### Large Eddy Simulations of Pool Fires at different Cross-Wind Velocities with a Large Adjacent Object

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## Introduction

The present investigation is focused on Large Eddy Simulation (LES) of a liquid-fuelled fire in the vicinity of a large object in a crosswind. Both experimental and computational configurations are intended to reproduce the scenario of an aviation fuel spill fire that occurs close to a plane fuselage. In LES, the large turbulent flow structures are fully resolved and only the dissipation scales require modelling. Flow in the plume region is associated with the large scale structures, and motion of the large eddies are expected to make the most significant contributions to the transport of heat, radiation, chemical species and soot (Novozhilov, 2001). Thus, LES may be able to offer higher levels of accuracy than Reynolds-averaged techniques in simulating the fire behaviour. Recent calculations using LES for different conditions (McGrattan et al., 1998; Desjardin et al., 1999) also show some encouraging results; however there is still a significant degree of modelling required in LES. This is related to the closure of the subgrid Reynolds stress and combustion models which require information at the molecular level. Use of LES for three-dimensional and unsteady fire problems also implies a significant increase in computational run time compared to Reynolds Averaged techniques. The aim of the present study is to investigate the capabilities of an LES code for three dimensional and time-dependent calculations of fire behaviour in the fuel spill scenario outlined above. Modelling issues are also identified in order to initiate further developments in the code, for this application. The computational domain and boundary conditions are defined according to the experimental configuration used in tests run by the Fire Research Group at the University of Waterloo. This setup consists of a 2-m-diameter pool fire fuelled with kerosene and located 1-m-upstream of a 2.7-m-diameter culvert in a large enclosure. Crosswind velocities ranging from 4 m/s to 13 m/s are imposed on the fire and culvert. At the initial stage of our study (Devaud et al., 2004), time-averaged temperatures and velocities were compared with experimental data for a cross-wind velocity of 13 m/s. The computational results showed reasonable agreement. However, these first results indicated some sensitivity of the simulations to the size of the enclosure modelled, the input wind profiles and the details of the computational grid. In this work these issues have been addressed. New results for different fire scenarios with various cross-wind velocities are presented and compared to the experimental data for the corresponding conditions.

# Computational details

The LES code used in this study is Fire Dynamics Simulator (FDS) made available through NIST (McGrattan et al., 2004). FDS solves the filtered Navier Stokes equations valid for low-speed, buoyancy-driven flows. Large variations in density, but not in pressure, are allowed. The transport equations are discretized in space using second-order central differences and in time using an explicit, second-order, predictor-corrector scheme. The parallel version of the

code is used to run the simulations on several processors and information is passed between the processors through the Message Passing Interface (MPI) program. The unresolved subgrid Reynolds stress is modelled using a standard Smagorinsky model (Smagorinsky, 1963), i.e.

$$\mu_{sgs} = \rho \ C_s^{\ 2} \ \Delta^2 |S| \tag{1}$$

where  $\mu_{sgs}$  is the subgrid scale eddy viscosity, |S| is the rate of strain,  $C_s$  is the Smagorinsky constant,  $\rho$  the density,  $\Delta$  the filter width defined as  $(\Delta_x \ \Delta_y \ \Delta_z)^{1/3}$ ,  $\Delta_x$ ,  $\Delta_y$  and  $\Delta_z$  the grid spacing in x, y, and z directions respectively. The subgrid diffusivity,  $D_{sgs}$  is related to  $\mu_{sgs}$ by

$$D_{sgs} = \frac{1}{\rho} \frac{\mu_{sgs}}{Sc},\tag{2}$$

where Sc is the subgrid Schmidt number. Throughout these simulations unless specified otherwise  $C_s$  and Sc are kept constant and equal to 0.2 and 0.5 respectively (McGrattan et al., 2004).

