INTER-COMPARISON AND VALIDATION OF RANS AND LES COMPUTATIONAL APPROACHES FOR ATMOSPHERIC DISPERSION AROUND A CUBIC OBSTACLE

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INTRODUCTION

A comparative study between two different computational fluid dynamics approaches is presented for the flow case of atmospheric dispersion of a passive gas release around a ground-based cubical obstacle. Open field experimental data have been used as a validation reference for the simulations. The computational simulations have been performed using a) the widely applied Reynolds-Averaged Navier-Stokes (RANS) approach using a *k-l* turbulence model of the code ADREA-HF and b) Large Eddy Simulation (LES) using the classical Smagorinsky turbulence model. The purpose of this study is to compare the performance of the two well-established modelling approaches in describing flow and dispersion in relatively complex conditions as a first step, with the perspective of their application in more realistic urban configurations. The comparison concerns flow characteristics, as the dimensions of the recirculation zone, dispersion characteristics, as the plume lateral dimensions and the peak concentrations, as well as the use of computer resources. Regarding dispersion, both average concentrations and standard deviations of concentrations are calculated by the models and inter-compared.

MODELS AND METHODS

Description of models

The details of the numerical procedures used in the LES approach for the present study can be found in *Grigoriadis et al.* (2003, 2004). The full set of the Navier-Stokes equations are solved for an incompressible fluid. The solution of the derived Poisson's equation is achieved by a direct pressure solver which is using an efficient combination of FFT's and cycling reductions. The direct solver has been combined with *the immersed boundary method* (*Grigoriadis et al.* 2003), so that geometrically complicated domains can be treated. Time advancement was based on the second order Adams-Bashforth scheme, with a variable time step which is dynamically computed according to the convection (CFL) and viscous time scale (VSL) criteria: CFL<0.2 and VSL<0.05. The implemented solution strategies lead to performances of the order of 0.9μs/node/time-step on personal computers (Linux, Intel Xeon@3.6 GHz).

For the RANS approach the computational fluid dynamics code ADREA-HF, developed by the Environmental Research Laboratory, has been used for the simulations presented in this article. The purpose of ADREA-HF is to simulate the dispersion of buoyant or passive pollutants over complex geometries. ADREA-HF is a finite volumes code that solves the Reynolds-averaged equations for the mixture mass, momentum, energy, pollutant mass fraction and the variance of the pollutant mass fraction. Turbulence closure is obtained through the eddy viscosity concept, which is calculated by a 1-equation *k-l* model. The turbulent kinetic energy *k* is calculated by a transport equation. The effective length scale *l* depends on the flow stability and on the distance from solid boundaries, so in the general case it is three-dimensional. For the simulations presented in this article, a uniform length scale approach has been adopted, taking into account the shortest distance from the solid boundary. For the pollutant concentration variance, a three-dimensional transport equation is also solved. Details on the modelling approach regarding the concentration variance are included in *Andronopoulos et al.* (2002).

Experimental configuration and computational simulations

The field experiments are described in detail by *Mavroidis, I. and R.F. Griffiths* (2000) and *Mavroidis et al.* (2003). In the trials simulated here a cubical model building (H=1.15m) was positioned normal to the mean wind direction. The surrounding terrain was flat and the atmospheric conditions were neutral (Pasquill category D). The tracer gas (ammonia in the present cases) was released from a point source, at a distance 2H upwind of the building, at a height 0.5H, pointing towards the building. The gas detectors were positioned downwind of the building (Figure 1). Three cases have been selected for the present simulations: Case E03, with the gas source located at the building centreline and Cases E04 and E10, with the source located H/2 and H off the centreline in the lateral direction (Figure 1).

