LARGE EDDY SIMULATION OF ONE-METER METHANE POOL FIRE USING ONE-EQUATION SUB-GRID SCALE MODEL

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Abstract
A numerical study simulating the time-dependant flow field structures of a one-meter buoyant methane pool fire is carried out using a fully-coupled Large Eddy Simulation (LES) model, which incorporates the one-equation sub-grid scales (SGS) turbulence model. Based the mixture fraction approach and infinity fast chemistry assumption, the velocity profile and turbulence characteristics are calculated and compared against experimental measurements. The predicted time-averaged velocity is in good agreement with the experimental data. The computed velocity time history is better predicted than the previous study, where Smagorinsky SGS model was utilized. In addition, the time-averaged turbulence velocity fluctuations are predicted higher than the experimental values. These over-predicted results are attributed to the SGS model which directly controls the turbulence mixing in small eddies.

Introduction

The overall fire problem involves many complex processes including buoyancy driven flow field, turbulent combustion, radiation heat transfer, solid and liquid fuel vaporization, pyrolysis and decomposition, and interactions between structural materials and the fire. Due to the restrictions and difficulties associated with experiments, especially for large-scale fires, numerical simulation is an essential research tool. On the other hand, the simulation of fires using computational fluid dynamics (CFD) is challenging due to the need to resolve several length scales from those characteristics of the combustion processes to those characteristics of the mass and energy transport throughout an entire domain. At this point, three different CFD techniques have been used for fire modelling: Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), and Reynolds-Averaged Navier-Stokes (RANS). DNS method solves the transport equations without sub-grid models. This technique demands fine spatial and temporal resolution. Due to its computational cost, it is limited to small laminar flames and sometimes small turbulent jets. DNS is still impractical for simulating of large scale fires.

LES and RANS employ several models of the unresolved sub-grid dissipative processes in fire phenomena. These models which are called turbulence models differ in scope. LES attempting to compute as much of the resolvable length and time scales (the large eddies) as possible, whereas RANS averages over significantly larger spatial and temporal scales than those that are characteristic of the given numerical grid or the fundamental frequency of the fire.

Macroscopic fire simulations based on RANS approaches have been widely adopted in earlier studies [1–3]. Nevertheless, the RANS models have been known to be unable to solve the scale dependent dynamic behaviors, which are predominant during the pulsation cycle of buoyant fires [4]. Alternatively, LES approach has recently become the central focus of fire modeling [5–9]. Based on the spatial filtering technique, LES can provide information to match scales that are resolved on computational mesh while the microscopic information is indirectly calculated by the formulation of the SGS turbulence model. Due to the importance

and dynamic behaviors of large eddies on the flow field, the temporal vortical structures are expected to be better captured by the LES compared to the RANS approach [7].

Baum et al. [7] have pioneered the study of buoyant plume modelling using LES turbulent model. Their study obviously confirmed the potential of the application of LES in buoyant fire simulations. More comprehensive LES fire models were presented by Rawat et al. [8] and have been validated against the experiment on a one meter diameter pool fire by Tieszen et al. [10]. Rawat et al. [8] adopted the unsteady flamelet approach in order to include the complex chemistry of methane into the sub-grid scale combustion model.

Recently, Fire Dynamic Simulator (FDS) which is a CFD model of fire-driven fluid flow has been developed by National Institute of Standards and Technology (NIST) [11,12]. The model solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires.

Wen et al. [13] applied FDS to simulate a medium-scale methanol pool fire. They successfully predicted the mean values of temperature and axial velocity. However, some difficulty in calculating the pulsation frequency was reported. They concluded that the limitation of the computer code could have been originated from the simplified pressure treatment within FDS. Wang et al. model a series of purely buoyant fire plumes with heat release rates from 14 to 58 kW and compared the results with experiments. Their study has been done using OpenFOAM platform. The good agreements in all aspects examined of their simulation show that their CFD model performs well for small-scale fire plumes.

