A NUMERICAL LAGRANGIAN MODEL OF CONCENTRATION FLUCTUATIONS

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INTRODUCTION

The evaluation of pollutant dispersion in turbulent environmental flows can support public and private institutions to provide forecasts and scenarios of pollution reduction. The knowledge of concentration fluctuations is useful to determine the range of the expected values of concentration, not only the mean, which can be unsatisfactory for accidental releases. Furthermore, concentration fluctuations are also important to simulate chemical reactions in a more realistic way, according to the instantaneous concentrations, instead of their means. So a numerical model has been developed by integrating a macromixing (*Thomson, D.J., 1987*) and an IECM (Interaction by Exchange with the Conditional Mean) scheme (*Pope, S.B., 1998; Luhar, A.K. and B.L. Sawford, 2005; Sawford, B.L., 2006*) to determine the moments of concentration for a passive scalar in 3D turbulent flows. The wind tunnel experiments of *Fackrell, J.E. and A.G. Robins* (1982) simulating the Atmospheric Neutral Boundary Layer have been reproduced. Our results have been compared with these measurements and with *Cassiani, M. et al.'s* (2005) numerical simulations.

THE EXPERIMENT

The *Fackrell, J.E. and A.G. Robins* (1982) experiments of dispersion of a passive scalar (a mixture of propane and helium) have been performed in a wind tunnel with a bottom surface of approximately 24x9 m^2 and a boundary layer height h =1.20 m. Both transversal (along y-axis) and vertical (along z-axis) components of the mean velocity, respectively $\overline{v}$ and $\overline{w}$, have been neglected, while for the average wind velocity $\overline{u}$ along the longitudinal axis x the standard neutral logarithmic profile:

$$\overline{u} = \frac{u_*}{k} ln(z/z_0) \qquad (1)$$

has been adopted. Here, u_*=0.188 m/s is the friction velocity, k=0.4 the von Karman constant and z_0=0.000288 m the roughness length. The standard deviations s_u, s_v, s_w of the velocity components u, v, w and the dissipation rate e of turbulent kinetic energy (TKE) have been interpolated according to the available measurements (Figure 1). The position of the pollutant point source is y_s=0 and z_s=0.19h. The "ground level" has been assumed at z_g=0.06 m. The numerical simulation is based on the same hypothesis of the laboratory model and utilises measurements and interpolations of turbulence parameters as input data.

THE NUMERICAL MODEL

The macromixing scheme is based on the so called "Well-Mixed" condition proposed by *Thomson, D. J.* (1987). This model describes the motion of fictitious trajectories of marked fluid particles. For high Reynolds numbers, the balance of the mean concentration is unaffected by the value of molecular diffusivity. 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 founded behaviour of the model in inhomogeneous turbulence too.
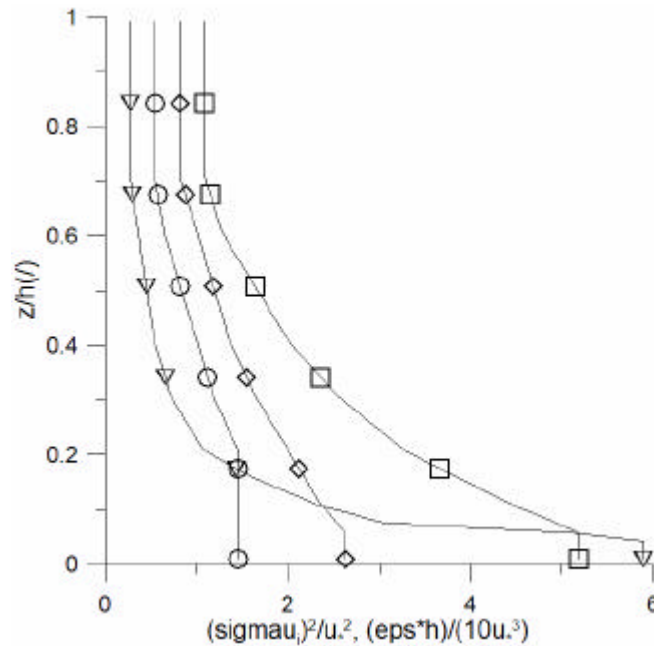
Fig. 1; Interpolated profiles from Fackrell, J.E. and A.G. Robins (1982) measurements of velocity variances s_u^2 (squares), s_v^2 (diamonds), s_w^2 (circles) and TKE dissipation e (triangles).