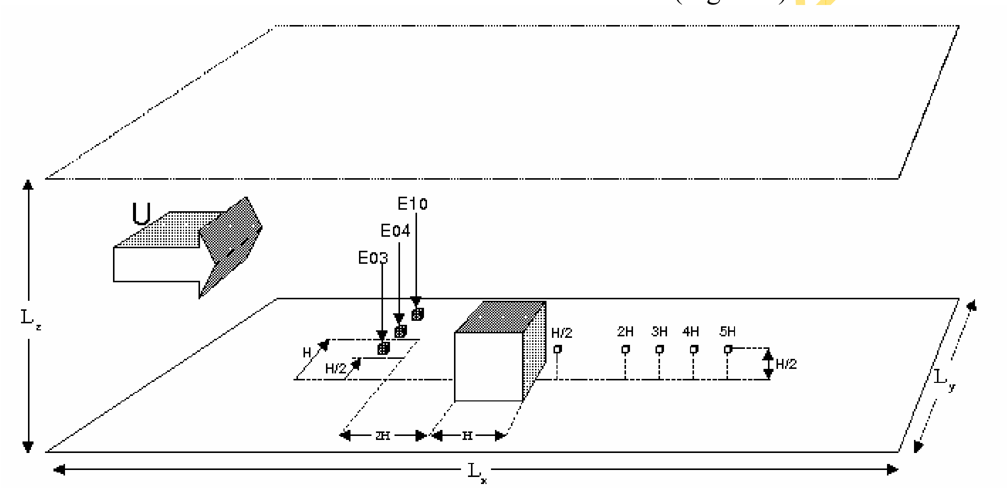

Fig.1; Simulated cases: dimensions, gas source (dark points), gas detectors (light points)

For the LES computations the domain dimensions were set to (L_x, L_y, L_z)=(20H, 12H, 6.5H) for all cases with the square obstacle of dimension H located at a distance 9H from the inlet plane and symmetrically across y-direction (Figure 1). Two different grid resolutions have been computed the first using a grid with 129x96x64 cells and a finer one with 182x128x96 cells. Using the coarser resolution, a total of one CPU-day was enough for a full computation of 100000 time steps starting from an unrealistic initial solution. That corresponded to a time interval of 27 flow-through times T_c, where T_c is the time needed for a hypothetical particle to cross the domain travelling with the bulk flow speed. The statistical results presented here have been gathered after an initial transient time of 16 T_c for another 11 T_c so that stationary statistics had been achieved.

For the RANS computations the domain dimensions were set to (L_x, L_y, L_z)=(17H, 16H, 7.5H). The grid resolution was 105 x 81 x 30 cells. The computations were performed as for a transient problem, until a steady-state situation was reached. This required about 8 hours CPU time on a Xeon 3.2GHz computer.

RESULTS AND DISCUSSION

The calculated flow is examined first. In Figure 2, a horizontal cross section, at height 0.5H is presented. It can be seen that the recirculation area predicted by the LES model (defined by the 0 value of the horizontal velocity component) is larger than the one predicted by the RANS model. There are also two flow-separation zones at the lateral building sides, which are predicted by the LES model, but not by the RANS. The above are indications that the RANS model is characterized by a higher degree of momentum diffusion in comparison to the LES model, resulting to smaller gradients in the flow and, therefore, concentration fields.

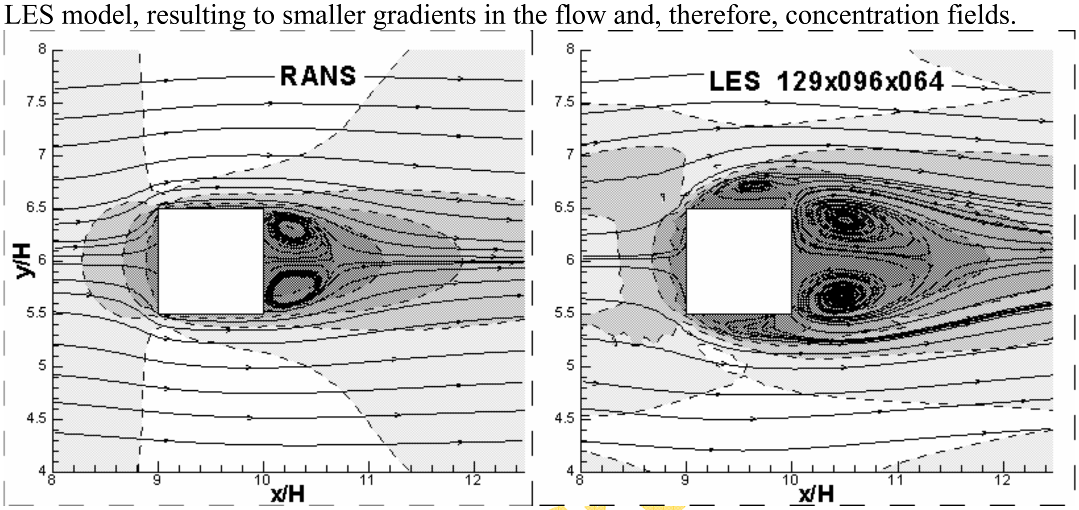

Fig. 2; Calculated flow field at horizontal cross section at height 0.5H. Streamlines and velocity contours are shown

The calculated tracer gas concentrations downwind of the obstacle are examined next, in comparison with the experimental values (Figure 3).