The aim of this paper is the use of one-equation SGS model for LES on the simulation of large-scale pool fire and compare the results with the previous Smagorinsky model and experiments. The present study is carried out using OpenFOAM [15] platform. OpenFOAM is a set of object-oriented, open source CFD toolboxes written in C++. It represents the modern point of view in CFD techniques for industrial applications, including conservative finite volume, unstructured polyhedral mesh, etc. These advanced CFD features are important for modelling large scale and complex geometry fires.

Mathematical Formulation

The fluid motion of the pool fire is considered as a low-speed flow. Also, the contribution of acoustic waves is assumed to be negligible to the flow dynamics [4]. The low-Mach-number Favre-filtered mass, momentum, energy and scalar conservation (i.e. mixture fraction) equations in a Cartesian coordinate system with turbulence model can be written as:

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j}=0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}\right)\right)-\frac{\partial}{\partial x_j}\left(\widetilde{\bar{\rho}u_iu_j}-\bar{\rho}\tilde{u}_i\tilde{u}_j\right)+\rho g_i \quad i=1,2,3 \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{h}}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_i\tilde{h})}{\partial x_j}=\overline{\frac{Dp}{Dt}}+\frac{\partial}{\partial x_j}\left(\frac{K}{C_p}\frac{\partial \tilde{h}}{\partial x_j}\right)-\frac{\partial}{\partial x_j}\left(\bar{\rho}\left(\widetilde{hu_j}-\tilde{h}\tilde{u}_j\right)\right)+q_r+q_{comb} \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{Z}}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z})}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}D\frac{\partial \tilde{Z}}{\partial x_j}\right)-\frac{\partial}{\partial x_j}\left(\bar{\rho}(\widetilde{Zu_j}-\tilde{Z}\tilde{u}_j)\right) \tag{4}$$

where ρ is the mixture density, u_i is velocity vector, p is pressure, h is sensible enthalpy and Z is mixture fraction. In equation (2), $\widetilde{\bar{\rho}u_iu_j}-\bar{\rho}\tilde{u}_i\tilde{u}_j$ is the unresolved SGS turbulence stress which arises from Favre-filtered and should be modelled using equation (5) [16].

$$\overline{\tau}_{ij,SGS} = \overline{\rho}\widetilde{u_i u_j} - \overline{\rho}\tilde{u}_i\tilde{u}_j = -2\mu_T^{SGS}\tilde{S}_{ij} + \frac{1}{3}\tau_{kk}\delta_{ij} \tag{5}$$

$$\tilde{S}_{ij} = \frac{1}{2}\left(\frac{\partial\tilde{u}_i}{\partial x_j} + \frac{\partial\tilde{u}_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial\tilde{u}_k}{\partial x_k}\delta_{ij} \tag{6}$$

$$\mu_T^{SGS} = \overline{\rho}C_S\Delta^2\left|\tilde{S}_{ij}\right| \tag{7}$$

In the above equation, Δ is the filter size, C_s is the Smagorinsky constant and $\left|\tilde{S}_{ij}\right| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$. Also, τ_{kk} may be ignored for the practical calculation [16].
The SGS enthalpy flux and scalar flux correlations are modelled in a approach similar to the SGS turbulence stresses by the standard gradient diffusion hypothesis as:

$$H_j = -\overline{\rho}(\widetilde{hu_j} - \tilde{h}\tilde{u}_j) = \frac{\mu_T^{SGS}}{\mathrm{Pr}_t}\frac{\partial\tilde{h}}{\partial x_j} \tag{8}$$

$$M_j = -\overline{\rho}(\widetilde{Zu_j} - \tilde{Z}\tilde{u}_j) = \frac{\mu_T^{SGS}}{Sc_t}\frac{\partial\tilde{Z}}{\partial x_j} \tag{9}$$

