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STREET CANYON CONCENTRATION ESTIMATION COUPLING THE RANS MODEL MISKAM AND THE MICROMIXING LAGRANGIAN MODEL LAGFLUM

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Abstract: The stationary three-dimensional Lagrangian stochastic model LAGFLUM has been coupled with MISKAM to simulate numerically the higher statistical moments of concentration for a passive scalar in the 3D turbulent flow corresponding to MUST wind tunnel experiment. LAGFLUM is based on the coupling of a macromixing scheme founded on the well-mixed condition, while the micromixing scheme utilizes the IECM (Interaction by Exchange with the Conditional Mean) (Pope, S.B., 1998). LAGFLUM can be easily coupled with common 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 next two sections describe MISKAM and LAGFLUM models, the successive one presents the main results of the concentration.

Key words: concentration fluctuations, LAGFLUM, MISKAM, COST 732, MUST.

INTRODUCTION
Street canyon concentration modelling represents a useful numerical tool for urban air quality management. 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) (Yee, E. and C.A. Biltoft, 2004) wind tunnel experiment. The results show a reasonable agreement between simulated and measured statistical moments of concentration.

THE MISKAM MODEL
The flow field in this study is calculated using the MISKAM code. 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. The model consists of a flow and a dispersion part: calculated flow fields serve as inputs for an Eulerian advective dispersion simulation. In this paper the MISKAM flow field results are used to drive the LAGFLUM code.

MISKAM model description
MISKAM solves the three-dimensional motion equations with Boussinesq-approximation 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.

Flow simulation of the MUST case
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 of the MUST case was performed in the framework of the European COST Action 732 (Eichhorn, J. and M. Balczó, 2008). From several grids a fine one was selected as it gave the best agreement with wind tunnel data reported by Leitl, B. et al. (2007). The simulation domain is shown in Figure 1. Grid axes are parallel to the container walls, and wind direction is -45 degree.
Coupling technicalities

MISKAM simulation results of the variables \( k \) and the three components of the mean velocity vector \( \mathbf{u}, \mathbf{v}, \mathbf{w} \), respectively along the \( x, y \) and \( z \) axis, from the denser simulation grid are linearly interpolated to the cell centres of the LAGFLUM grid. Variances of \( u, v \) and \( w \) were determined as \( 2/3 \, k \). A problem emerges from the aligned positions of buildings in the different grids (Figure 2) which might cause deviations in the results near the container walls.

Figure 1. MISKAM domain of the MUST case (left); inlet boundary conditions (right).

Figure 2. MISKAM grid (left); LAGFLUM grid with MISKAM (grey) and aligned (red) building positions.

Figure 3. The horizontal wind speed (arrows) and turbulent kinetic energy \( k \) (colour map) at \( z=H/2 \).

Grid resolution is 0.5 x 0.5 x 0.5m in the region of the container blocks with a total number of 4.8 million (400 x 400 x 30) grid cells. 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 reference velocity \( u_{ref} \) was set to 1 ms\(^{-1} \) at \( z_{ref} = 7.29 \) m. A good fit to wind tunnel data was
stochastic differential equations have been integrated (hereinafter the Einstein notation applies): well-mixed condition ensures a well-founded behaviour of the model also in inhomogeneous turbulence. The following set of mean conditioned on the velocity are unaffected by the value of molecular diffusivity. Therefore, polluted fluid particles, marked fluid particles. As pointed out by Pope, S.B. (1998), for high Reynolds numbers the mean of concentration and the values of above 0.66 might be seen as state-of-the-art. With these results however MISKAM 6 performed well in comparison (excellent) while for W only 0.19 (poor). Turbulent kinetic energy \( k \) gave a hit rate value of 0.59 (near good). Hit rate were fair for variables of lateral and vertical wind velocity. Calculated hit rates for the mean velocity component \( U \) were 0.81

\[
\frac{dU_i}{dt} = a_i \left( \mathbf{X}, U \right) dt + b_i \left( \mathbf{X}, U \right) d\xi_j,
\]

where \( U_i \) and \( X \) indicate the particle velocity and position respectively, the subscripts refer to the axis direction, and the \( d\xi_j \) are the increments of independent Gaussian Wiener processes with mean zero and variance \( dt \). The functions \( a_i \) and \( b_{ij} \) in stationary cases can be calculated as follows:

\[
a_i = -B \left( \mathbf{X}, U, \right) \phi a_i,
\]

\[
2B_{ij} = \delta_{ij} C_{ij} \varepsilon,
\]

\[
\phi \frac{g_a}{g_a} = \frac{1}{2} \left( \mathbf{V} \cdot \nabla \right) u_i \mathbf{V} - \mathbf{V} \cdot \nabla u_i = \frac{1}{2} \mathbf{V} \cdot \nabla \mathbf{V} + \mathbf{V} \cdot \nabla u_i = \frac{1}{2} \mathbf{V} \cdot \nabla \mathbf{V} + \frac{1}{2} \mathbf{V} \cdot \nabla u_i = \frac{1}{2} \mathbf{V} \cdot \nabla \mathbf{V} + \frac{1}{2} \mathbf{V} \cdot \nabla u_i = \frac{1}{2} \mathbf{V} \cdot \nabla \mathbf{V} + \frac{1}{2} \mathbf{V} \cdot \nabla u_i = \frac{1}{2} \mathbf{V} \cdot \nabla \mathbf{V} + \frac{1}{2} \mathbf{V} \cdot \nabla u_i.
\]