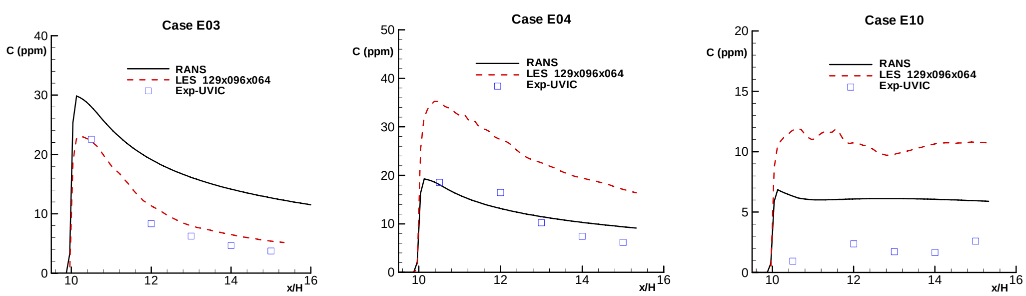

Fig. 3; Tracer-gas concentrations downwind of the obstacle

In the symmetrical case (E03), the RANS model predicts higher values of concentrations than the LES model, which however is in better agreement with the observations. In the cases E04 and E10 with the off-centreline source, it is the LES model that over-predicts the concentration values. In the last case (E10) the experimental values are much lower as compared to cases E03 and E04, a feature which neither of the models is able to simulate. However, both models capture rather well the shape of the concentration variation with downwind distance: decrease for E03 and E04, constant level for E10, with the LES model providing a better representation of the experimental results.

The standard deviation of concentrations downwind of the obstacle calculated by the model is shown in Figure 4, together with the experimental values.

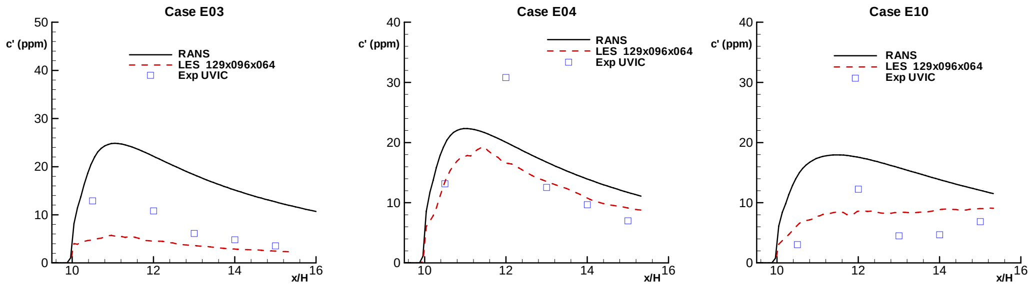

Fig. 4; Standard deviation of tracer-gas concentration downwind of the obstacle

For experimental cases E04 and E10, the LES model gives a better agreement with the observed values than the RANS model. For case E03 the LES model under-estimates the values close to the building. The RANS model over-estimates the values of the concentration standard deviation in all cases. The high peak value observed in case E04 is not captured by any of the models.

The influence of the building and of the lateral source displacement on the crosswind plume shape is shown in Figure 5 for the concentration and in Figure 6 for the concentration standard deviation. Crosswind profiles are drawn, as calculated by the LES and RANS models, at 3 locations: middle of the building, 2H downwind and 4H downwind (of the downwind building side).