An alternative strategy to the basic SGS models is the development of a one-equation model, which uses a transport equation for the SGS kinetic energy. The SGS viscosity can be expressed in terms of the SGS kinetic energy as:

$$\mu_T^{SGS} = \overline{\rho}C\Delta\sqrt{k_{SGS}} \tag{10}$$

where the constant C = 0.069 represents a theoretically value [16]. A transport equation to determine the distribution of SGS kinetic energy accounting the effects of convection, diffusion, production, and destruction can be formulated as:

$$\frac{\partial}{\partial t}(\overline{\rho}k_{SGS}) + \frac{\partial}{\partial x_i}(\overline{\rho}\tilde{u}_i k_{SGS}) = \frac{\partial}{\partial x_i}\left(\overline{\rho}C_{\alpha k}\Delta\sqrt{k_{SGS}}\frac{\partial k_{SGS}}{\partial x_i}\right) + P_{k_{SGS}} - D_{k_{SGS}} + B_{k_{SGS}} \tag{10}$$

where $P_{k_{SGS}}$ is the regular production term, $D_{k_{SGS}}$ is the destruction term, and $B_{k_{SGS}}$ is the production due to buoyancy. The description of these terms can be found in [16].
The combustion model applies the mixture- fraction approaches using infinitely fast chemistry and single step reaction assumptions, i.e., chemical reactions are faster than the time scales for diffusion and flow. Therefore, combustion takes place as soon as fuel and oxidizer meet. The mixture fraction Z is a passive scalar defining the local fuel/oxidizer ratio as:

$$Z = \frac{sY_f - Y_o + 1}{1 + s} \tag{11}$$

where Y_f and Y_O are the mass fractions of fuel and oxidizer, respectively, and s is the stoichiometric air-fuel mass ratio. The mixture fraction 'Z' should satisfied the transport equation (4). Additionally, a similar transport equation for Y_f is solved, reading

$$\frac{\partial \bar{\rho}\tilde{Y}_f}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Y}_f)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\bar{\rho}\left(D+\frac{\nu_t}{Sc_t}\right)\frac{\partial \tilde{Y}_f}{\partial x_j}\right)+R \tag{12}$$

where R is the source term and represents the fuel consumption rate. It can be modeled by the following equation [17]:

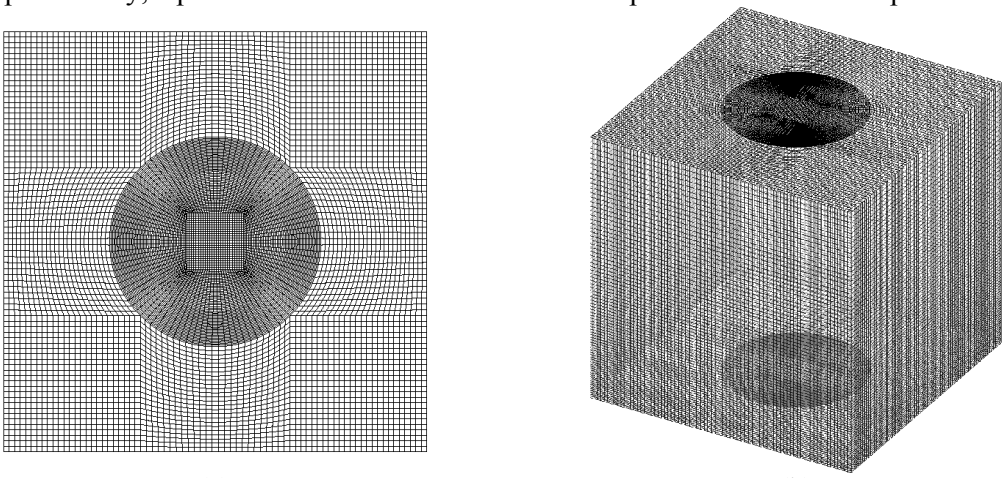
$$R=\frac{\rho}{\Delta t C_c}\min(\tilde{Y}_f,\frac{\tilde{Y}_O}{s}) \tag{13}$$

where Δt is the time step and C_c is the model constant. The combustion source term in energy equation can be found by Eq. 13:

$$q_{Comb}=-R\Delta h_C \tag{13}$$

Computational model and boundary conditions

The numerical study of a large-scale one-meter diameter methane pool fire was carried out and the results were validated by using experimental measurements of Tieszen et al. [10]. The computational domain of square cube with 3m×3m×3m length in each direction was employed for the simulation. A methane-fuelled burner with 1m diameter was placed on the center of the floor level of the domain. A methane inlet mass flow rate 0.053 kg/m^{2}s was specified which corresponds to 2.07MW heat release rate. Two non-uniform mesh distributions of 850000 and 956250 cells were utilized within the computational domain with finer grid cells around the fuel inlet for better capturing all the necessary macroscopic large-scale features of the fire. No significant difference of the predicted results was observed with these two grid resolutions. Therefore, the grid resolution with 850K cells is used for better trade-off between the accuracy and computational time. The mentioned domain is shown in Fig. 1. The traction-free boundary condition was employed for all lateral boundaries [4]. For the top boundary, a pressure inlet/outlet condition was imposed for all the transport variables.



(a) (b)

Figure 1. Computational domain of current study (a): top view (b): 3-D view

Results and discussions

The transient simulation was performed for about 60 seconds. In each time step, the Courant–Friedrichs–Lewy (CFL) number is checked at the end of the prediction step. The time step is calculated at the end of the prediction step using a CFL of 0.4.

As pointed out by Tieszen et al. [10], the pulsating behavior of pool fire, which is called puffing, has a leading effect on the fire flow field. Therefore, the puffing phenomenon corresponded to the vertical velocity is studied first. Vertical velocity at X=0 and Y=0.505 m is plotted as a function of time in Fig. 2. The results are in a good agreement with the experimental study of Tieszen et al. [10] using PIV.

The predicted time history of vertical velocity in location appears much smoother than the dispersion measurement points where a more chaotic behavior with strong fluctuation of the velocity have been observed. It is due to the nature of the LES models. Because LES uses the spatial filtered technique and only resolved large eddy motions over sub-grid length. Actually, the SGS models directly affect on the motion of eddies in sub-grid scale. Therefore, better capturing of the pulsating behavior required significant improvement of the grid resolution or even use of DNS technique. The results also compared to those by Xin et al. [18] who used FDS, which utilized Smagorinsky SGS model, for the same fire scenario. Xin et al. [18] results under-predict the maximum vertical velocity. The same conclusion can be seen in Cheung and Yeoh [4]. The current results, which are shown in Fig. 2, show better agreement with the experiments [10] than the previous study. It seems that the improvement in the modeling of sub-grid motion of eddies can be obtained using one-equation SGS model.