\( C_{ij} \) is the Kolmogorov constant, assumed equal to 4, \( g_a \) is the probability density function of the Eulerian velocity \( \mathbf{u}_i \) (corresponding to \( \mathbf{v}, \mathbf{w} \)), \( \delta_{ij} \) is the Kronecker delta and \( V_{ij} \) is the one-point velocity covariance matrix of the turbulence (due to lack of data this matrix has been considered diagonal) and \( \varepsilon \) is the rate of \( k \). \( \varepsilon \) has been computed as a function of \( k \) (Stull, R.B., 1988):

\[
\varepsilon = 0.1 k \left( \frac{\partial u_i}{\partial x_j} \right)^2
\]

Fifteen million particles have been released, in order to calculate both the mean \( \tau \) and conditional mean concentration \( \langle \epsilon | \mathbf{U} \rangle \)

In the second phase of the model run the IECM micromixing equation has been integrated. A large number of particles should be released all over the domain, uniformly distributed. Every particle should be initialized with the conditional mean concentration of the starting cell, in order to reproduce the motion of the whole fluid. Since the fluid motion has a predominant direction of motion, we can start the particles, in a more efficient way, only from the pollutant source and from the boundary of the plume. Sixty million particles have been released; they move according to the macromixing scheme (1,2) and exchange pollutant mass through the micromixing process. In this way all the particles (non conservative) have their own representative instantaneous concentration: their statistical computation in every cell of the domain gives, in theory, all the concentration moments. In practise the lower order moments are better simulated and we focus here on the mean, variance and skewness. The micromixing model adopted is the IECM:

\[
\frac{d\mathbf{C}}{dt} = \frac{\mathbf{C} - \langle \epsilon | \mathbf{U} \rangle}{t_w}
\]

where \( \mathbf{C} \) is the instantaneous particle concentration and \( t_w \) is the mixing time scale. Since the simulation represents a large number of realisations of the turbulent regime, the conditional mean in (7) 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. The mixing time scale is assigned consistently with the asymptotic mixing constraints (Cassiani, M. et al., 2005):

\[
\tau_m = \mu \left[ \frac{1.225}{\varepsilon} \frac{\sigma_0^{2/3}}{f L^{2/3}} + \sqrt{2T_L t_f} \right]
\]

where \(\mu=0.75\) is the micromixing constant, \(T_L = \frac{4k}{3C_p\varepsilon}\) is the Lagrangian integral time scale, \(\sigma_0\) is the source length scale and \(t_f\) is the mean flight time of the particles, calculated on each cell during the macromixing process. The 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.

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 4). All the values of mean and standard deviation of the concentration have been normalized with the reference scale \(Q/\mu u_{ref}^3\), where \(Q\) is the source mass rate.

Figure 4. Comparisons between (left) the simulated normalized mean concentration and (right) the corresponding wind tunnel measures (squares) at \(z=H/2\).

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 flux 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 5. 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 5). 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. The agreement is further confirmed by the transversal profiles of the standard deviation of concentration reported in Figure 6a.

Figure 5. As in Figure 2, but for the normalized standard deviation of concentration.
Finally, Figure 6b 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 velocities used in the concentration normalization procedure (MISKAM utilizes a low reference velocity in order to approach the Reynolds number of the wind tunnel experiment).

![Figure 6b](image_url)

**Figure 6.** Comparison between simulated (full squares) and measured (open squares) standard deviation (a) and skewness (b) of the concentration.

**CONCLUSIONS**

The numerical 3D model LAGFLUM (LAGrangian FLUctuation Model) based on the “well mixed” macromixing scheme (Thomson, D.J., 1987), and the IECM micromixing scheme (Pope, S.B., 1998) has been presented. The model has been applied to the wind tunnel experiment of Bezpalcova, K. (2007) and Leitl, B., et al., (2007) on passive pollutant dispersion in presence of obstacles (MUST experiment). The LAGFLUM input data have been obtained by using the output of the MISKAM model 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 to furnish a practical tool for the investigation of concentration fluctuations in very complex urban environments.

**REFERENCES**


