A LAGRANGIAN STOCHASTIC MODEL FOR ESTIMATING THE HIGH ORDER STATISTICS OF A FLUCTUATING PLUME IN THE NEUTRAL BOUNDARY LAYER

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Abstract: We use a Lagrangian stochastic micromixing model to predict the concentration fluctuations of a continuous release in a neutral boundary layer. We present the computational algorithm that implements the Interaction by Exchange with the Conditional Mean (IECM) model and we compare the numerical solutions with the experimental values in order to evaluate the reliability of the model. The influence of the source size on the concentration probability density function (PDF) in the near and far-field is discussed and some shortcomings of the model are pointed out.

Key words: *turbulent mixing; concentration fluctuations; Lagrangian stochastic modelling; atmospheric turbulence*

INTRODUCTION

The impact assessment of risks related to the dispersion of flammable gases and toxic substances requires a reliable description of the concentration probability density function (PDF) and estimations of the higher order moments of the concentration. Recent studies have shown that this can be achieved by means of Lagrangian stochastic micromixing models which simulate the effects of molecular diffusivity on the pollutant concentration fluctuations. Cassiani et al. (2005a) and Postma et al. (2011a) simulated the dispersion of a point source in the neutral boundary layer and compared the concentration fluctuation intensity with the experimental profiles provided by Fackrell and Robins (1982). The dispersion in the convective boundary layer (Cassiani et al., 2005b) and in the neutrally stratified canopy flow (Postma et al., 2011b) was also analysed. To our knowledge the first four concentration moments are numerically estimated only in homogeneous turbulence (Sawford, 2004), whereas the other authors restrict the analysis to the mean and standard deviation of the concentration field. Here we take advantage of recent wind tunnel experiments (Nironi et al., 2013) and we evaluate the accuracy of a Lagrangian stochastic micromixing model in estimating the first four concentration moments in a fluctuating plume in neutral boundary layer.

MODEL EQUATIONS

The temporal evolution of the velocity and position X_i of an ensemble of independent fluid particles is governed by the following differential stochastic equations:

$$dU_i^t = a_i(X_i^t, U_i^t, t)dt + b_{ij}(X_i^t, U_i^t, t)d\zeta_j \quad (1)$$

$$dX_i^t = (\langle u_i \rangle + U_i^t)dt \quad (2)$$

where U_i' is the Lagrangian velocity fluctuation related to the Eulerian mean velocity $\langle u_i \rangle$, $d\zeta_j$ is an incremental Wiener process (Gardiner, 1983) with zero mean and variance dt; a_i and b_{ij} are, respectively, the deterministic and stochastic-diffusive acceleration components, which are determined according to the well-mixed condition (Thomson, 1987).

The micromixing model takes into account the effects due to the molecular diffusivity. Each particle is characterised by a concentration C that evolves following the IECM model:

$$\frac{dC}{dt} = -\frac{C - \langle C|\mathbf{X}, \mathbf{U}\rangle}{t_m} \quad (3)$$

where $\langle C|\mathbf{X}, \mathbf{U}\rangle$ is the mean scalar concentration conditioned on the local position and velocity. The scalar micromixing time t_m represents the temporal scale of molecular diffusion. The parameterisation of t_m follows the formulation proposed by Cassiani et al. (2005a) and it is assumed to be proportional to the time scale of the relative dispersion process depending on velocity variance, kinetic energy dissipation rate, source size and particle flight time.

NUMERICAL MODELLING

The coupling between the Lagrangian stochastic model (equations (1) and (2)) and the micromixing model (equation (3)) is performed by the code SLAM (Safety Lagrangian Atmospheric Model). The micromixing time and conditional mean concentrations are estimated during a pre-processing step, computing the trajectories of a small ensemble of particles released at the source location. Afterwards, we consider the molecular diffusivity effects on the concentration fluctuations by simulating the influence of the background particles. This strategy allows us to obtain a multitude of concentration values and, therefore, suitably approximate the concentration

PDFs. The numerical experiments follow the approach of Cassiani et al. (2007); at the initial time-step a set of particles is uniformly distributed in the whole computational domain and each particle moves in accordance with the equations (1) and (2). During this motion the particle concentration changes (equation (3)) assuming a large variety of values that allows us to compute the high order statistics. In order to increase the solution accuracy, a time-averaging is performed. A suitable choice of the boundary conditions allows us to correctly reproduce the dispersion of the passive scalar and keep constant the number of particles during the simulations:

- top and lateral boundaries, the particle velocity and position are perfectly reflected and the concentration is absorbed;
- ground, the particles are elastically reflected and they conserve their concentration;
- inflow/outflow, periodic conditions are applied to the particle position and the absorption of the concentration is imposed;
- source, the influence of the source is taken into account by marking the near-source particles with a scalar concentration C_{src}:

$$C_{src} = \frac{Q}{2\pi\sigma_0^2\langle u_x\rangle}\exp\left(-\frac{r^2}{2\sigma_0^2}\right) \tag{4}$$

where Q is the source mass-flow, $\langle u_x\rangle$ is the horizontal mean velocity at the source location (x_s, y_s, z_s), σ_0 is the source size and $r^2 = (y-y_s)^2 + (z-z_s)^2$ is the distance from the particle to the source in yz-plane.

The computational algorithm is made of the following steps:

1. Pre-processing (equations (1) and (2)):
   - simulation of the trajectories of an ensemble of particles released at the source location;
   - estimate of the conditional mean concentration $\langle C|\boldsymbol{X},\boldsymbol{U}\rangle$ and micromixing time t_m.
2. Simulation of the concentration fluctuations (equations (1), (2) and (3)):
   - instantaneous release of a uniform particle distribution in the whole domain;
   - initialization of the particle properties ($\boldsymbol{X}$, $\boldsymbol{U}$, C);
   - main time loop:
     - loop on all the particles:
       - update particle velocity and position;
       - apply boundary conditions;
       - update particle concentration;
     - update cell-centred statistics;
   - update time-averaged statistics.

Such micromixing model requires the tuning of some free parameters in order to get a suitable accuracy in the solutions (Postma et al., 2011a): the Kolmogorov constant C_0, that influences the Lagrangian integral scales, the Richardson constant C_r and the micro-mixing constant μ_t, that affect the micromixing time scale, and the initial source distribution σ_0, that depends on the source diameter. It is worth noting that this approach requires a large amount of computational resources due to the elevated number of particles.

NUMERICAL EXPERIMENTS

Experimental set-up

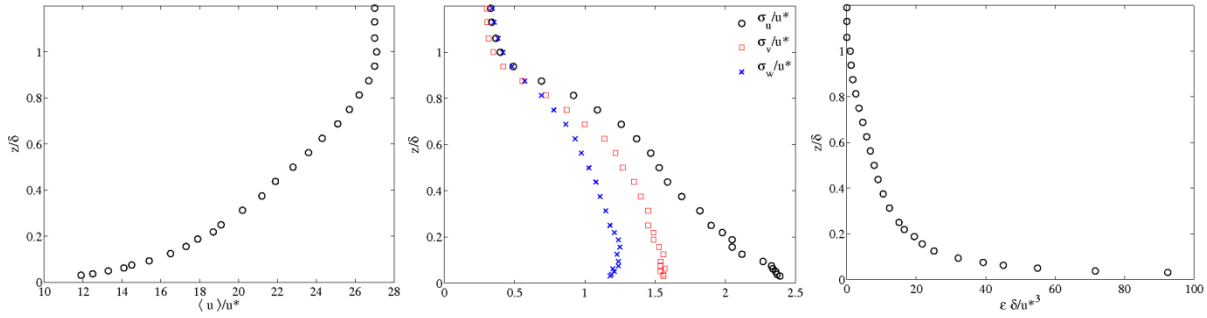

Figure 1: Non-dimensional vertical profiles of a) mean longitudinal velocity, b) r.m.s of the velocity components, c) turbulent kinetic energy dissipation rate (u^* is the friction velocity).

The numerical model is tested against a new experimental data set investigating the dispersion of a passive scalar emitted from a continuous point source in a neutral boundary layer (Nironi et al., 2013). The velocity field is characterised by the profiles shown in Figure 1 and obtained through Hot Wire Anemometry measures.

The experiments provide the concentration PDFs at increasing distance from the source location through measures of a passive scalar (ethane) concentration performed by means of a Flame Ionization Detector (FID).