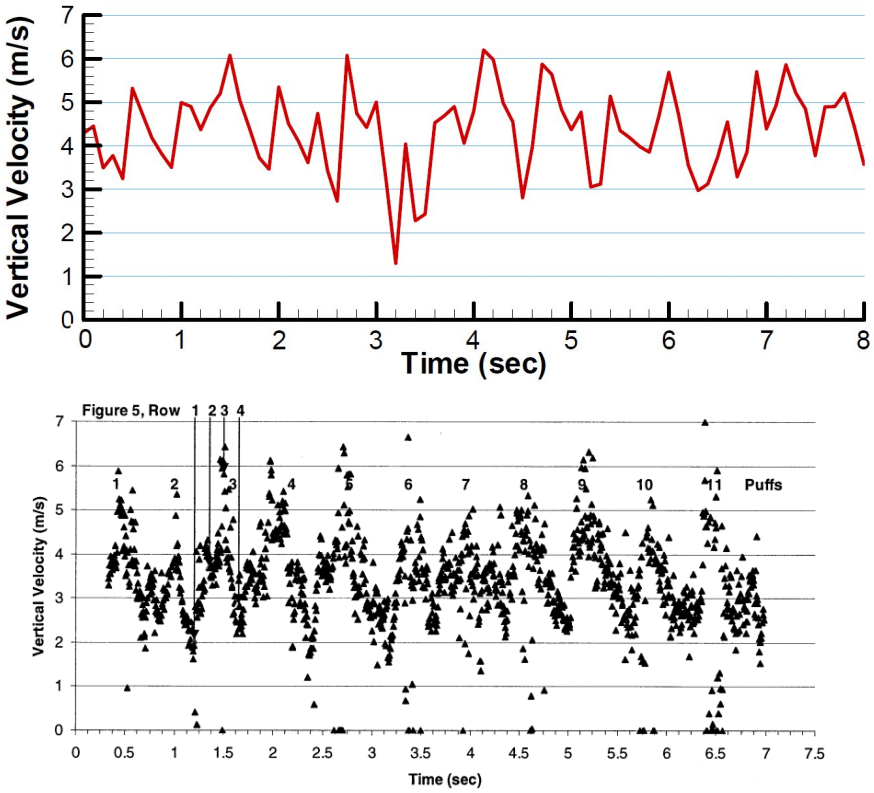
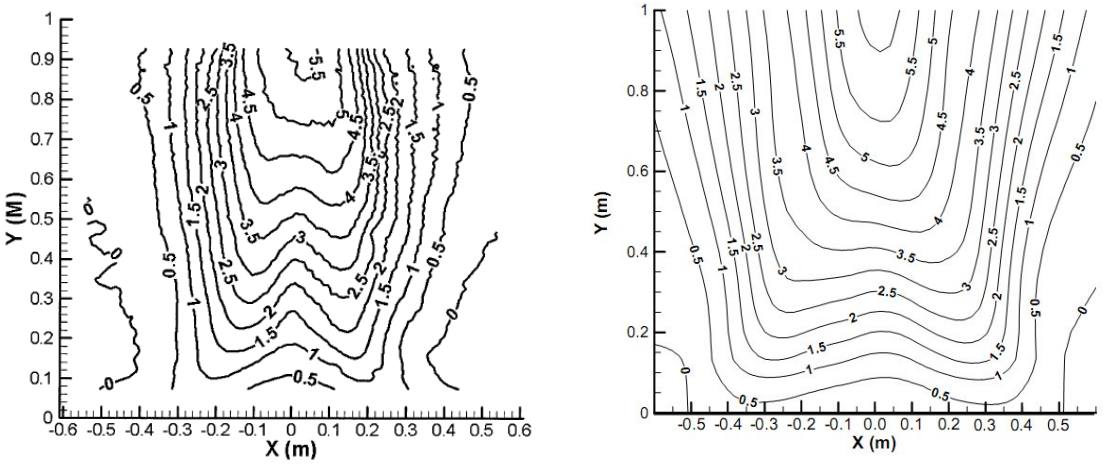


Figure 2. Calculated time history of the vertical velocity at the centre-point of fire, (a): Present work, (b): PIV, Tieszen et al [10] (X=0, Y=0.505)

For better comparison between the measured data by Tieszen et al. [10] and the present study, a quasi steady state of the solutions was obtained when the physical time arrived at 50 second. The time-averaged values of each quantity then extracted over 15 seconds on the instantaneous solutions. The comparison of time-averaged vertical and horizontal velocity contour at the center-plane of the fire regime are shown in Fig. 3. Generally, the predicted time-averaged velocity components are in a good agreement with the experiments. It can be

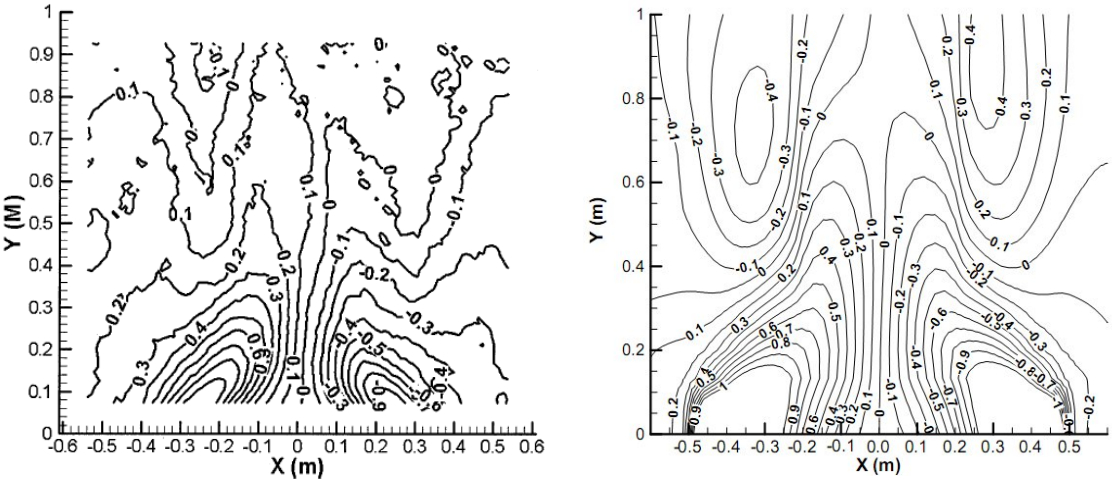
observed from Fig. 3 (a) and (b) that there is a gap between the velocity regions, which are wider in the predicted results than the measurements. Therefore, the current model slightly over-estimates the velocity spread over the fuel source.

