Modelling of temporal combustion behaviour in a large-scale buoyant pool fire with detailed chemistry consideration

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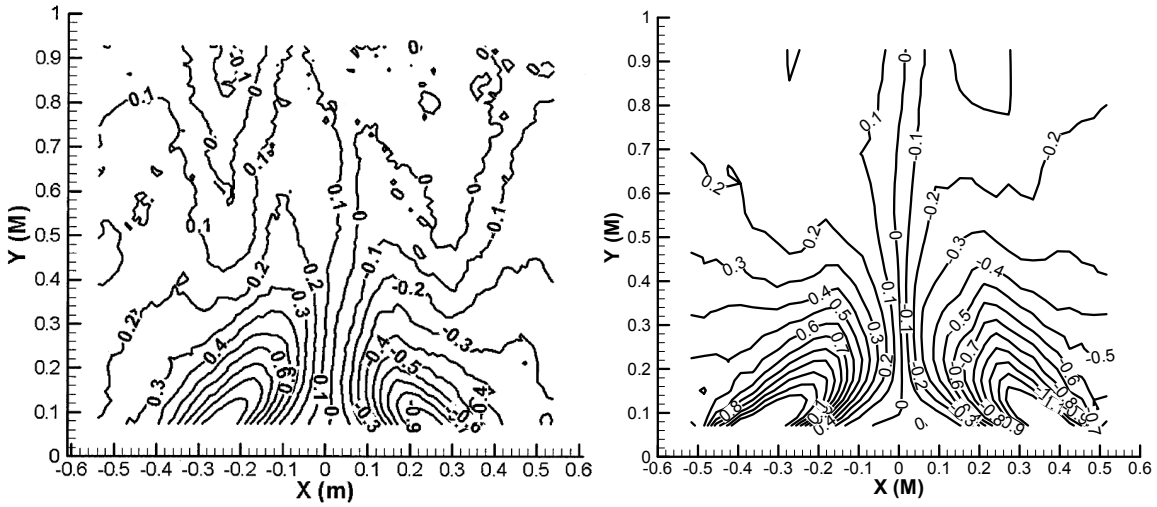
Abstract: Accurate prediction of the consequence of fire is crucial for fire safety analysis and assessment of designs for fire protection measures. Based on the previous study, a fully-coupled large Eddy simulation (LES) has been carried out to simulate the temporal combustion behavior of a large-scale buoyant pool fire. Although the pulsation effect of fire was properly captured, a single chemical reaction was adopted which could pose inappropriate interpretation of instantaneous heat release rate and vorticity generation. Combustion of fire involves hundreds of chemical reactions where the embedded kinetics plays a predominant role of the resultant heat release rate and species concentrations. Due to its complexity and intensive computational requirement, combustion kinetics simulations were used to be limited for combustion in laboratory scale. Most the existing fire models (e.g. Fire Dynamics Simulator – FDS) therefore only consider one or just few chemical reactions in simulation. With advancement of computer technology, integrating kinetics in fire modelling has become feasible. To investigate the influence of chemical kinetics on the vortical structures of fire, a LES model coupled with detailed chemical kinetics has been developed based on laminar flamelet approach. The flamelet library was evaluated based on the chemical mechanism for C1-C2 hydrocarbons combustion with soot formation. Numerical predictions are then compared and validated against previous numerical predictions and experimental data. Based on the preliminary results, the predicted time-averaged velocity and temperature profile has been found to be in good agreement with the experimental data whilst the temporal fluctuation of temperature and velocity are better captured in comparison to previous results with single step reaction.