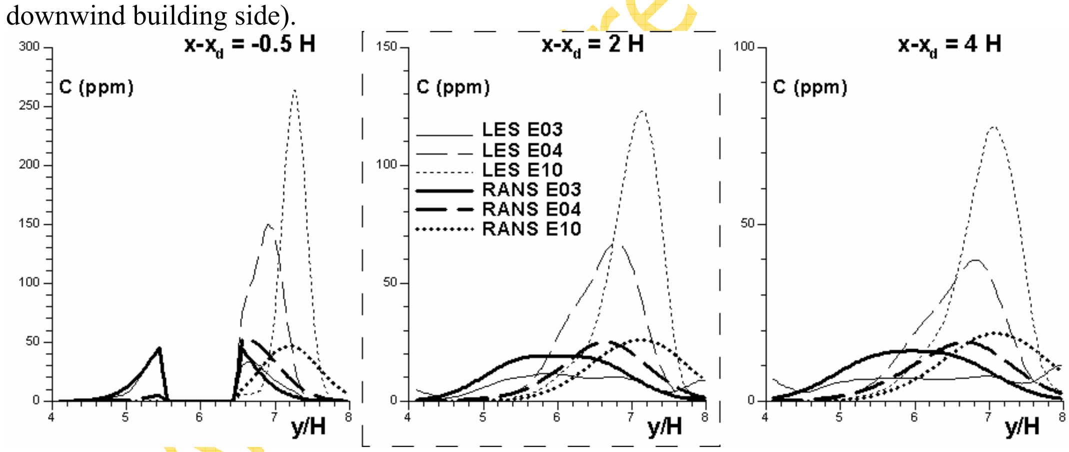

Fig. 5; Crosswind concentration profiles calculated by the two models

The LES model predicts much higher concentration peaks than the RANS model for the cases with the laterally displaced source (E04 and E10). For case E03 however, it is the RANS model that predicts the highest concentrations downwind of the building. Both models predict an increase of the peak concentration as the gas source is laterally displaced (from E03 to E10). However this increase is much steeper for the LES model. The effect of the building is an increase of the crosswind plume dimension or of the lateral dispersion of the tracer gas. This effect is most pronounced in case E03, where the building is placed on the plume centreline and decreases as the source is displaced laterally. Thus, in cases E04 and E10 the plume is less spread in the crosswind direction and the peak concentrations are higher, approaching the characteristics of the plume in an unobstructed flow. This feature is more enhanced in the LES model and is in agreement with experimental results from the field and the wind tunnel (*Mavroidis et al.*, 2003). A similar behaviour is observed for the standard deviation of concentrations calculated by the model (Figure 6).

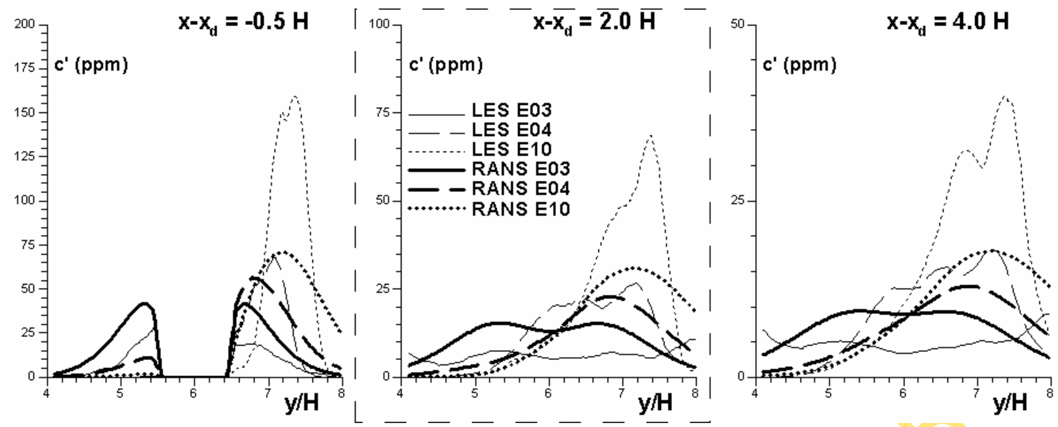

Fig. 6; Crosswind profiles of calculated concentration standard deviation

CONCLUSIONS

The comparative study between two different computational fluid dynamics approaches (LES and RANS) as applied for the flow case of atmospheric dispersion of a passive gas release around a ground-based cubical obstacle, has revealed several interesting features, also in relation to the open-field experimental data used as a validation reference for the simulations. Regarding the flow field, the LES model appears less “diffusive”, as it predicts a longer recirculation area downwind of the building and two flow-separation zones at the building sides. The complex features of the wind flow around the cubical obstacle are reproduced better with the LES model than with the RANS simulation, although at the disadvantage of greater computation time. Regarding the tracer gas concentration patterns, the shape of the downwind variation with distance is well captured by both models. Differences exist in the values predicted for the different simulated cases. The LES model predicts higher plume centreline values than the RANS model as the gas source is displaced in the crosswind direction. The same is true for the standard deviation of concentrations. However, for the case with the gas source located on the building centreline, the concentration and standard deviation values predicted by the RANS model are higher than those calculated by the LES model. These differences, which are attributable to the fact that the LES model resolves better the large-scale turbulence features observed in atmospheric flows, need to be further explored by looking more in detail at calculated quantities that are related to turbulent diffusion.

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