The horizontal velocity clearly affects on the width of the fire plume (Fig. 4 (a) and (b)). An over-predicted result of the horizontal velocity can be seen in Fig. 4 (b) compared to measurements. Therefore, wider fire scenario predicted using the present model. The same numerical errors can be found in the numerical study of Cheung and Yeoh [4] and Xin et al. [18]. Insufficient grid resolution for LES model over the fuel source to better capture the microscopic eddies, assumption of infinity fast chemistry, single-step chemical reaction, and inaccurate prediction of turbulence viscosity are influenced on the turbulence-mixing rate of the flow field and the heat release rate of the fire. Due to these sources of error, imprecise results are obtained.



a ~~B~~b

Figure 3. Comparison of time-averaged vertical velocity contour captured from PIV [10] (a) and present one-equation LES model (b)

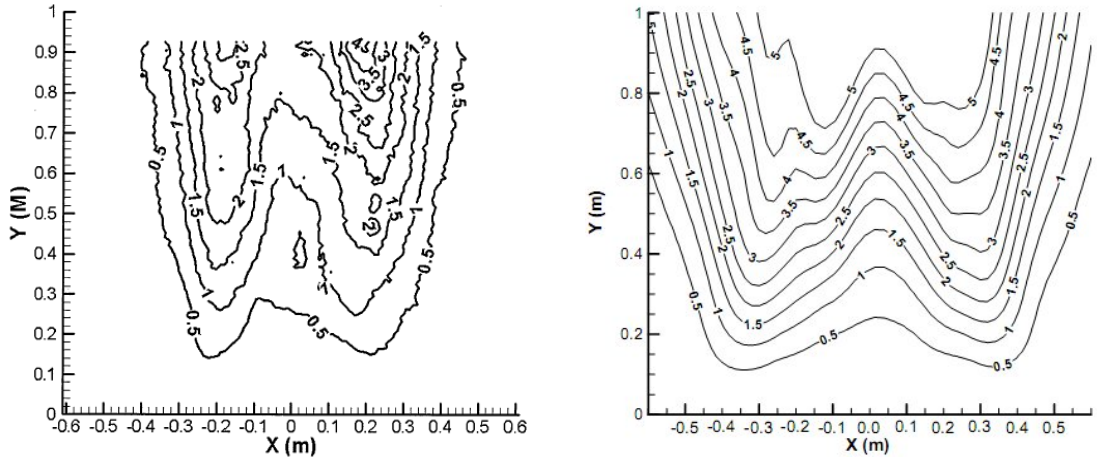


a b

Figure 4. Comparison of time-averaged horizontal velocity contour captured from PIV [10] (a) and present one-equation LES model (b)