Comparison of time-averaged horizontal velocity contour captured from PIV measurement of Tieszen et al. (2002) (left) and the present LES model (right) at the centre-plane of the fire

Keywords: *Large eddy simulation, Buoyant pool fire, turbulent combustion*

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1. INTRODUCTION

In the past decades, with the rapid advancement of computing hardware, research studies on fire using numerical modelling techniques have received considerable attention among researchers. One of the great advantages of fire modeling is its capability in capture the fire behavior and its associated smoke and generation of other toxic gases. This allows fire engineers to carry out fire safety assessment and design of an appropriate fire protection system without substantial cost for fire testing in scaled or on-site measurements. Therefore, accurate prediction of the consequences of fire; specifically the spread of smoke, transient temperature distribution and its associated velocity field, is particularly crucial. Nevertheless, fire dynamics generally involves numerous tightly coupled phenomena associated with convective and diffusive process, buoyancy and entrainment induced fluid motion, turbulent mixing of chemical species and chemical combustion processes where in-depth understanding is yet to be fully attained (Drysdale, 1999). Aiming to investigate the complex chemico-physical phenomena in practical fire, this paper presents a numerical study on the temporal combustion behaviour of a large-scale buoyant pool fire where air flow structure and the fire behavior is dominant by the buoyancy force.

Based on previous experimental and numerical studies, it is well know that a buoyant pool fire usually exhibits a unique periodic oscillatory motion close to their origin. Such temporal fluctuation of temperature and velocity is referred as "puffing" or pulsation behaviour (Bryan and Nelson, 1970; Portsche, 1975 and McCaffrey, 1983). Tieszen et al. (1996) identified three mechanisms primarily responsible for the vortical structures in fire as depicted in Figure 1.

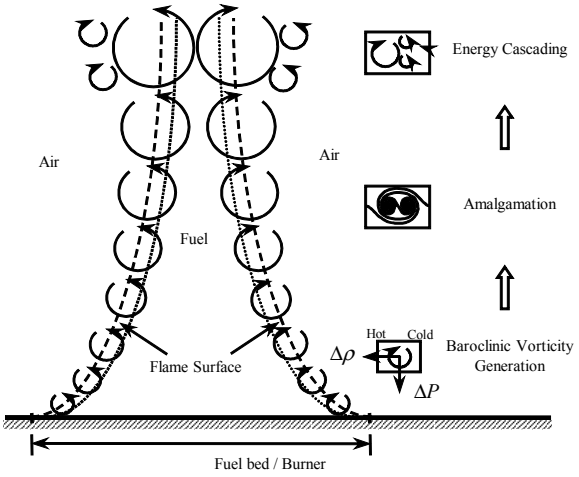

Figure 1. A schematic of the mechanisms contribute to the three stages of vortical structure development.

As depicted, small-scale vorticity is generated near the fuel bed by the baroclinic vorticity generation. This vorticity gradually becomes larger-scale through amalgamation until it finally collapses due to turbulent energy cascading. Apparently, the vortical structures of fire can be generated in a wide range of length scales where exothermic combustion, fluid motions and the spatial distribution of density and pressure occur in highly non-linear unsteady conditions. It is envisioned that chemical reactions in the fire could be subjected to highly fuel rich conditions where various intermediate species could be generated. To properly resolve aforementioned chemico-physical phenomenon, this paper presents our preliminary numerical results in attempting to incorporate detailed chemistry considerations into our LES fire model.

2. NUMERICAL METHODOLOGY

2.1. Mathematical Framework

Following our previous study (Cheung and Yeoh, 2009), the low-Mach-number Favre-filtered mass, momentum, energy and scalar conservation equations in a Cartesian coordinate frame were adopted governing equations (Knio et al., 1999). The filtered viscous stress tensor, species diffusion vector and heat flux vector in terms of resolved quantities are modelled according to Newton's, Fick's, and Fourier's laws (Warrantz, 1996). A value of 0.7 is applied to the molecular Prandtl number, the molecular Schmidt numbers for mixture fraction and its variance; while the Schmidt numbers for soot quantities according to Sivathanu

and Gore (1994) are set to 700. The SGS momentum stress is modelled according to the Smagorinsky-Lilly formulation (Smagorinsky, 1963).

