

Computational fluid dynamic on the temperature simulation of air preheat effect combustion in propane turbulent flame

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Abstract. this paper presents results obtained from the application of a computational fluid dynamics (CFD) code Fluent 6.3 to modelling of temperature in propane flames with and without air preheat. The study focuses to investigate the effect of air preheat temperature on the temperature of the flame. A standard k- ϵ model and Eddy Dissipation model are utilized to represent the flow field and combustion of the flame being investigated, respectively. The results of calculations are compared with experimental data of propane flame taken from literature. The results of the study show that a combination of the standard k- ϵ turbulence model and eddy dissipation model is capable of producing reasonable predictions of temperature, particularly in axial profile of all three flames. Both experimental works and numerical simulation showed that increasing the temperature of the combustion air significantly increases the flame temperature.

1. Introduction

Combustion modelling has played an important role not only in the design, but also in the operation of a turbulent combustion system. In order to accurately predict the temperature in such system, an integrated model that at least represents turbulence and combustion phenomena, as well as radiation heat losses is required. The ability to apply such an integrated model, of demonstrated accuracy, aiming at reaching maximum combustion efficiency and minimizing heat losses, emission of pollutants in relation to safety and environmental considerations, would represent a major step-forward in our ability to design and manage combustion processes. However, it is important to note that the modelling could not stand alone, since modelling requires verification. Therefore, experimental works are required the modelling not only for the purpose validation but also for providing better understanding on the phenomena being studied.

Numerous experimental works have been performed in an attempt to study the effects of air preheat on the combustion process. Gupta [1] conducted an experimental study on the structure of turbulent propane – air diffusion flames with preheated air and found out that the emission NO_x was observed to be less with high preheat temperature and low oxygen concentration in the oxidizer. Sadakata [2]



also confirmed that by increasing the temperature of combustion air up to 573 K, the emissions of thermal and fuel NO were not significantly increased. Although previous works mentioned that air preheating did not significantly affect the NO concentrations in a flame, recent experimental works emphasize different findings. Lim [3] investigating the effects of air preheat on the structure and emission of counter-flow methane –air diffusion flame have shown that the peak concentrations of CO and H₂ increased by 20 per cent, and that of NO increased by 70 per cent, as the air temperature was increased from 300 to 560 K. In another study, Fuse [4] also observed that the increase in air temperature increased the NO formation in diffusion flames. However, they found out that NO formation can be decreased, even with high air temperature, if concentration of oxidizer is significantly reduced. With respect to the temperature of the flame, all above studies confirmed that the flame temperature increases due to the use of air preheat. Since air preheat could be produced from waste heat sources, the use of air preheat will not only improve the combustion efficiency but also could reduce the heat loss in an industry. Therefore, it is important to investigate if the modelling could also produce similar increase of flame temperature when the combustion is supplied with air preheat.

A number of combustion models, ranging from simple to complex approaches, have been proposed in the literature, and research to develop new models and improve the existing ones is on-going. Those approaches that have been proposed for modelling combustion in turbulent flames have their own advantages and disadvantages. Although numerous models are available, modelling of non-premixed turbulent combustion using the eddy dissipation model (EDM) still receives great attention due to its simplicity and low computer resource usage. Therefore, for predictions of temperature in the propane flames being studied, this model was employed for the sake of keeping the computational cost at an acceptable level without losing an acceptable degree of accuracy.

In this paper, the results of the application of a computational fluid dynamics (CFD) code Fluent 6.3 to modelling of air preheated propane non-premixed flames are presented. The objective of the present work is the assessment of the EDM combustion model, available directly in the code to represent the temperature profile in the turbulent propane flames, with and without air preheat. Turbulence of the flame is calculated using a standard k- ϵ model. Validation is achieved by comparing the computed temperature predictions against available experimental data of propane flames with and without preheated air [5,6].