The following hypothesis have been assumed: the turbulent dispersion in x direction is negligible ($s_u << \overline{u}$), the turbulent fluctuations of velocity components are uncorrelated ($\overline{u'_i u'_j} = 0$ if $i \neq j$), the flow is steady ($\partial/\partial t = 0$) and horizontally homogeneous ($\partial/\partial x = \partial/\partial y = 0$), the transversal components of the mean velocity ($\overline{v} = \overline{w} = 0$) are negligible and the probability density function of the velocity components is Gaussian.

According to *Thomson, D.J.* (1987), the particle velocity can be described by the stochastic differential equations:

$$dU = 0 \qquad (2)$$

$$dV = \frac{V}{2s_V^2}\left(-C_0 e + W\frac{\partial s_V^2}{\partial z}\right)dt + \sqrt{C_0 e}\,dx_V \quad (3)$$

$$dW = \frac{1}{2s_W^2}\left[-C_0 e W + \left(s_W^2 + W^2\right)\frac{\partial s_W^2}{\partial z}\right]dt + \sqrt{C_0 e}\,dx_W \qquad (4)$$

where U, V and W are the Lagrangian particle velocities and $C_0 = 5$ is the Kolmogorov constant. dx_V and dx_W are the increments of a Gaussian Wiener process with mean zero and variance dt. The mean concentrations have been calculated from the particle trajectories obtained from the increments (2-4). In order to evaluate the higher statistical moments of concentrations, a micromixing scheme simulating the pollutant mass exchanges between a fluid particle and its surrounding environment has been implemented. A large number of non-polluted particles have been released over the whole domain: they reproduce the motion of the whole fluid and can be used to evaluate the other moments of concentration. A little ensemble of particles initially polluted move according to the macromixing scheme 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 first ones are better simulated and we focus here on the variance. The micromixing model adopted here is the IECM (*Pope, S.B.*, 1998):

$$dC/dt = (C - \langle c|\mathbf{X},\mathbf{U}\rangle)/t_m \qquad (5)$$

where C is the instantaneous particle concentration, $\langle c|\mathbf{X},\mathbf{U}\rangle$ is the mean concentration conditioned on the particle position and particle velocity vectors and t_m is the mixing time scale, assigned in the form proposed by *Cassiani, M. et al.* (2005). As the simulation represents a large number of experiments in turbulent regime, the conditional mean (in eq.5) might imply that particles change pollutant mass only with the surrounding particles belonging to the same experiment or to a similar one. The IECM scheme guarantees that the mean concentrations given by the macromixing model are unaffected by mixing, according to the balance equation of pollutant mass. A finite difference form of eq. (5) is:

$$C(t + \Delta t) = C(t)exp(-\Delta t/t_m) + \langle c|\mathbf{X},\mathbf{U}\rangle[1 - exp(-\Delta t/t_m)] \qquad (6)$$

where Δt is the integration time step. At each time step the macromixing model estimates both the unconditional and the conditional mean concentrations. The latter is necessary for the IECM scheme to evaluate the instantaneous concentrations. At a given time step U is the same for all the particles and, according to *Cassiani, M. et al.* (2005), corresponds with the average weighted over the particle concentrations. The source mass rate is $Q = 0.471$ mg/s. The transversal section of the domain is divided into 60x60 grid cells, while the longitudinal dimension of the grid cell is $\Delta x = U \, \Delta t$. Ten ranges of velocity for each component have been assumed to estimate the conditional means, and 10,800,000 particles (3,000 of which initially polluted) have been released to calculate significant statistics. Δt was chosen equal to 1/25 of the Lagrangian integral time scale.