2.2. Detailed Combustion Modelling

For the combustion, detailed chemical mechanism – GRI-Mech 3.0 is adopted to resolve the laminar flamelet of fuel combustion. GRI-Mech 3.0 is an optimized detailed chemical reaction mechanism tailored to handle chemical reaction processes for C1-C2 hydrocarbon fuels with soot formation consideration. The mechanism consists of 325 elementary chemical reactions with associated rate coefficient expressions and thermo chemical parameters for the 53 species. Based on the mechanism, a flamelet library with a range of scalar dissipation was construction using the commercial chemistry simulation package - CHEMKIN. The main role of a SGS reaction model for turbulent non-premixed combustion is designed to incorporate the effect of subgrid fluctuations in the thermo-chemical variables on the filtered chemical source term. On the basis of the mixture fraction-based approach, all the species mass fractions can be taken to be functions of only the mixture fraction. Using this assumption, Bilger (1977) derived the expression for the rate of reaction for the *i*th species, which can also be found in Kuo (1986) see Eqn. (1) The instantaneous heat release rate is determined for *N* species from Eqn. (2).

$$\omega_i = -\frac{1}{2}\rho\chi\frac{d^2Y_i}{dZ^2}, \text{ where } \chi \text{ is the instantaneous scalar dissipation.} \quad (1)$$

$$\omega_T = -\sum_{i=1}^{N} h_{fi}^{o}\omega_i \text{ where } h_{fi}^{o} \text{ is the } i\text{th species standard heat of formation} \quad (2)$$

where ρ, Y_i and Z are the density of air, mass fraction of *i*th species and mixture fraction respectively. In LES, the flame is typically not spatially resolved by the computational grid. It is assumed that at the subgrid level there exists a statistical ensemble of laminar diffusion flamelets each satisfying universal state relationships. Under near-equilibrium conditions, the state relationships could be represented such as those of equilibrium chemistry assumption or experimental state relationships established by Sivathanu and Faeth (1990). In order to predict highly non-equilibrium flame events such as lift-off or extinction, the state relationships need to be modified by the consideration of the scalar dissipation and to distinguish between burning and extinguished flamelets – the strained laminar flamelet approach. More details regarding the SGS reaction model can be found in our previous work Cheung and Yeoh (2009).

2.3. Soot formation and radiation modelling

The two-equation semi-empirical soot model by Moss et al. (1988) that incorporates the essential physical processes of soot nucleation, coagulation and surface growth is adopted. The Nagle and Strickland-Constable rate (1962) for soot oxidation is adopted as the limiting mechanism for oxidation by O_2. Luminous thermal radiation from combustion products and soot is treated by solving the filtered radiative transfer equations (FRTE) for a non-scattering grey gas using the Discrete Ordinates Method (DOM) with S4 quadrature scheme. The filtered gas absorption coefficient for the combustion products (CO_2 and H_2O) as well as the unburnt methane fuel can be approximated by the Weighted Sum of Gray Gases Model (WSGGM) according to Beer, Foster and Siddall (1971).

2.4. Numerical details

Similar to our previous study Cheung and Yeoh (2009), the finite volume method is employed to discretize the above filtered governing equations on a collocated gird. Second-order central differencing is adopted for all spatial derivatives approximations. The advancement of the solution in time is achieved numerically by using the predictor-corrector approach. Numerical simulation was conducted of a 1-m diameter methane pool fire experiment of Tieszen et al. (2002). A cubic computational domain of 3 m length was employed for the simulation. A methane fuelled burner with 1m diameter was centrally placed on the floor level of the domain. A methane inlet velocity of 9.7cm/s was specified at the burner corresponding to a fire of 2.07MW heat release rate measured in the experiment. For the heat release considered in this investigation, the characteristic length of the pool fire is approximately of the order of 1.3m and thus a non-uniform Cartesian mesh of 96^3 control volumes was generated within the domain. Finer grid cells with the minimum spacing of 1.4 cm were generated above the burner to better capture all the finer-scale features of the vortical flame structure. The traction-free boundary condition was employed for all lateral boundaries. For the top boundary, a zero gradient condition was imposed for all the transport variables. To prevent flow entering the

domain from its top, which might incur numerical instabilities, velocities with negative values were forced to zero.