2. Methodology

2.1 Target flame

Three turbulent non-premixed propane flames with and without air preheats considered in the present study have been experimentally reported by Nishida and Mukohara [5], and Jurng et al [6], respectively. The important characteristics of each of these flames are presented in TABLE I. Further details with regards to the flame geometry, methods of data collection and processing can be found in the relevant references.

Table 1. Operating conditions for air-propane and preheated air propane flames

Air exit temperature	298 K	323 K	773 K
Absolute pressure/atm	1	1	1
Fuel exit velocity/ms ⁻¹	16	30.0	30.0
Reynolds number	11000	13000	13000
Fuel exit temperature/K	298	298	298
Nozzle diameter/mm	3.0	2.0	2.0
Co-flow air velocity/ms ⁻¹	0	0.4	0.96

2.2 Turbulent flow field calculation

Since the flow of the flames being studied is turbulent in nature, the flow is characterized by fluctuating velocity fields. These fluctuations affect other transported quantities within the flame such as momentum, energy, and species concentration, and cause the transported quantities to fluctuate as well. Since these fluctuations can be of small scale and high frequency, they are too computationally expensive to simulate directly in practical engineering calculations. Instead, the instantaneous (exact) governing equations can be time-averaged, ensemble-averaged, or otherwise manipulated to remove the small scales, resulting in a modified set of equations that are computationally less expensive to solve. However, the modified equations contain additional unknown variables, and turbulence models are needed to determine these variables in terms of known quantities. For the purpose of propane flames calculation, a standard k - ε turbulence model was used to represent the flow field within the flame. As the k - ε turbulence model is categorized into two-equation models, it requires the solution of two transported equations for k and ε [7], in conjunction with the mass and momentum conservation equations.

Calculation of turbulent kinetic energy, k and turbulent dissipation rate, ε is required during the combustion calculation under EDM approach. The turbulent kinetic energy and turbulent dissipation rate can be calculated using Equation 1 and 2, respectively.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M \quad (1)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = & \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \\ & C_{1\varepsilon} \frac{\varepsilon}{k} (G_k C_{2\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} \end{aligned} \quad (2)$$

In these equations, G_k is turbulent kinetic energy in average velocity gradient, G_b is kinetic energy related in driving force. Y_M is contribution in compressible turbulent dilatation contribution to overall dissipation rate. $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ is constant, σ_k and σ_ε is Prandtl number turbulent for k - ε .

Standard turbulence modeling constants in the standard k - ε modelling appropriate to asymmetric flows were employed, although to ensure the accurate prediction of the spreading rate of the jets, an adjustment was made to the value of $C_{\varepsilon 2}$ from 1.92 to 1.86 to affect an increase in the dissipation rate of turbulence kinetic energy

2.3 Combustion calculation

The Eddy Dissipation Model (EDM), a combustion model originally developed by Magnussen and Hjertager [8], is based on the assumption that the chemical reactions occur in regions where the dissipation of turbulence energy takes place. The region of the flow where this dissipation occurs is in fine structures or small turbulence scales, which are treated as perfectly stirred reactors. To find the amount of fine structures in the flow, Magnussen [9] uses an energy cascade model which accounts for finite Reynolds number effects and the influence of molecular dissipation processes on the reaction rates of combustion. Combustion is treated as a single-step reaction. In later developments, EDM models have been developed to account for finite-rate chemistry [9]. The main advantage of the EDM approach clearly lies in its simplicity and low computational cost due to the use of a conserved scalar concept, e.g. mixture fraction, which allows decoupling of the chemistry terms and the flow field.

Although Hjertager et al. [10] reported that the standard EDM model is not suitable for liquid-phase reactions; it has found extensive application in the simulation of turbulent reacting flows. Magnussen [9] applied detailed chemistry to investigate the performance of the EDM for the prediction of soot formation and destruction in an acetylene diffusion flame. Gran and Magnussen [11] used the model to simulate a non-premixed bluff body stabilized flame, and good agreement with experimental data was reported, and its performance was comparable to that of a transported PDF model. Chakraborty et al. [12] also used the model to simulate H₂/air combustion in a scramjet

combustor. Here, the EDM model with detailed chemistry and finite rate single-step chemistry was found to capture well all essential features of the reaction rate profile distribution, with similar order of magnitude peak values. In Giacomazzi et al. [13], the EDM model is used to describe single-step combustion chemistry close to the dissipation scales in the context of LES and RANS predictions of a bluff-body C₃H₈/air premixed flame.

