A STATIONARY 3D LAGRANGIAN STOCHASTIC NUMERICAL MODEL FOR CONCENTRATION FLUCTUATIONS

Andrea Amicarelli[1,2], Giovanni Leuzzi[1], Paolo Monti[1] and David J. Thomson[3]

[1]DITS, Università di Roma "Sapienza", Via Eudossiana 18, 00184 Roma, Italy
[2]DIPIA, ISPESL (National Institute for Occupational Safety and Health), Via Fontana Candida 1, 00040 Monte Porzio Catone, Roma, Italy
[3]Met Office, FitzRoy Road, Exeter, EX1 3PB, UK

Abstract: A stationary three-dimensional Lagrangian stochastic numerical model has been developed by coupling a macromixing with a micromixing scheme, to determine the mean and the variance of concentration for a passive scalar in 3D turbulent flows. The macromixing scheme is based on the "well-mixed" condition (Thomson, 1987). The micromixing IECM (Interaction by Exchange with the Conditional Mean; Pope, 1998; Sawford, 2006) scheme has been integrated to calculate the higher moments of concentration. The model has been tested by comparison with the MUST (Mock Urban Setting Test) wind tunnel experiment by Bezpalcova (2007) and Leitl et al. (2007), which corresponds to the atmospheric dispersion experiment by Yee and Biltoft (2004). In both these experiments the dispersion of a passive tracer in a 3D stationary flow field, in presence of obstacles, has been analysed. The mean and the variance of concentration, calculated by the numerical model presented here, show a reasonable agreement with the experimental results.

Key words: *concentration fluctuations, micromixing, IECM, MUST.*

1. INTRODUCTION

Knowledge of concentration fluctuations is useful to determine the range of the expected values of concentration for microscale dispersion and to assess the hazard in the case of a strong non-linear relationship between concentration and damage (i.e. accidents). Furthermore, knowledge of concentration fluctuations permits a better simulation of chemical reactions, which depend on the instantaneous concentration, rather than the mean. The IECM (Interaction by Exchange with the Conditional Mean) model (Pope, 1998; Sawford, 2006) is one of the more promising methods to estimate the concentration fluctuations. IECM micromixing models have been applied to several case studies: one-dimensional scalar dispersion in grid turbulence from line or area sources (Sawford, 2004) and for multiple reacting pollutants (Sawford, 2006), one-dimensional multiple scalar dispersion in convective boundary layers from area sources (Luhar and Sawford, 2005), one-dimensional dispersion from area sources in canopy turbulence (Cassiani et al., 2005c), two-dimensional dispersion from point or line sources in neutral boundary layers (Cassiani et al., 2005a; Dixon and Tomlin, 2007) and in convective boundary layers (Cassiani et al, 2005b), and from single or multiple sources in canopy turbulence (Cassiani et al, 2007a; Dixon and Tomlin, 2007; Cassiani et al., 2007b).

In this context the three-dimensional stochastic model LAGFLUM (LAGrangian FLUctuation Model) has been developed, by coupling a macromixing with a micromixing scheme, to determine the most significant statistical moments of concentration for a passive scalar in 3D turbulent flows. The macromixing scheme is based on the "well-mixed" condition (Thomson, 1987). This model describes the motion of fictitious trajectories of marked fluid particles to estimate the averaged concentrations. To take account for concentration fluctuations, the IECM micromixing equation has been integrated. All the particles move according to the macromixing scheme and exchange pollutant mass through the micromixing process. So they have their own representative instantaneous concentrations: their statistical computation in each cell of the domain can furnish all the concentration moments.

The model has been tested by comparison with the MUST wind tunnel experiment by Bezpalcova (2007) and Leitl et al. (2007). In that experiment the dispersion of a passive tracer in 3D, stationary flow fields in the presence of obstacles, has been analysed. In the present paper, after a short description of the experiment, the LAGFLUM equations have been reported. In the last section some results of the comparison have been shown.

2. THE EXPERIMENT

The dispersion of a passive pollutant (ethane) has been performed inside an obstacle array in the WOTAN wind tunnel of the Environmental Wind Tunnel Laboratory (EWTL) at the Meteorological Institute (University of Hamburg, Germany). It is described in detail in Bezpalcova (2007) and Leitl et al. (2007) and reproduces the MUST field experiment.