The source is located at z_s/δ=0.19 and two diameters, d_s/δ, are taken into account, 3.75e-3 and 7.5e-3 (δ is the boundary layer depth).

Computational set-up

The numerical experiments concerned a preliminary study of the influence of the discretization parameters. We performed some simulations on a uniform grid, varying the cell dimensions and the time-step length, and we verified that the solutions are affected by neither the time-step length nor the space discretization (Figure 2). Table 1 summarizes the parameter values adopted in the simulations in order to have a satisfactory agreement with the experimental measures.

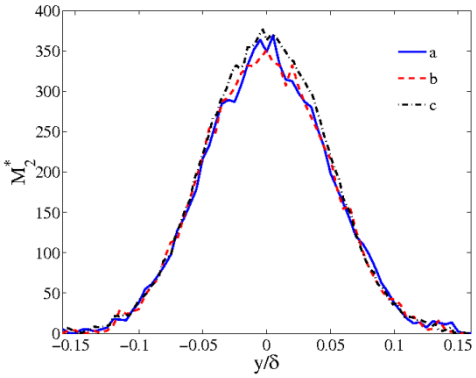

Table 1: Free parameter values adopted in the simulations.

C_0	σ_0	C_r	μ_t	velocity classes
5.0	$\sqrt{(2/3)}d_s$	0.3	0.6	3 x 3 x 3

Figure 2: Non-dimensional concentration standard deviation M_2^* vs. y/δ at the source height and x/δ=0.625; (a) Δt = 1.0e-3, Δx = 0.02, $\Delta y = \Delta z$ = 5.0e-3; (b) Δt = 5.0e-4, Δx = 0.02, $\Delta y = \Delta z$ = 5.0e-3; (c) Δt = 1.0e-3, Δx = 0.01, $\Delta y = \Delta z$ = 3.0e-3.

Results

The measures show that the source size does not affect the mean concentration whereas it influences the higher order moments (Fackrell and Robins, 1982). This influence is significant in the near-field (Figure 3) and it gradually becomes negligible for increasing distances from the source (Figure 4).

In order to test the reliability of the model, we computed the first four centred concentration moments and we compared them with the corresponding experimental values after a suitable adimensionalisation:

$$M_i^* = \left[\frac{1}{N_c}\sum_{p=1}^{N_c}(C_p - C_c)^i\right]^{1/i}\frac{u_\infty \delta^2}{Q} \tag{5}$$

where u_∞ is the velocity at the boundary layer height, N_c and C_c are the number of particles and the mean concentration in the cell, respectively, and C_p is the particle concentration.

In the near-field (Figure 3) the model is able to reproduce the influence of the source size on the concentration fluctuations showing a good agreement with the experimental values; in particular, Figures 3b-3d shows that the differences in the concentration PDFs due to the source diameter are correctly simulated. In the far-field (x~500÷1000 d_s) the model suitably simulates the negligibility of the source size on the computed standard deviation and the agreement with the experimental values is satisfactory (Figure 4a and 4b). On the contrary, some discrepancies occur on the higher order moments: the numerical solutions overestimate the experimental results and some differences due to the source diameter persist (Figures 4c and 4d). Indeed the loss of influence of the source size is delayed with respect to the experiments. If we define the relative difference between the computed moments for the two source sizes *S1* (d_s/δ=7e-3) and *S2* (d_s/δ=3.75e-3) as

$$D_{rel} = \sqrt{\frac{\int_{-\infty}^{\infty}[(M_i^*)_{s1} - (M_i^*)_{s2}]^2 dy}{\int_{-\infty}^{\infty}[(M_i^*)_{s1}]^2 dy}} \tag{6}$$

we observe that D_{rel} reduces from x/δ =3.75 and x/δ =5 (Figure 5) as shown in Table 2.

Table 2: Relative difference between the third and fourth moments at different distances x/δ.

x/δ	D_{rel} M_3^*	D_{rel} M_4^*
3.75	0.17	0.36
5.0	0.12	0.29

The reasons for this delay can be reasonably attributed to the shortcomings of the micromixing model that can be related to the formulation of the micromixing time scale.