The eddy dissipation model (EDM) proposed by Magnussen and Hjertager [8] was developed for the prediction of gaseous combustion reactions in turbulent flows. The combustion reaction is treated as a single-step irreversible reaction with finite rate for fuel F, oxidant O and product P, as illustrated in Equation 3.



The EDM assumes reaction to be much faster than mixing, and therefore the rate of combustion is entirely determined by the turbulent mixing rate ε/k and by the limiting ingredient needed for reaction, either the fuel or oxidizer or product. The model requires the solution of two variables, the mass fraction of species and the mixture fraction, where the source term in mass fraction of species equation is solved using Equation 4.

$$\bar{w}_\alpha = A \bar{\rho} \frac{\varepsilon}{k} \min \left[\bar{Y}_F, \frac{\bar{Y}_O}{s}, B \frac{\bar{Y}_P}{(1+s)} \right] \quad (4)$$

Where k and ε are the turbulence kinetic energy and its dissipation rate obtained from the turbulence flow field calculation, and s is the stoichiometric coefficient of the reaction given as Equation 3. The constants A and B are often set to 4.0 and 0.5, respectively, for gaseous combustion reactions.

2.4 Numerical computation

With respect to numerical simulation, the flame geometry was created using GAMBIT software. The calculation of flow and mixing fields was achieved by equations under the standard k - ε turbulence modeling with the use of the commercial CFD code FLUENT ver. 6.3. The combustion calculation which solved the energy and species concentration was performed by utilizing EDM that is embedded in the FLUENT code. Computations were performed using a laptop computer of 2.00 GB RAM having a 2.13 GHz of speed. The computation time for each flame took around 4 to 6 hours.

3. Result and discussion

Figure 1 demonstrated axial and radial predictions of axial temperature for the propane flame without air preheating compared to experimental data [6]. The solid line represents the simulations resulting from the use of k - ε standard turbulence model and EDM model. The centreline axial temperature predictions in the flame display qualitatively good agreement with the experimental data, particularly further downstream of the flame. As a consequence, the predicted temperature in radial direction in the area closer to the nozzle significantly deviated from the experimental data. However, the radial temperature predictions further downstream are in line with measurements. This could be due to adjustment of spreading rate through modifying the constant $C_{\varepsilon 2}$ of the standard k - ε turbulence model.