We choose the x-axis to be in alignment with the obstacle array. The reference wind speed outside the array is u_{ref} (z=7.3m) = 8 ms^{-1}, oriented at 45° clockwise to the x-axis. Here we always refer to the full scale values (the wind tunnel scale is 1:75). All the velocities were measured with the two-dimensional Laser-Doppler technique. Figure 1 shows the numerical domain used in our simulations together with the obstacle arrangement, the pollutant source (violet), and the meteorological monitoring points. The numerical domain used is the part of the wind tunnel domain nearby and to the leeward of the pollutant source. It represents almost a quarter of the wind tunnel domain. The obstacles have all the same dimensions (12.5x2.5x2.5 m^3), except the smallest one in Figure 1 (which is 3.5 m tall).

Although the obstacle array is a little irregular, an average distance between the obstacles of 12.9 m along x-axis and 7.9 m along the y-axis can be recognised. Even if there were more obstacles in the wind tunnel than are included in our simulation, the extra obstacles were all downwind of our numerical domain. The meteorological dataset is composed of a coarse network (green), some vertical profiles (red) and a fine network (blue). The coarse network cover the whole wind tunnel domain at the height of the obstacles (z=H=2.5 m), and at z=2H and z=H/2. It collects the mean and the standard deviation of the horizontal velocities ($\bar{u}$ and σ_u along x, $\bar{v}$ and σ_v along y) at 847 monitoring points. 18 profiles of the standard deviation of the vertical velocity (σ_w), $\bar{u}$ and σ_u are measured at 497 monitoring points. The fine network lies entirely within the numerical domain, records measures of $\bar{u}$, σ_u, $\bar{v}$ and σ_v at 4 heights (z=H/3, H/2, 2H/3, H), and is composed of 376 monitoring points.

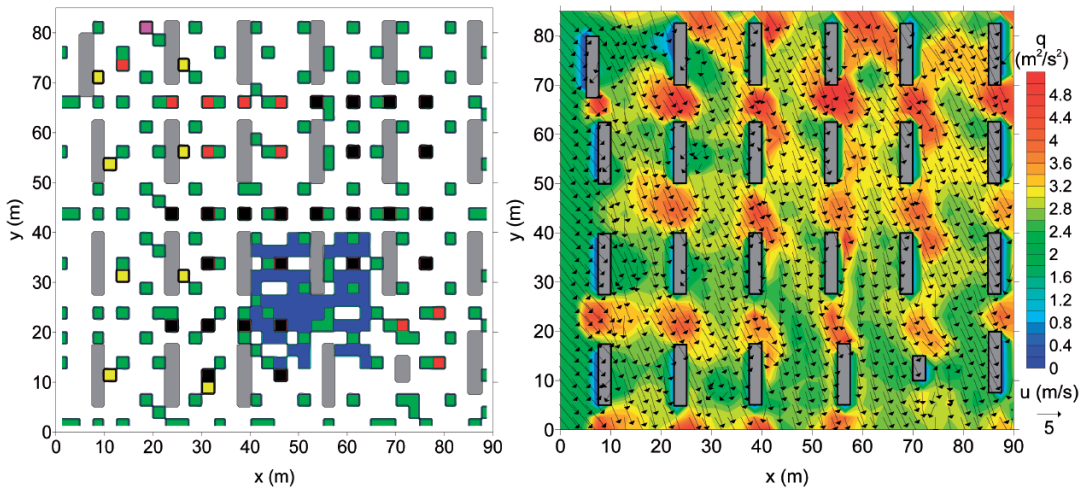

Figure 1. On the left. the numerical domain with the horizontal coordinates of the meteorological monitoring points (grey: obstacles, red: profiles, green: coarse network, blue: fine network, violet: pollutant source). On the right: the horizontal wind speed (arrows) and turbulent kinetic energy q (colour map) at z=H/2.

All these monitoring points values have been interpolated to a numerical grid aligned with the coordinate axes using the inverse distance method. We use a three-dimensional interpolation for the mean horizontal velocities. Furthermore, in the first meter above the ground, a neutral logarithmic profile has been assumed with a roughness (z_0) equal to 0.0165 m. The vertical mean velocity ($\bar{w}$) has been computed from the balance equation for the air mass. The horizontal velocity variances have been referred onto the new reference axis, keeping the same horizontal kinetic energy, but neglecting, on first approximation, the correlation between the horizontal components of velocity (which corresponds here to take σ_u equal to σ_v). Their variances were then interpolated as previously described for the means. The vertical velocity variance is only available from profile measurements. So a first vertical interpolation was performed for each profile, and then a two-dimensional horizontal interpolation at every level was made. In Figure 1 (right panel) both the horizontal velocity and the turbulent kinetic energy q, interpolated at H/2 are shown. The pollutant source is located at x_s=17.44 m, y_s=77.72 m, z_s=0.15 m, with a diameter D=0.75 m. The mean and the standard deviation of concentration ($\bar{c}$ and σ_c) were measured with a Fast Ionization Flame Detector (frequency=150 Hz) in 80 monitoring points, belonging to the numerical domain, at the height z=H/2.