A reaction model must be incorporated into the code to calculate the species concentrations and temperatures. In FDS, the chemistry is assumed to be very fast so that chemical time scales are much smaller than any turbulence scales. The conserved scalar, mixture fraction is used in order to tabulate major species concentrations based on a flamelet approach (Peters, 1984). A simplified one-step ideal mechanism is employed and concentrations of fuel, oxygen, nitrogen,  $CO_2$ ,  $H_2O$ , CO and soot are calculated based on a linear relationship with mixture fraction. Kerosene is used as the fuel. The heat release is calculated based on the consumption of oxygen. Constant CO and soot yields are set equal to 0.012 and 0.042 respectively (McGrattan et al., 2004). Given the finite-rate kinetics for CO and soot formation use of a direct relationship between mixture fraction and CO-soot concentration is questionable; for simplicity, these assumptions are used here. Finally the effect of radiation is included by setting a constant radiative fraction heat loss to 0.4 based on preliminary calculations using the radiative transport equation.

The computational domain and flow configuration are shown in Fig.1. The domain has dimensions of 18.0 m x 15 m x 12.80 m and reproduces the configuration of the experimental test enclosure (Lam , 2004). The 2-m-diameter pool is approximated by a series of rectangular blocks which follow the round contour of the pool. The pool is located 5 m downstream of the wind inlet which has dimensions of 7.8 m x 5.6 m. The large object is a 2.7-m-diameter cylinder with a length of 11 m. It is placed 1m downstream of the pool edge as it was in the experiments. The exit door has dimensions of 7.8 m x 7.2 m. The roof starts at z=7.4 m and peaks up to z=12.80 m. It should be noted that the floor is raised by 0.10 m and the pool surface is located at z=0.2 m but the edges around the pool are at z=0.3 m, to plausibly mimic the lip effect that occurred during the fire tests. Based on the experimental velocity profiles measured for the cross-wind (Weisinger, 2004), a "plug flow" is set at the wind inlet. Several values of cross-wind velocities are tested: 4.4, 6.2, 9.0 and 13 m/s.

Previous calculations (Devaud et al., 2004) used two different non-uniform computational grids with filter widths ranging from 0.147 to 0.178 m and the results showed that the time-averaged temperature profiles were grid-dependent. Here, the grid is significantly refined and is uniform in all directions; therefore avoiding any problem of permutation for the Fourier transforms in the code. The filter width is 0.1 m, which produces a grid of  $3.456 \times 10^6$  cells. The calculations are run in parallel on 3 Xeon 3.0 GHz processors. This is accomplished using 3 meshes, each of which is defined with the boundaries as far as possible from the reaction zone. Due to the improved grid resolution, the computational domain also includes more



Figure 1: Computational domain

detail such as the culvert supports, the calorimeters and the cable box, which were present during the experiments and can represent significant obstacles to the fire development.

# (a) Simulated Temperature contours at y=0 (a) Simulated Temperature contours at y=0

# Results

Figure 2: Instantaneous profiles for a cross-wind of 9 m/s

Simulations of fire behaviour were run for 200 s test time. Each such simulation takes approximately 175 CPU hours. Due to these long run-times, results are concentrated on cross-wind velocities of 9 m/s and 13 m/s. Relative to the buoyant acceleration of the fire plume, the simulations qualitatively reproduce the experimental observations (Fig.2). Due to the strong cross-wind the fire is tilted well underneath the culvert. Maximum temperatures are expected to occur close to the floor. Fig.3 shows the vertical profile of the experimental and simulated time-averaged temperatures at y = 0, x = 7.0 m and at t =138 s for a cross-wind velocity of 9 m/s. Quantitatively, the peak of the time-averaged temperatures closely match the experimental values (both magnitude and location) but the vertical spreading rate (z direction) is underpredicted. At heights above 1-1.5 m above the floor the experiments indicate temperatures on the order of 200C whereas the simulations show temperatures around 20C because the numerical predictions decrease more rapidly with height above the floor. Much as has been noted in application of  $k - \epsilon$  models to fire plume predictions, this would suggest that the turbulent mixing is not accurately captured. In LES, several modelling constants



Figure 3: Time-averaged temperature profiles at x=7.0 m and y=0.0

are also empirically determined and may be tuned on a case by case basis. In this example, the Smagorinsky constant was increased to 0.3. The temperature profiles are also in Fig.3. Clearly this change did not improve the model predictions and resulted in overpredicting both the magnitude and location of the peak in the fire. Therefore, further investigation of the influence of these other parameters is currently underway. This should lead to increased understanding of these constants in LES models of fire development and optimization of the methods for future application.

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