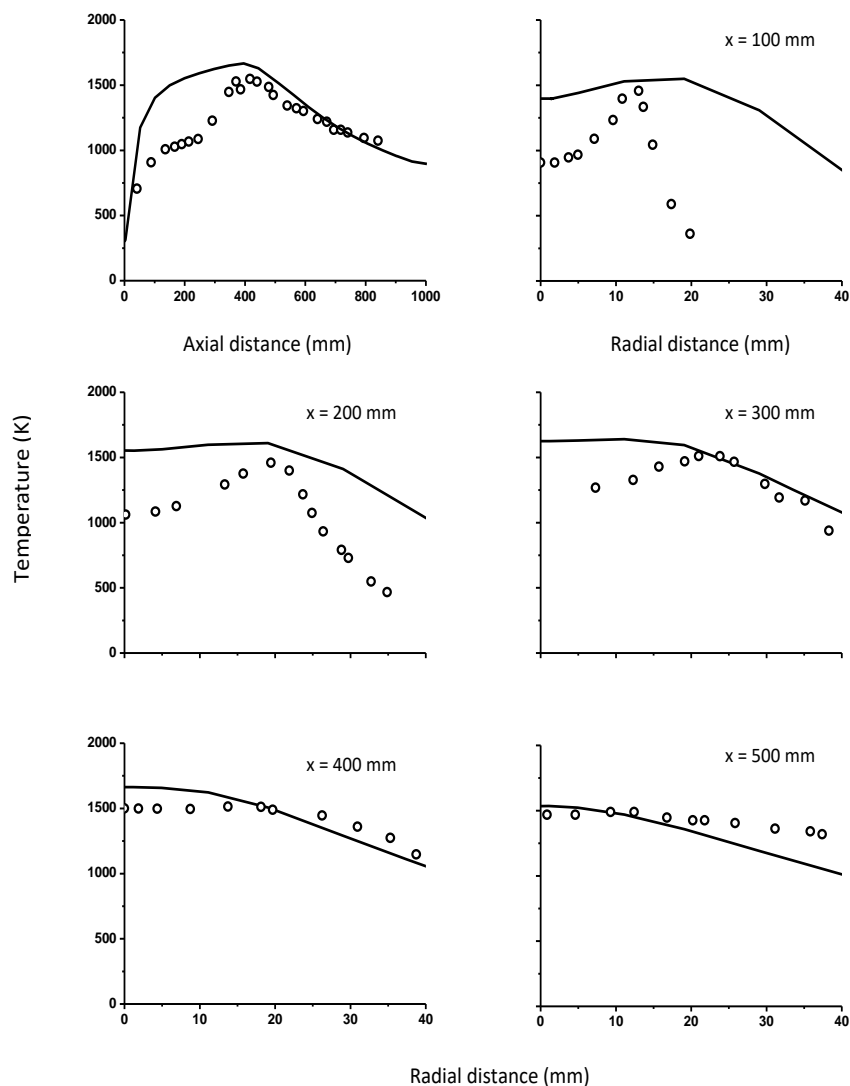


Figure 1. Axial and radial profiles of temperature for propane flame, $T_{air} = 298$ K (symbol – measured, solid line – predicted with EDM model)

Temperature predictions calculated using Eddy Dissipation Model showed that the centreline temperature predictions in the propane flame without preheating display qualitatively good results in comparison to the experimental data. The peak temperature in axial profile slightly over predicted. The evolution of the computed axial temperature is in line with the measurements along the core of the flame. Overall, the position and value of peak temperature is qualitatively and qualitatively well captured by the EDM model. This agreement is achievable not only due to the conformity of flow field predictions with experimental data but also due to the correct selection radiation model to represent the combustion.

