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LANGRANGIAN MODELING EMBEDDED IN RANS CFD CODES FOR CONCENTRATIONS AND CONCENTRATION FLUCTUATIONS PREDICTIONS FROM AIRBORNE HAZARDOUS RELEASES IN URBAN ENVIRONMENTS

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Abstract: A dispersion modeling of airborne pollutants in urban environments using RANS CFD codes is usually based on mean and variance concentration Eulerian transport equations. An alternative could be to use simple Lagrangian approaches with the detailed flow parametrization provided by the CFD codes. The Lagrangian approaches have been approved quite successful at least in regional scale and/or mild topography. The present work can be considered as a first step towards a systematic testing of the performance of the abovementioned Lagrangian approaches at local scale environments characterized with canopies of high geometry complexities such as urban environments. The present work is based on the MUST wind tunnel experiment. The Lagrangian approach was implemented in the ADREA-HF CFD code. The obtained results are quite encouraging not only with respect the concentration mean but the variance as well.

Key words: *concentrations, concentration fluctuations, langrangian, CFD-RANS.*

INTRODUCTION

Dispersion modeling of airborne pollutants in urban environments using RANS CFD codes is usually based on mean and variance concentration Eulerian transport equations. An alternative could be to use simple Lagrangian approaches based on Langevin Equation (Thomson, 1987) fully coupled with the detailed flow parametrization provided by the CFD codes. The main advantages with respect to the Lagrangian approach are (a) they can produce concentration time series like LES, generating concentration statistics, (b) the particle path geometry being independent on the flow grid, can theoretically recognize better the complex terrain subgrid features, (c) the short time releases including instantaneous ones, can be directly simulated and (d) the numerical diffusion error experienced in the corresponding Eulerian models are here non existent. The main disadvantage is that these simple approaches are not based on first principles making necessary the extensive testing on the specific type of problems to be addressed.

The simple Lagrangian approaches have been approved quite successful at least in regional scale and/or mild topography (e.g. Stohl et al, 2005). Applications in build up domain have also been performed mainly in connection with diagnostic wind field (e.g. Kaplan and Dinar, 1996; Tinareli et al., 2007) with satisfactory results. Attempts also have been made to couple with the wind field produced by RANS-CFD approach using more complicated formulation of the Langevin Equation (e.g. Wilson et al, 2007). To the authors knowledge the relevant effort up to now was on predicting concentrations and not concentration fluctuations.

The present work can be considered as a first step towards a systematic testing of the performance of simple Lagrangian approaches coupled with CFD-RANS wind field at local scale environments characterized with canopies of high geometry complexities such as urban environments, with the following objectives: (a) examine the possibility of predicting not only mean concentrations but concentration variance as well and (b) keep the Langevin equation formulation as simple as possible.

THE PRESENT MODEL

The initial Langevin formulation follows the one of Kaplan and Dinar, (1996) suitable for build up domains. The turbulent dispersion parameterization is derived from the wind field CFD-RANS primary parameters: the turbulent kinetic energy (k) and the turbulent energy dissipation (ε).

Following Efthimiou and Bartzis, (2011), the Langrangian time scale (T_L) has been assumed isotropic given by the relationship:

$$T_L = C_T\, k/\varepsilon, \qquad C_T = 0.5$$

In general, the fluctuation velocity components standard deviation are different in the various directions, especially near the solid surfaces. However, they are of the same order of magnitude. Therefore, in the present model, as a first approximation, the standard deviations in the *x*-, *y*- and *z*- direction are assumed equal.