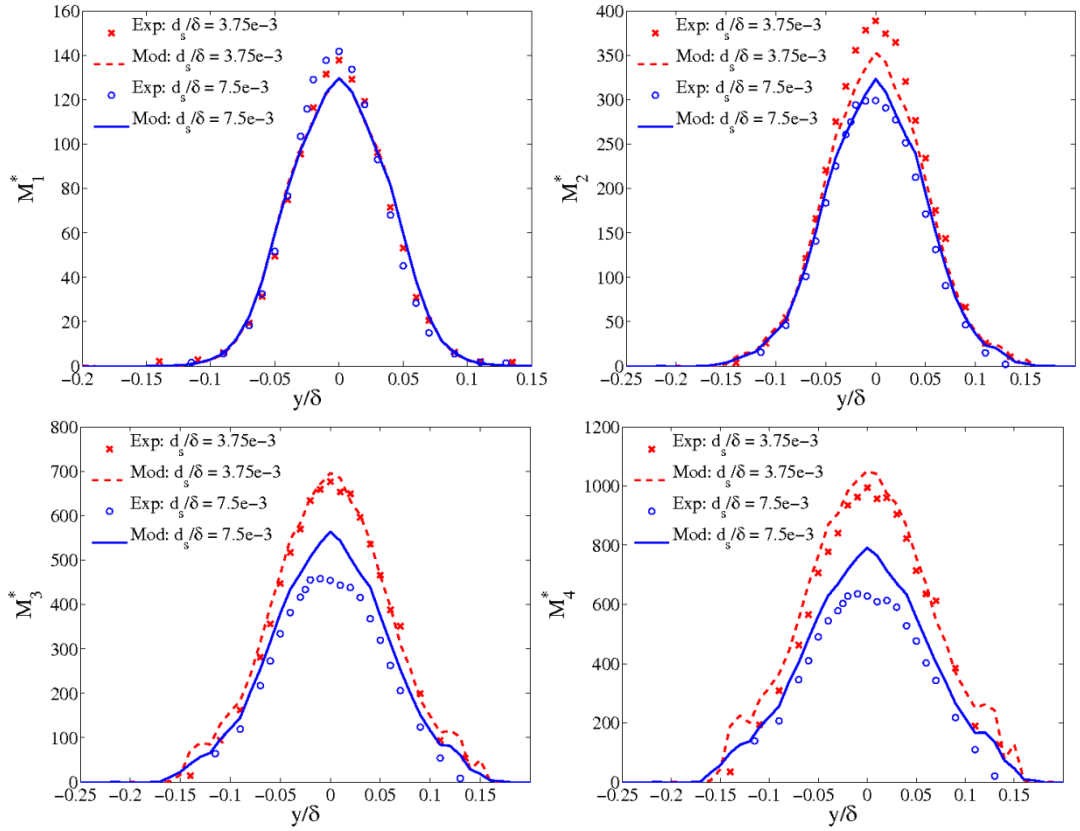

Figure 3: Non-dimensional concentration statistics vs. y/δ evaluated at the source height and $x/\delta = 0.625$.