3. THE MODEL

LAGFLUM utilises both macromixing and micromixing schemes. The mean concentration is computed during the first phase of the model run and then the concentration variance is computed. The macromixing scheme is based on the so called "well-mixed" condition. This model describes the motion of fictitious trajectories of marked fluid particles. For high Reynolds numbers, the mean of concentration and the mean conditioned on the velocity are unaffected by the value of molecular diffusivity, as pointed out by Pope (1998). Therefore, polluted fluid particles, which do not exchange pollutant mass with the surrounding ones, can be utilised to estimate the averaged concentrations. The well-mixed condition ensures a well-founded behaviour of the model in inhomogeneous turbulence. The following set of stochastic equations have been integrated (hereinafter the Einstein notation applies):

$$dU_i = a_i(\boldsymbol{X},\boldsymbol{U},t)dt + b_{ij}(\boldsymbol{X},\boldsymbol{U},t)d\xi_j \quad (1)$$

$$dX_i = U_i dt \quad (2)$$

where U_i and X_i 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:

$$a_i = -B_{ij}\left(V^{-1}\right)_{jk}\left(U_k - \overline{u_k}\right) + \frac{\phi_i}{g_a} \tag{3}$$

$$2B_{ij} = b_{ik}b_{jk} = \delta_{ij}C_0\varepsilon \tag{4}$$

$$\frac{\phi_i}{g_a} = \frac{1}{2}\frac{\partial V_{il}}{\partial x_l} + \overline{u_l}\frac{\partial \overline{u_i}}{\partial x^l} + \left(\frac{1}{2}\left(V^{-1}\right)_{lj}\overline{u_m}\frac{\partial V_{il}}{\partial x_m} + \frac{\partial \overline{u_i}}{\partial x_j}\right)\left(U_j - \overline{u_j}\right) + \frac{1}{2}\left(V^{-1}\right)_{lj}\frac{\partial V_{il}}{\partial x_k}\left(U_j - \overline{u_j}\right)\left(U_k - \overline{u_k}\right) \tag{5}$$

C_0 is the Kolmogorov constant, assumed equal to 3, g_a is the probability density function of the Eulerian velocity, δ_{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 ε is the rate of dissipation of the turbulent kinetic energy. According to Beljaars (1987), Kitada (1987), and Detering and Etling (1985) has been computed as a function of the turbulent kinetic energy (q):

$$\varepsilon = 0.3q\sqrt{\left(\frac{\partial \overline{u}_i}{\partial x_j}\right)^2} \tag{6}$$

Twenty million of particles have been released, in order to calculate both the mean $\overline{c}$ and conditional mean concentration $\langle c|\boldsymbol{U}\rangle$. 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. So, all these particles 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 and variance. The micromixing model adopted is the IECM:

$$\frac{dC}{dt} = -\frac{C - \langle c|\mathbf{U}\rangle}{t_m} \tag{7}$$

where C is the instantaneous particle concentration and t_m is the mixing time scale. As 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 et al., 2005a):

$$t_m = 0.8\left(\frac{3}{2}\right)^{-\frac{1}{2}}\left[\left(\frac{3}{2}\right)^{\frac{1}{2}}\frac{{\sigma_0}^{2/3}}{\varepsilon^{1/3}} + \sqrt{2T_L t_f}\right] \tag{8}$$

where $T_L = 4q/3C_0\varepsilon$ is the Lagrangian integral time scale, σ_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.

4. RESULTS

Some preliminary results of the numerical simulation have been compared with the wind tunnel measurements of concentration on the horizontal plane at half obstacle height (Fig. 2). 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 three-dimensional 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 as the pollutant fluxes from the zones above the array begin to be important. Unfortunately, the low resolution of the flow data cannot accurately reproduce the recirculation zones downwind of the obstacles. Furthermore both the mean and the variance of the velocities have been interpolated with a geometrical method, which does not fulfil the momentum balance nor the turbulent kinetic energy balance. Nevertheless the comparison between numerical and experimental results shows a satisfying agreement. Both the plume shape and the concentration levels seem to be correctly reproduced, just a small underestimation of the pollutant dispersion across the plume axis occurs. The standard deviations of the concentration are shown in Figure 3. In comparison to the mean, they show an accentuated channelling effect and a wider lateral spread of fluctuations in the neighbourhood of the source (Fig. 3).

