CONCENTRATION ESTIMATION COUPLING THE MICROMIXING LAGRANGIAN MODEL

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INTRODUCTION

The estimation of the mean concentration of traffic pollutants has been usually the main task of urban dispersion models. Nevertheless concentration fluctuations could be relevant at the micro-scale and are of primary importance for accidental releases.

The Reynolds-Averaged-Navier-Stokes (RANS) meteorological model MISKAM (Microscale Flow and Dispersion) has been coupled with the micromixing Lagrangian dispersion model LAGFLUM (LAGrangian FLUctuation Model).

This modelling system has been validated on the MUST (Mock Urban Setting Test) wind tunnel experiment by Bezpalcova, K. (2007) and Leitl, B. et al. (2007), where the dispersion of a passive tracer in a 3D stationary flow field, in presence of obstacles, was analysed. The turbulent flow field used as input for LAGFLUM was obtained from MISKAM. It solves the Reynolds averaged Navier-Stokes equations with a modified k-ε turbulence closure in a non-uniform Cartesian grid. In particular mean velocities and turbulent kinetic energy evaluated with MISKAM, by modelling the MUST experiment, have been furnished to LAGFLUM.
The MISKAM 3D RANS model is widely used in environmental assessment practice in Europe because of its simple model setup and the ability to gain results fast on personal computers. MISKAM solves the three-dimensional motion equations with Boussinessq-approximatation using the standard k-ε turbulence closure in which the production rates of turbulence kinetic energy and dissipation are replaced following suggestions by Kato, M and B.E. Launder (1993) and López, S.D. (2002). Grid type of Arakawa-C is used, with buildings represented as blockouts. The applied new version 6 introduced revised numerical schemes, with which high numerical diffusion of the upstream scheme used earlier could be avoided. A detailed description of the model can be found for example in Eichhorn, J. and A. Kniffka (2010). The model was extensively validated in the last years, comparison to simple geometries were performed by Eichhorn, J and A. Kniffka (2010) and by Olesen, H. et al. (2009). The implemented vegetation model was evaluated by Balczó, M. et al. (2009). The model also participated in several round tests of urban measurement datasets.
LAGFLUM (LAGrangian FLUctuation Model)

The LAGFLUM is a 3D Lagrangian model for the evaluation of the most significant statistical moments of concentration of a passive scalar. LAGFLUM is based on the coupling of a macromixing with a micromixing scheme. The macromixing scheme is founded on the well-mixed condition (Thomson, D.J., 1987), while the micromixing utilises the IECM (Interaction by Exchange with the Conditional Mean) (Pope, S.B., 1998):

$$\frac{dC}{dt} = -\frac{C - \langle c | U \rangle}{t_m}$$

the conditional mean of the concentration is consistent with the particles exchanging pollutant mass only with the surrounding particles belonging to a similar realisation (i.e. with a similar velocity at the particle location). The IECM scheme guarantees that the mean concentrations given by the macromixing model are unaffected by mixing, according to the balance equation for the pollutant mass. LAGFLUM can be easily coupled with common k-ε models, from which it carries out all the input data.
MUST AND NUMERICAL SET-UP

The MUST was a full-scale wind and dispersion measurement campaign on an arrangement of 120 standard shipping containers in a Utah desert area. The MISKAM simulation domain of the MUST case is shown in Figure 1. MISKAM simulation results of the turbulent kinetic energy $k$ and the three components of the mean velocity vector, from the denser simulation grid are linearly interpolated to the cell centres of the LAGFLUM grid. The velocity variances were determined as $2/3 \ k$. The default boundary condition types of MISKAM are used: no-slip conditions were applied on the surfaces using wall functions, outflow boundaries had no-flux conditions. At the inlet boundaries a logarithmic profile was generated with an initial roughness length $z_0$. On the top boundary constant variable values taken from the top of the inlet profile are prescribed.

Figure 2 shows the fields of horizontal wind speed and $k$ interpolated in LAGFLUM cells. The LAGFLUM numerical domain of (90*85*21 m$^3$) is divided into (36*34*42) cells with a horizontal spacing of $dx=dy=2.5$ m and a vertical one equal to $dz=0.5$ m. The pollutant source has been approximated with a continuous point emission. Furthermore, a geometrical reflection has been assumed for the particles hitting the ground or the obstacles.
Figure 1. MISKAM domain of the MUST case (left); inlet boundary conditions (right).
Figure 2. The horizontal wind speed (arrows) and turbulent kinetic energy $k$ (colour map) at half building height ($z=H/2$)
**RESULTS**

The results of the numerical simulation have been compared with the wind tunnel measurements of concentration on the horizontal plane at half obstacle height (Figure 3). All the values of mean and standard deviation of the concentration have been normalized with the reference scale $Q/H^2u_{ref}$, where $Q$ is the source mass rate. The centre of mass of the plume is not aligned with the wind speed reference direction, but it is rotated clockwise. In fact the obstacles channel the wind as it enters the array, due to their thin shape and the narrow canyons. However, as the distance from the source increases, the plume axis tends to the reference wind direction, because the pollutant fluxe from the zones above the array begins to be important. The comparison between numerical and experimental results shows a satisfying agreement. Both the plume shape and the concentration levels seem to be correctly reproduced, with the exclusion of a small underestimation of the pollutant dispersion across the plume axis. The standard deviations of the concentration are shown in Figure 4. In comparison to the mean, they show an accentuated channelling effect and a wider lateral spread of fluctuations in the neighbourhood of the source (Figure 4). Such behaviour is visible also in the measured data and confirms the good performances of the model, which seems to properly reproduce the dissipation of the concentration fluctuations along the particle trajectories.
Figure 3. Comparisons between (left) the simulated normalized mean concentration
(right) the corresponding wind tunnel measures (squares) at $z=H/2$. 
The agreement is further confirmed by the transversal profiles of the standard deviation of concentration reported in Figure 5a. Finally, Figure 5b shows the transversal profiles of the concentration skewness. A general overestimation with respect to the measurements occurs. However, as pointed out by Bezpalcova, K. (2007), discrepancies in the comparison of the higher moments of the concentration might be present, due to the different reference velocity used in the concentration normalization procedure (MISKAM utilizes a low reference velocity in order to approach the Reynolds number of the wind tunnel experiment).

**CONCLUSIONS**

The LAGFLUM model has been coupled with MISKAM model and applied to the MUST experiment. The simulated values of mean and variance of concentration show a reasonable agreement with the corresponding measurements; both shape and concentration levels are reproduced satisfactorily. The concentration skewness calculated by LAGFLUM has the same order of magnitude of the measured one. Since LAGFLUM can be easily coupled with common k-ε models, it seems furnish a practical tool for the investigation of concentration fluctuations in very complex urban environments.
Figure 4. As in Figure 3, but for the normalized
standard deviation of concentration.
REFERENCES

Figure 5. Comparison between simulated (full squares) and measured
(open squares) standard deviation (a) and skewness (b) of the concentration.