3. RESULTS AND DISCUSSIONS

3.1. Velocity distribution

A quasi-steady state solution was obtained when the physical time arrived at 30s. Time-averaged field quantities were then extracted by performing time-weighted averaging calculation over 8s of instantaneous solutions. Figure 2 illustrates the predicted and measured time-averaged vertical velocity profiles at different centre-line locations (i.e. Y=0.2, 0.4 and 0.6m) above the methane burner. In general, the predicted velocity profiles agreed reasonably well with the measurement. Especially at the location Y=0.6m, the maximum error of prediction is 18% which is within the ±20% uncertainly bounds of the measurements. On the other hand, noticeable discrepancies were observed at the vicinity of burner surface (i.e. Y=0.2). As illustrated in the figures, the distance between two velocity peaks was considerably over-predicted. Meanwhile, vertical velocities at the fire centre were also under-predicted. This indicates that the temperature and chemical reaction rate at the location could be under-estimated.

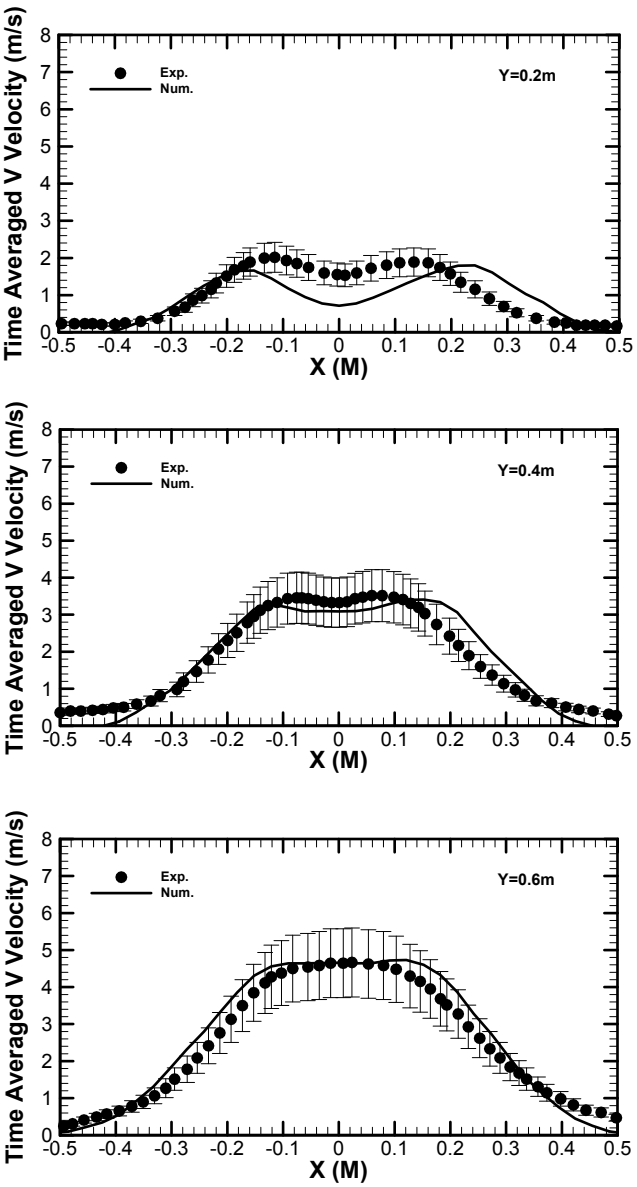

Figure 2. Predicted and measured time-averaged vertical velocity at different centre-line locations: (top) Y=0.2m; (middle) Y=0.4m and (bottom) Y=0.6m.