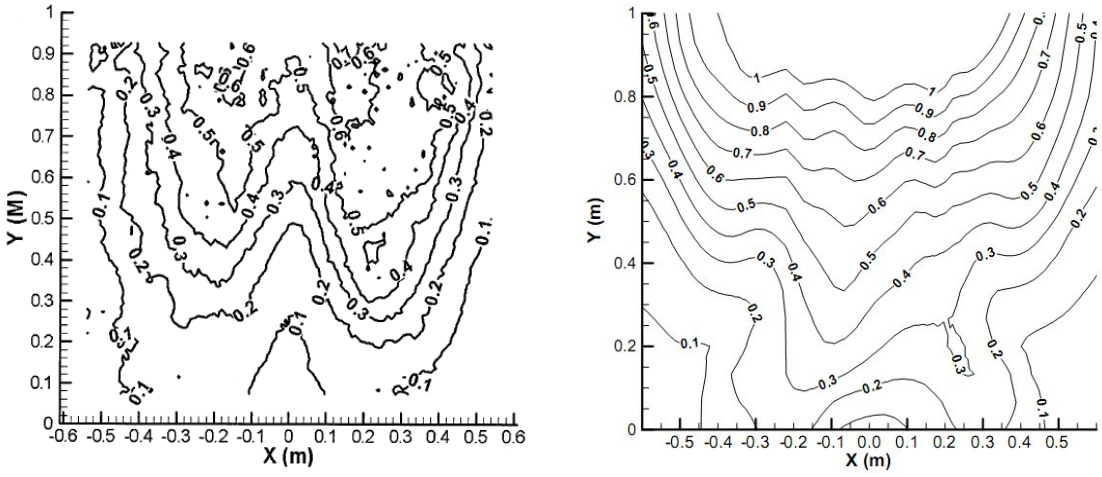
For better understanding of these effects, the predicted and measured turbulence quantities' distributions over the center-plane of the fire plume are compared in Fig. 5 and 6. As depicted, the turbulence statistics are over-estimated at the center of the fuel inlet using the

present model. Far from the fuel inlet, this over-prediction is also appeared. Xin et al. [18] evaluate the effect of the Smagorinsky constant on the turbulence fluctuation of the same fire plume. They show that the Smagorinsky constant controls the turbulence diffusion, especially when a coarse grid is selected. The same situation is also appeared in our study. For capturing better results, a comprehensive study about the effect of the constant coefficient in equation 10 on the flow field behavior or a dynamic SGS procedure is under developed by the authors.



a B

Figure 5. Comparison of time-averaged vertical velocity fluctuation ($\overline{v'^2}$) captured from PIV [10] (a) and present on-equation LES model (b)



a B

Figure 6. Comparison of time-averaged horizontal velocity fluctuation ($\overline{u'^2}$) captured from PIV [10] (a) and present on-equation LES model (b)

Unfortunately, there are no temperature measurements being ready by Tieszen et al. [10]. Therefore, the validation between numerical results and the temperature profiles are not made possible. However, we made some instantaneous iso-surface of temperature of the predicted results in Fig. 7. These instantaneous iso-surfaces show a period of puffing cycle. At the beginning of the puffing cycle, a vortex is generated near the fire source (Fig. 7(a)). The air enters into reaction zone due to the assistant of vortex motion (Fig. 7(b)). This entrainment of the air creates high local temperature around the fire plume. In addition, the vortex moves upward concerning buoyancy force, which is generated by high local temperature (Fig.

7(c),(d)). Therefore, a neck-shape body is made by the motion of the vortex. This neck-shape body makes a low-pressure region and pushes the vortex upward.