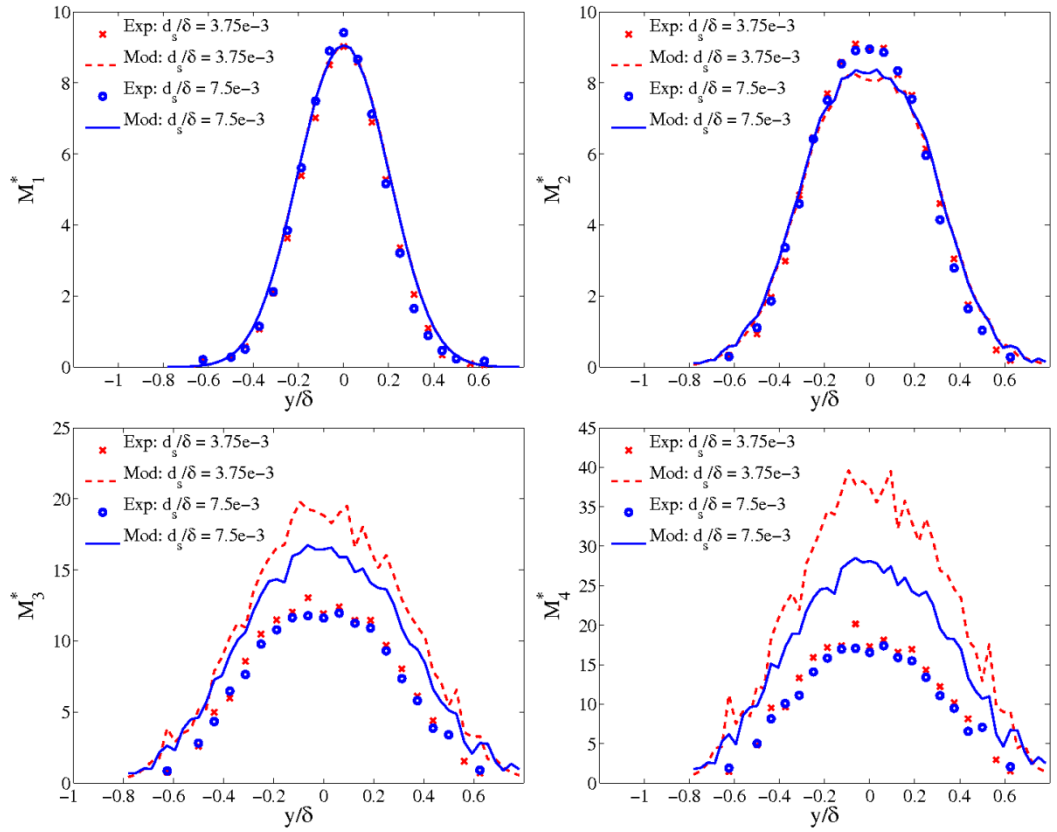

Figure 4: Non-dimensional concentration statistics vs. y/δ evaluated at the source height and $x/\delta = 3.75$.

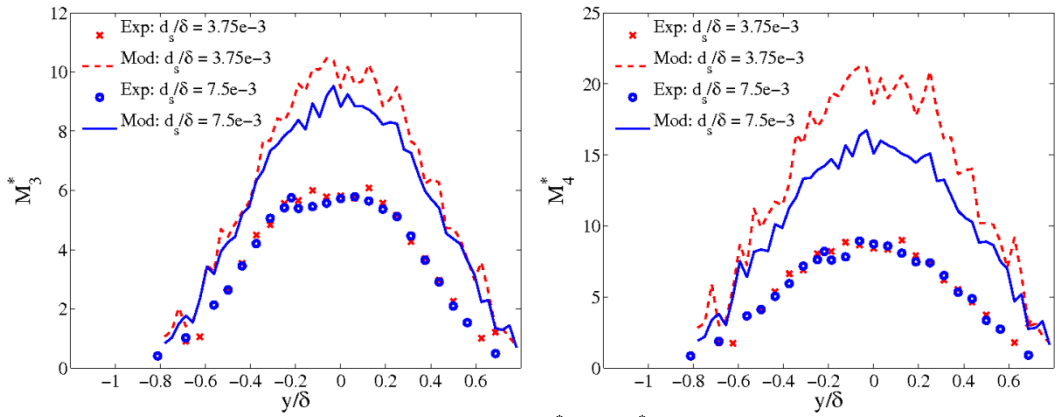

Figure 5: Non-dimensional third and fourth moments (M_3^* and M_4^*) of the concentration vs. y/δ evaluated at the source height and $x/\delta = 5$.

CONCLUSIONS

The ability of the Lagrangian stochastic micromixing model SLAM to estimate the concentration fluctuations was investigated. We simulated the dispersion of a fluctuating plume produced by a continuous release from a point source in the neutral boundary layer and we compared the numerical results with a new experimental data set. The numerical solutions show that the model is able to correctly simulate the concentration statistics in the near-field, reproducing the source size effects on the high order moments. In the far-field the numerical and experimental values of the mean and standard deviation of the concentration are in good agreement. Differently the model overestimates the third and fourth moments with respect to the experiments. Moreover, the experimental profiles show that the source size influence vanishes in the far-field after x~500÷1000 d_s, whereas in the numerical simulations such effect is delayed and it occurs at longer distances. This behaviour shows the shortcomings of the model and the need of further developments in order to improve the accuracy of the solutions.

The main shortcoming of such model is the high computational cost. The large number of particles, required to get a suitable accuracy in the numerical solutions, produces a large request of RAM and elevated CPU time; that limits the applicability of the model to real scale problems in complex geometries.

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