Aiming to compare our predictions thoroughly with the measurements, a more comprehensive depiction can be seen in Figure 3, where time-averaged horizontal and vertical velocity contour plots were compared with measured results. In general, the predicted time-averaged velocity contours are in good agreement with the measurements. As depicted, due to air entrainment, horizontal velocities in both directions meet at the center fire bed; forming two high velocity regions at the lower level. In between these two regions the horizontal velocity component is nearly zero; appearing as a gap in the figure. In comparison to the measurement, the predicted gap between two velocity regions has been slightly over-predicted. Such error could be attributed to the insufficient grid resolution for LES models to resolve the microscopic baroclinic vorticity generation near the burner surface. As this mechanism was observed to be responsible for the sequential up-scale turbulent energy transfer to large scale eddies, filtering of these small-scale turbulent motions by the LES models might cause under-prediction of the local turbulent mixing rate resulting in an inaccurate estimation of the local heat release, combustion and velocity spread rates. On the other hand, compared to our previous study (Cheung and Yeoh, 2009), noticeable improvements were found in the exiting numerical result. As single step chemistry and same numerical mesh were adopted in previous study, this shows that the inclusion of detailed chemistry resulted in considerable improvement in capturing the non-equilibrium combustion processes; especially near the fire bed where fuel rich conditions were likely.

For the vertical velocity contour, as shown in the figure, our model has successfully captured the overall distribution. Nonetheless, the width of the velocity plume is slightly over-predicted. Again, this could be caused by the prediction error of the horizontal velocity.