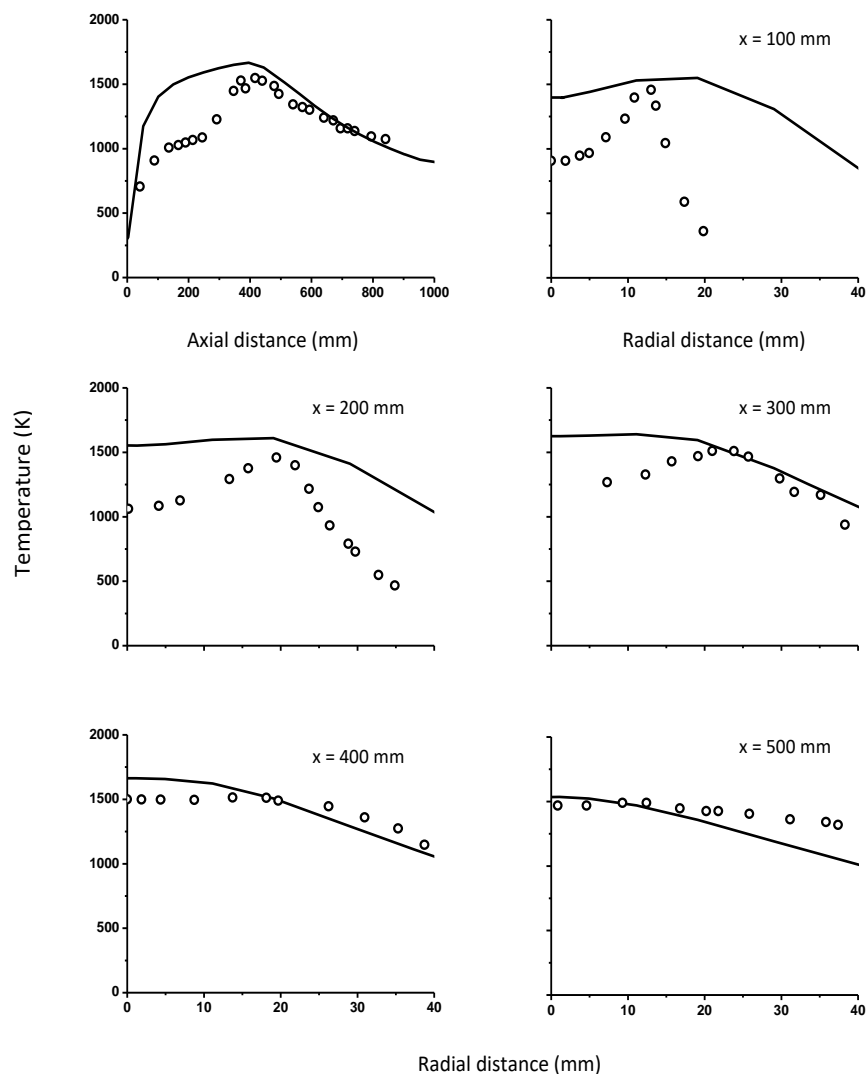


Figure 2. Axial and radial profiles of temperature for propane flame, $T_{\text{air}} = 323 \text{ K}$ (symbol – measured, solid line – predicted with EDM model)

Figure 2 presents graphs of temperature predictions compared with experimental data for flames with air preheating of 323 K. The calculated axial temperature profile predictions for the propane flame with air preheating of 323 K are in good agreement with the experimental data, indicating that the mixing field the lower air preheated propane flame is well represented by the application of the $k-\epsilon$ turbulence closure, as in the case of propane flame without preheating. In connection with temperature predictions, the results of upstream mean temperature predictions of the air preheated flames are not as satisfactory compared with experiment data, although the temperatures in the mid-flame region and its peak are well represented. Radial temperature profiles along with measurements for the lower air preheated propane flame in the position $x = 500 \text{ mm}$ are in good agreement with the experiments. However, closer to the nozzle, radial predictions of the temperature are not in agreement with the data.