RESULTS

The results of the first two moments of concentration have been compared with the measurements by *Fackrell, J.E. and A.G. Robins* (1982) and the simulations by *Cassiani, M. et al.* (2005); all the plots refers to y=y_s=0. At each time step the maximum of the standard deviation and the highest mean across the vertical profile have been evaluated. In Figure 2 their ratio has been reported as a function of downwind distance, normalised with the boundary layer height. The maximum of variance initially grows to its highest value, then tends to zero, according to the well-mixed condition. The maximum of the mean decreases for each downwind distance, until the well-mixed value has been reached. The simulation results are in satisfactory agreement with the measured values, which are a bit underestimated.

In Figure 3 the vertical profiles of mean concentrations (above) and concentration variances (below) have been plotted, both normalized on their time step highest values. Each profile has been evaluated at a fixed downwind distance. Ranging from left to right, they refer respectively to x/h = 0.96, 1.92, 2.88, 3.83, 4.79. While the maximum of concentration approaches the ground, the variance has its greatest values where the concentration gradient is higher. Its maximum value occurs for greater height as x grows. The simulated profiles of mean concentration are in good agreement with the measured profiles. On the contrary, some discrepancies occur in the variances comparisons, with a general underestimation of the normalized variance in the lower part of the domain. This might be due to an incorrect reflection scheme of the particles at the ground. Finally, the comparison between measured and calculated mean concentrations at two different heights ($z=z_s$ and $z=z_g$= 0.06 m) has been shown in Figure 4. The plots of the two levels tend to the same values in the last time steps

(approximately for $x/h > 5$), as the maximum reaches the ground. Also in this last case measured and simulated values are in reasonable agreement.
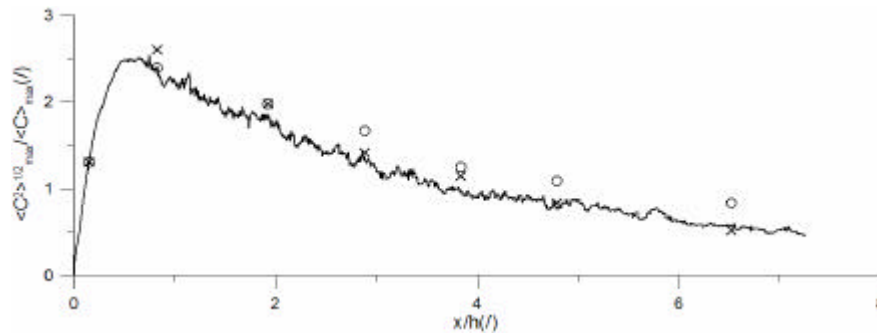

