *k-ω*, SST *k-ω* and RSM; Turbulence models derived from a more complex mathematical formulation such as Reynolds Stress Model (RSM) and RNG *k-ε* do not always produce better predictions than those models developed by simpler mathematical model such as standard *k-ε* turbulence model.

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