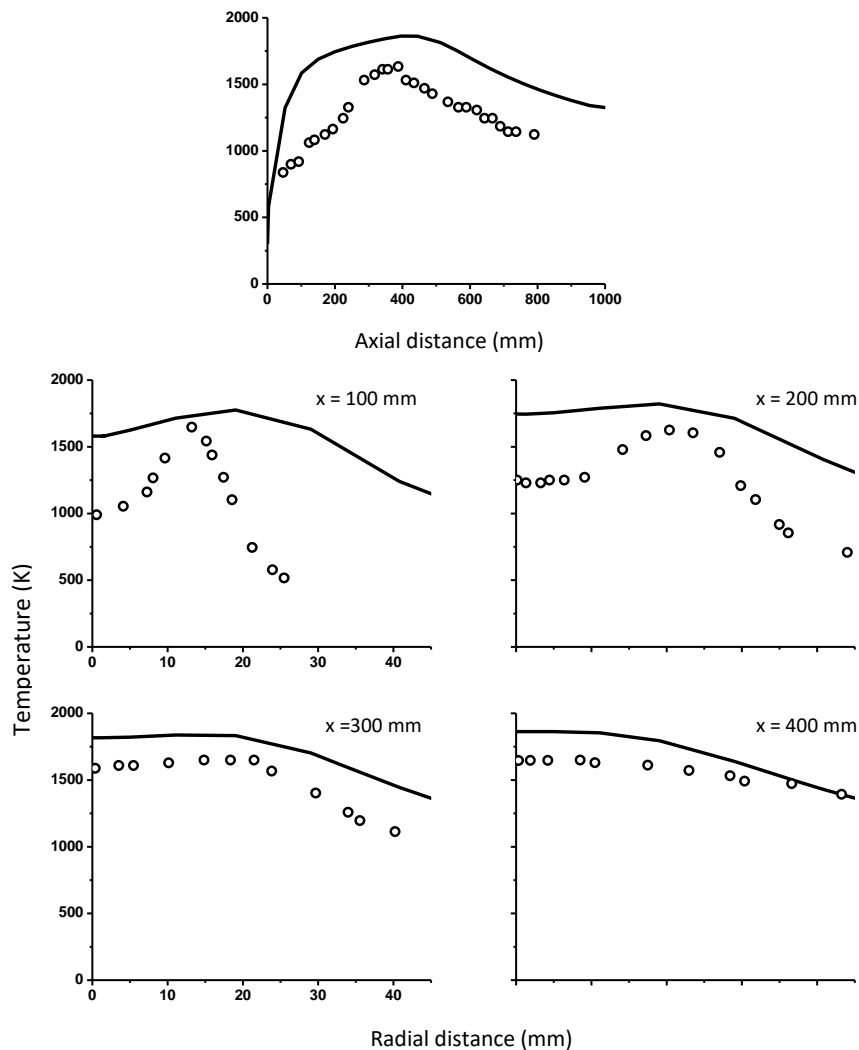


Figure 3. Axial and radial profiles of temperature for propane flame, $T_{\text{air}} = 332 \text{ K}$ (symbol – measured, solid line – predicted with EDM model)

Figure 3 represented predicted centerline and radial temperatures of the propane-preheat flame with air preheating of 772 K. Solid line and symbol represent temperature predictions and measurement, respectively. It is clearly seen that air preheating leads to an increase of centerline flame temperature, particularly up to the mid-flame zone. The temperature of air preheat flames increases sharply in core of the flame, leading to a shift of peak temperature and the predictions result is over prediction in the peak temperature. Further downstream, the radial profile of temperature predictions deviated significantly from measured data.

At this stage it is useful to compare the peak temperature in the three flames being studied. In the axial profile, it is clearly seen that the peak temperatures are as follows: 1862 K in the flame of 773 K air preheat, 1667 K in the flame of 323 K air preheat and 1652 K in the flame with no air preheat. As the temperature of the air preheats increases, the peak temperature also increases. As a consequence, the highest peak temperature among the three flames was observed in the flame of 773 K air preheat, reaching its peak at 450 mm and the lowest peak temperature among the three flames was in the flame with no air preheat having its peak at 400 mm.

It is seen that in all three flames, over prediction in temperature exists in the zone closer to the nozzle or in the rich fuel area, $x = 100$ mm. However, in the fuel lean area $x = 400, 500$ and 600 mm the result of prediction is getting better, reaching in closer agreement in measured data. On the contrary, Yunardi et al [14] could produce good result in rich fuel area but not in the lean fuel area when they used Conditional Moment Closure approach to calculate profile temperature coupled with a kinetic reaction scheme. However, it should be noted that Yunardi et al [15] demonstrated excellent temperature predictions in methane flame with the use of EDM model. It seems that the EDM model assuming single reaction step to represent the chemistry of combustion is suitable for simpler fuel like methane. With a more complex fuel, like propane, a single step reaction assumption is no longer applicable.

4. Conclusions

From the results and discussions, the following conclusions are drawn:

1. Increasing the temperature of the combustion air significantly increases the flame temperature. As a consequence, the flame of 773 K air preheat has the highest peak flame temperature of 1862 K and the flame of 298 K air preheat has the lowest peak flame temperature.
2. Although the position and the value of peak temperature in each flame is qualitatively predicted well by the EDM combustion model couple with $k-\epsilon$ turbulence model, the radial temperature predictions are not satisfactorily represented which much is caused by inability of the model to include finite rate chemistry to represent the combustion.

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