Fig. 2; Normalised concentration fluctuations (line) as a function of the dimensionless downwind distance, compared with Fackrell, J.E. and A.G. Robins's (1982) measurements (circles) and Cassiani, M. et al.'s (2005) simulations (crosses).
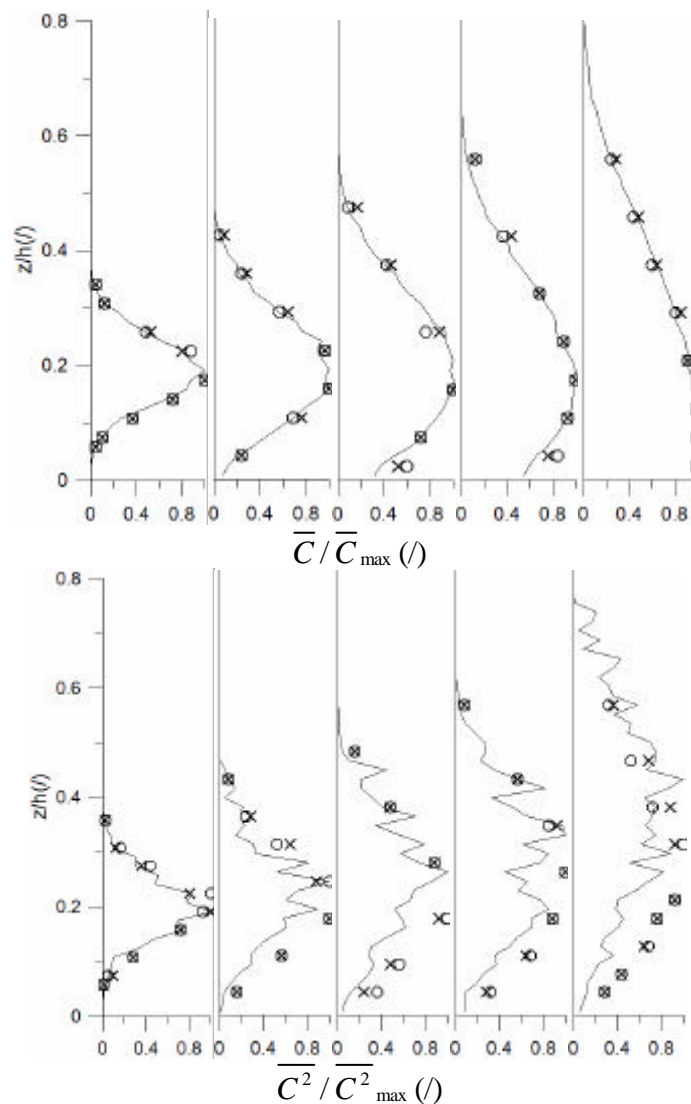

$$\overline{C} / \overline{C}_{max} \, (/)$$

$$\overline{C^2} / \overline{C^2}_{max} \, (/)$$

Fig. 3; Vertical profiles of the normalized mean (above) and variance (below) of concentration at five downwind distance (x/h=0.96, 1.92, 2.88, 3.83, 4.92), compared with Fackrell, J.E. and A.G. Robins 's (1982) measurements (circles) and Cassiani, M. et al.'s (2005) simulations (crosses).
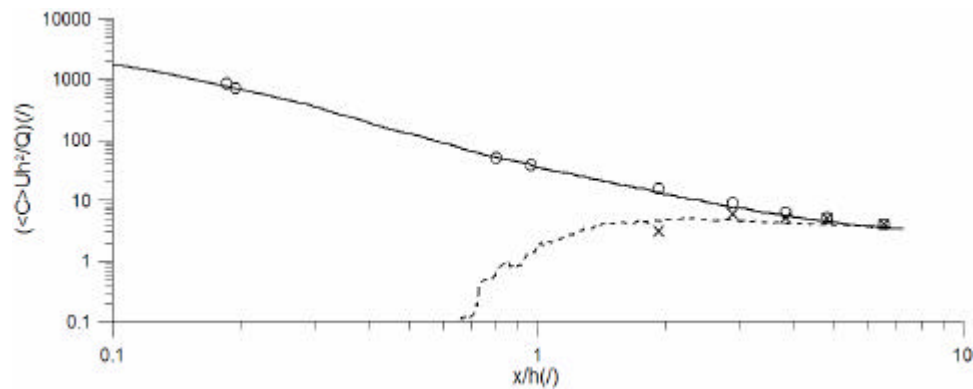
Fig. 4; Mean concentrations at the source elevation (continuous line) and in the proximity of the ground level (dashed line) compared with the correspondent Fackrell, J.E. and A.G. Robins's (1982) measurements (circles and crosses, respectively).

CONCLUSIONS

The numerical model presented here is a coupling of the *Thomson, D.J.* (1987) macromixing and the IECM micromixing schemes. It has been applied to the experiments by *Fackrell, J.E. and A.G. Robins* (1982) as an analogous numerical model by *Cassiani, M. et al.* (2005). The results, compared with the measurements and the available numerical simulations, give a satisfactory response to the test of the model for the estimation of the mean and the variance of the concentrations in Neutral Boundary Layer conditions. The mean concentrations are in good agreement in the whole domain. Furthermore, the comparisons show a satisfactory agreement for the maximal variances of the concentration fluctuations at various downwind distances. Some discrepancies have been observed in the lower part of the domain.

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