THE MUST WIND TUNNEL EXPERIMENT AND SIMULATION

The methodology has been validated against data of the MUST wind tunnel experiment (Bezpalcova and Harms, 2005) which have been scaled up for the conditions of the corresponding field experiment (Yee and Biltoft, 2004). Hence the CFD ADREA-HF code (Venetsanos et al., 2010) has been setup for the simulation in the field scale and all the experimental and computational parameters below are given in the field scale. In MUST experiment the obstacles were arranged in 12 rows, each consisting of 10 obstacles. The obstacles were nearly identical and had average length, width and height 12.2 m × 2.42 m × 2.54 m respectively. The contaminant's concentration has been measured by a 256-detectors array arranged along obstacle rows in the part of the domain covered by the plume (Fig. 1). All detectors were placed at the same height equal to 1.28 m. The wind flow was characterized by neutral stratification, wind speed at the roof level U_{ref} = 8 m/s, and wind direction -45^{o} (Fig. 1) in the experimental coordinate system. The contaminant originated from a point source located at the ground level (Fig. 1). The volume flow rate of gas at the source was $\approx 3.3 \times 10^{-6}$ m^3s^{-1}.

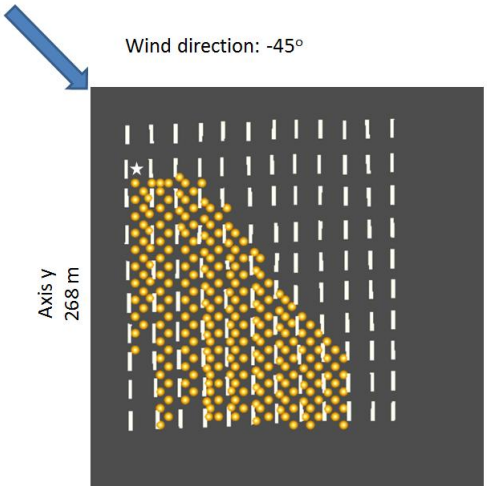
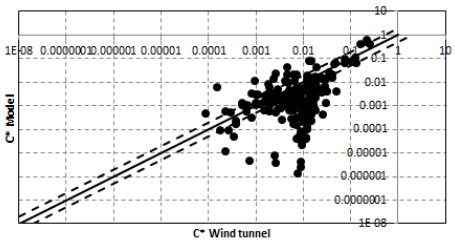


Figure 1. The computational domain of the MUST case. The sensors are presented with yellow circles. The source is depicted with a star. Small offsets of the containers are observed (see Biltoft, 2001).

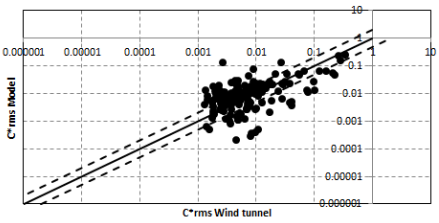
The wind flow problem was solved in a 3D rectangular computational domain with the *x*- and *y*-axes as presented in Fig. 1 and the *z*-axis in the vertical direction was extended up to 21 m. A 85 x 95 x 26 non uniform grid is used with 209,950 active cells.

RESULTS

The time step used for the simulations has been kept constant and intentionally low ($\Delta\tau$ = 0.05s) to minimize time filtering effects on concentration fluctuations. The time step was two orders of magnitude lower than the langrangian and the grid courant time scales. The comparison results for the Langrangian model are shown in Figures 2 (a) and 2 (b). Table 1 shows the comparison of the statistical indicators between the Langrangian and the corresponding Eulerian simulations.



(a) Mean concentrations



(b) concentrations standard deviation

Figure 2. Experiment and model concentration comparisons (a) mean (b) standard deviation.

Table 1. Experiment and model comparisons. The statistical indicators for the Langrangian and the Eulerian model .

		FAC2	FB	NMSE
mean	eulerian	0.283	-0.303	1.43
	langrangian	0.307	-0.206	6.89
std	eulerian	0.357	0.129	4.09
	langrangian	0.332	-0.058	3.98

CONCLUSIONS

The results in this particular application show that it is possible to estimate concentration fluctuations with the langrangian model. The obtained results for mean concentration and concentration fluctuations standard deviation are comparable with the Eulerian ones. However further testing is needed before definite results can be drawn.

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