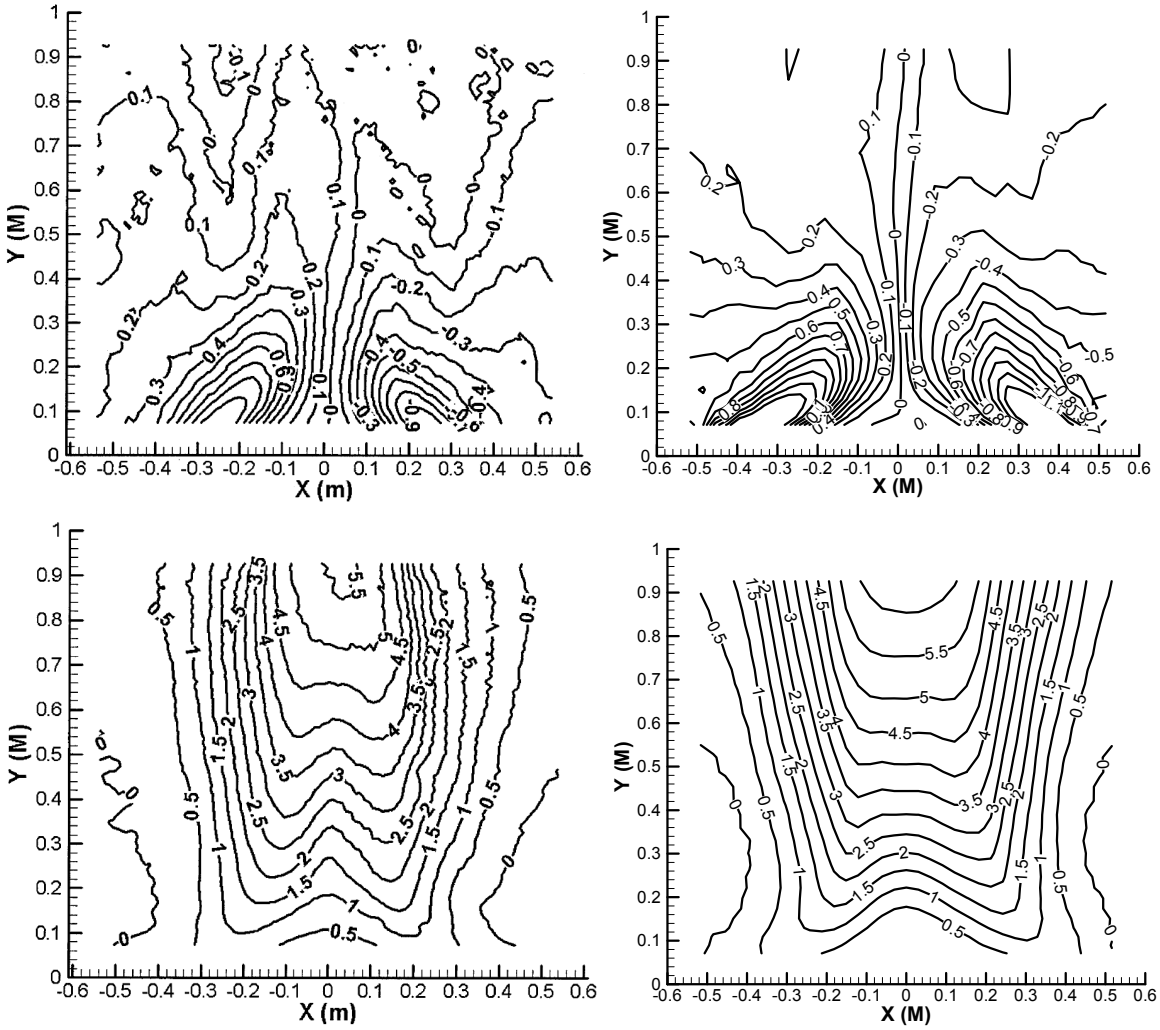

Figure 3. Comparison of time-averaged velocity component contours captured from PIV measurement of Tieszen et al. (2002) (left) and the present LES model (right) at the centre-plane of the fire: (a) U velocity (horizontal) and (b) V velocity (vertical).

3.2. Instantaneous temperature and velocity distribution

Figure 4 shows the instantaneous velocity field at the centre plane of the fire plume captured by the PIV measurement of Tieszen et al. (1996) and the present LES model. The three sequential PIV results on the left column clearly illustrate the relationship between large vortical structures (as pointed in the figure) and the puffing cycle. At the start of the cycle, turbulent eddies were firstly stemmed from the base of the fire which has been caused by baroclinic vorticity generation. Owing to the amalgamation of eddies and buoyancy forces, the size of vortical structures continuously increased and accelerated in vertical direction until it has been advected out of the image. A broad overview of the figure suggested that the predicted instantaneous velocity fields were in excellent agreement with the PIV measurements.

Velocity vectors of predicted results also exhibited similar behaviour / distribution to the experimental data. Special attention was paid to the simulated vortical structures at both sides of the fire. As depicted in the figure, the vortical structures were successfully captured by the present model. From the start to the end of puffing cycle, the simulated vortical structures were created at the fire base and continuously developed in size and convected upward away through the top of plot. The above development of the vortices was clearly aligned with the observations of PIV measurements. Vortex locations of the numerical results were also comparable to the measurement.