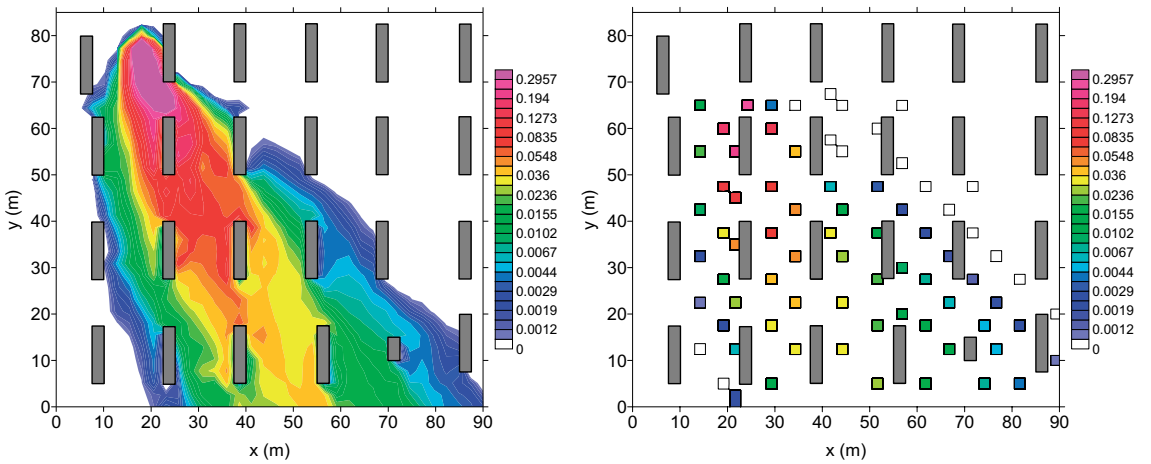

Figure 2. Comparisons between the simulated normalized mean concentration (left) and the corresponding wind tunnel measures (squares) (right) at $z=H/2$.

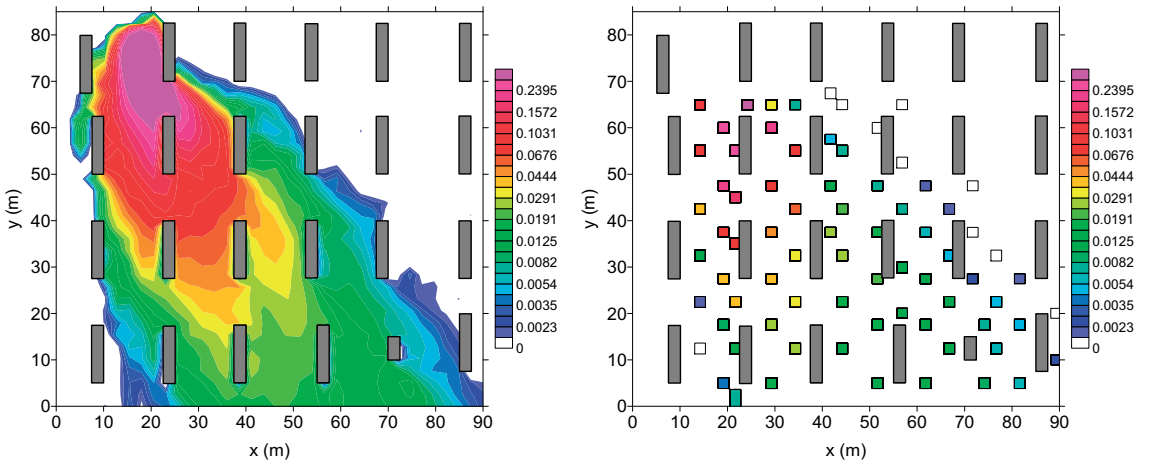

Figure 3. Comparisons between the simulated normalized standard deviation of concentration (left) and the corresponding wind tunnel measures (squares) (right) at $z=H/2$.

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.

5. CONCLUSIONS

The numerical 3D model LAGFLUM (LAGrangian FLUctuation Model) based on the "well mixed" macromixing scheme (Thomson, 1987), and the IECM micromixing scheme (Pope, 1998; Sawford, 2006) has been presented. The model has been applied to the wind tunnel experiment of Bezpalcova (2007) and Leitl et al., (2007) on passive pollutant dispersion in presence of obstacles. Starting from measured data, the wind field has been reconstructed by means of geometrical interpolation and the balance equation for the air mass. 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 model seems to furnish a valid tool for the investigation of concentration fluctuations in complex turbulent fields.

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