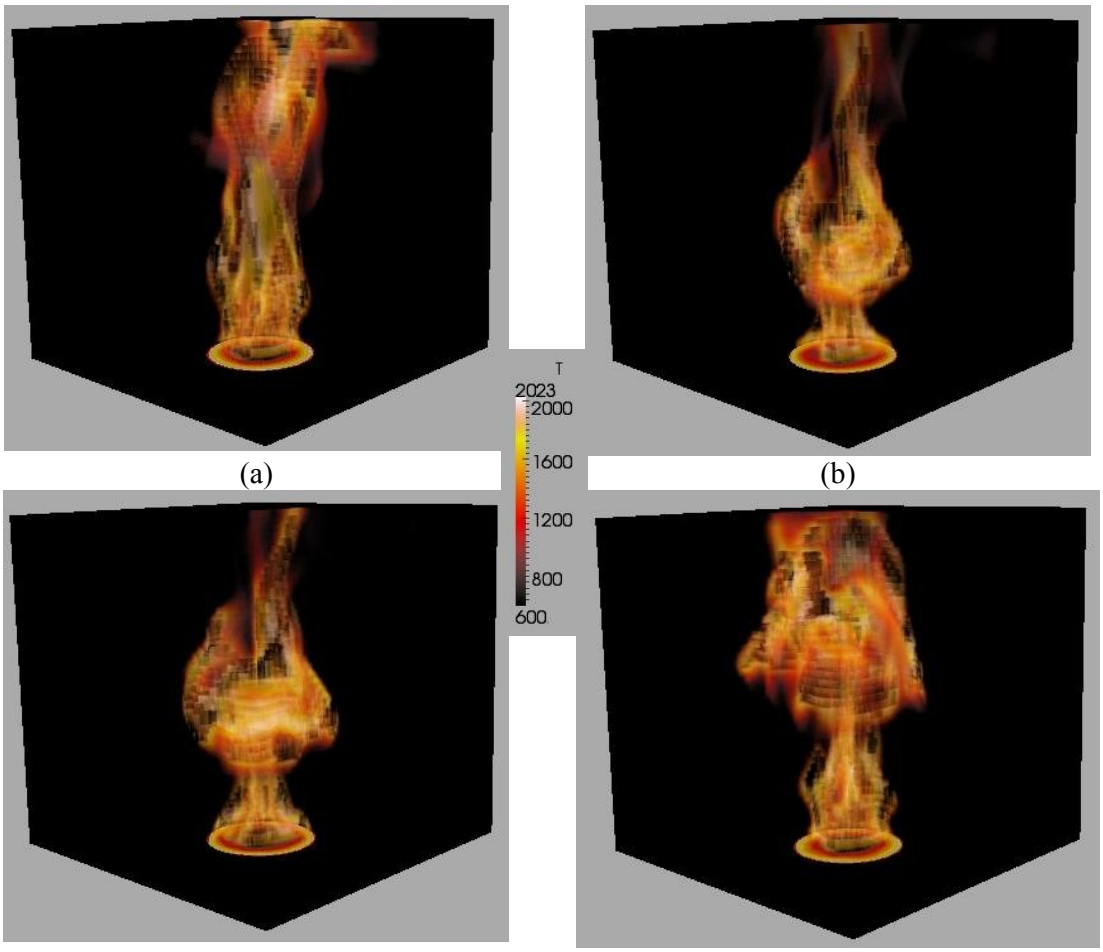


Figure 7. Instantaneous iso-surface temperature by present study with one-equation SGS model

Conclusion

Fully-coupled large eddy simulation of flow field structures for a one-meter buoyant methane pool fire has been done using a one-equation SGS turbulence model. For accounting combustion, the mixture fraction approach and infinity fast chemistry assumption is considered. The predicted velocity profile and turbulence characteristics are in good agreement with experimental measurements. An improvement to velocity time history profile has been obtained compared to previous numerical study, which incorporate Smagorinsky SGS model. In addition, over-predicted values for the time-averaged turbulence velocity fluctuations are computed by the current model, which mainly related to SGS model, coarse grid over the fuel inlet, single-step reaction and infinity fast chemistry assumption. Finally, the puffing cycle is evaluated by the motion of vortex regarding iso-surface temperature profiles.

Nomenclature

C Constant Coefficient

C_p Thermal capacity

D Diffusion Coefficient
h sensible enthalpy
H SGS enthalpy flux
k Turbulence kinetic
K conductivity
M SGS scalar flux
p Pressure
Pr Prandtl number
R Source term
q Heat value
s stoichiometric air-fuel mass ratio
Sc Schmidt number
t Time
u Velocity
Y Mass fraction
Z Mixture fraction
ρ Mixture density
μ Viscosity

Superscripts

com combustion
f fuel
i Coordinate direction
j Coordinate direction
o Oxidizer
r radiation
SGS Sub-grid scale
t Turbulence properties

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