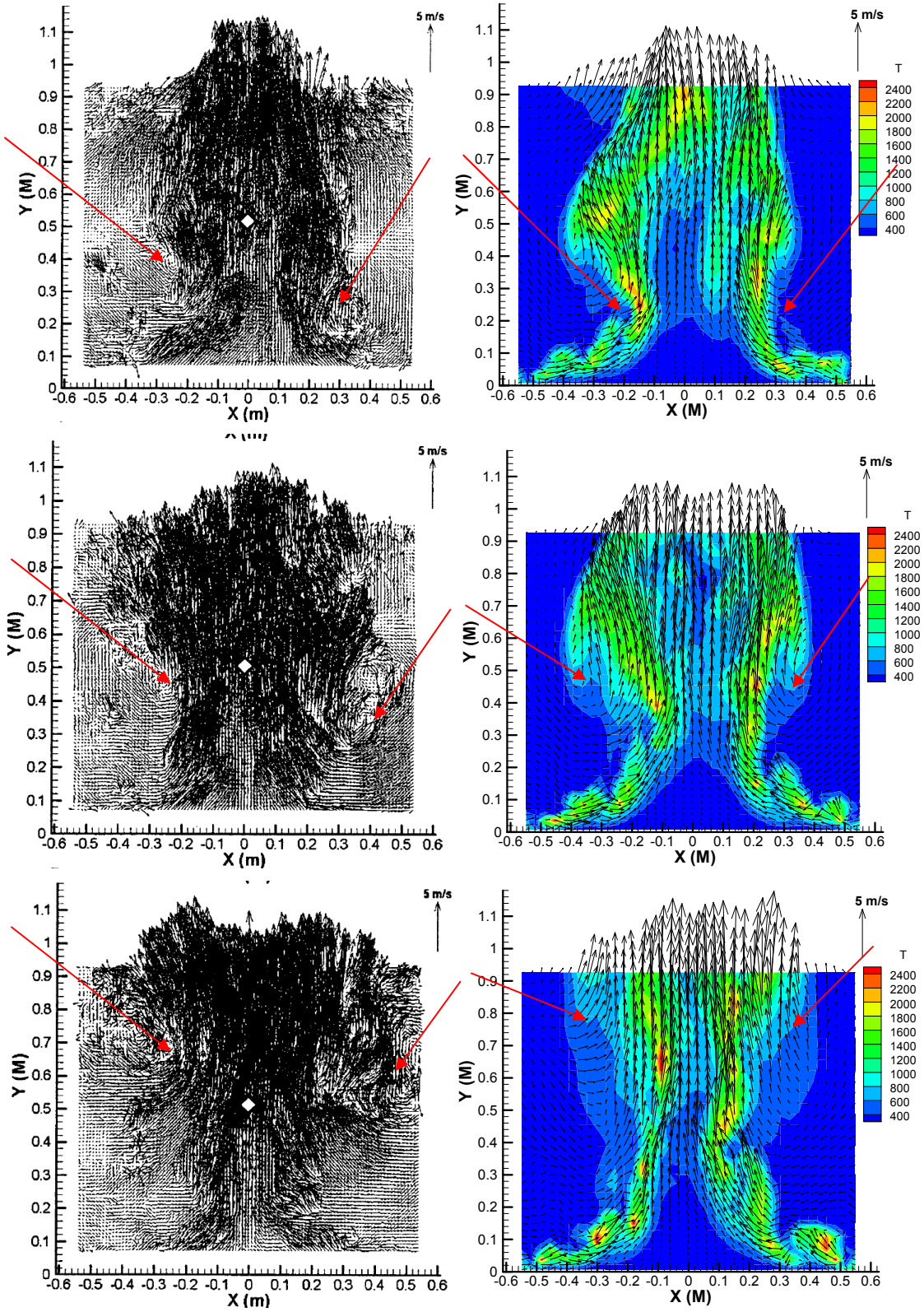

Figure 4. Three instantaneous temperature and velocity field at the centre plane of the fire plume captured by PIV measurement of Tieszen et al. (1996) (left) and the present LES model (right): (top) start; (middle) 1/4 and (bottom) 2/4 of puffing cycle.

4. CONCLUSION

A numerical study has been carried out to simulate the combustion of a large scale buoyant pool fire using a LES model including detailed chemistry and other essential radiation and soot formation considerations. Based on the presented preliminary results, the predicted time-averaged velocity and temperature profiles from the present model were in good agreement in comparison to experimental data. Noticeable prediction improvements were also found in comparison to our previous numerical results with only single step chemical reaction. Quantitative validations of the instantaneous velocity distribution were also presented with excellent agreement with experimental data. The encouraging results have demonstrated the great potential of the present model with detailed chemistry consideration. For future work, it is worthwhile to investigate if the detailed chemical kinetics could be replaced by with 2 or 3 thermally dominant lumped reaction steps.

ACKNOWLEDGMENTS

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