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## MODELLING CONCENTRATION FLUCTUATIONS IN A TURBULENT BOUNDARY LAYER: SENSITIVITY OF A LAGRANGIAN MODEL TO DISSIPATION RATE ESTIMATES

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**Abstract:** Lagrangian dispersion models require estimates of local production and dissipation rate of turbulent kinetic energy (t.k.e). Both quantities are hardly measurable in atmospheric flows. In laboratory experiments, although the t.k.e. production measurements can be easily achieved, the direct measurement of the dissipation ratio still represents a hard task. Therefore, this quantity is generally estimated indirectly, as a residual of the turbulent kinetic energy budget under a series of simplifying assumptions.

In this study we evaluate the sensitivity of a lagrangian model to different estimates of t.k.e. dissipation rate in simulating passive scalar dispersion in a turbulent boundary layer over a rough surface.

The estimates of t.k.e. dissipation are obtained by means of hot-wire anemometry velocity measurements in wind tunnel experiments. Two different estimates of epsilon are calculated. These values are used to simulate pollutant dispersion emitted by a linear elevated source with a lagrangian model which integrates a macromixing and a micromixing scheme. Comparison between numerical and experimental results allow us to discuss the performance of the model in predicting mean and fluctuating concentration and to define its sensitivity to the differences in the estimates of t.k.e. dissipation.

**Key words:** Lagrangian model, macromixing, micromixing, concentration fluctuation, turbulent boundary layer.

## INTRODUCTION

The impact assessment of accidental release of toxic or inflammable substances in the atmosphere requires the computation of the near field of the probability density function (p.d.f.) of their concentration, or at least the estimation of the first two moments of the p.d.f. - the mean and the variance. For this reason, a significant body of research work in the last years has been devoted to improve models for the estimate of the higher order moments of pollutant concentration p.d.f. in turbulent flows.

A strategy in order to estimate higher order moments of the pollutant concentration p.d.f. is to perform Lagrangian stochastic modeling of the dispersion of pollutant particles integrating a macro-mixing and a micro-mixing scheme (see for example Cassiani *et al.*, 2005a; Cassiani *et al.*, 2005b; Sawford, 2004, Luhar and Sawford, 2005; Amicarelli *et al.*, 2008).

These models usually require local estimates of the turbulent kinetic energy (t.k.e.), referred here as  $q$ , of its production  $p$  and dissipation  $\epsilon$ . Direct measurements of  $\epsilon$  are not easy to achieve, even in laboratory experiments. Therefore this quantity is usually estimated indirectly, assuming a series of simplifying assumptions. In this paper we test the sensitivity of LAGFLUM (Amicarelli *et al.*, 2008), a lagrangian code integrating a macromixing and a micromixing schemes, to different approximations in the estimate of  $\epsilon$ . These were achieved in laboratory experiments simulating pollutant dispersion in a neutral atmospheric boundary layer (Salizzoni *et al.*, 2009).

In the following paragraphs capital letters refer to lagrangian quantities. Eulerian time averaged variables are indicated with small letters, whereas the apex indicates fluctuating quantities. Overbars denote time averaging and brackets ensemble averaging.

## LAGFLUM: A LAGRANGIAN MODEL FOR CONCENTRATION FLUCTUATION

The LAGFLUM model combines a macromixing and a micromixing Lagrangian scheme in order to compute mean and standard deviation of passive tracer concentration. The mean concentration is computed during the first phase of the model run by the macromixing scheme, while the concentration variance is obtained by the micromixing scheme in a second phase using the already-computed mean concentration.

The macromixing scheme, is based on the so called “well-mixed” condition and describes the motion of marked fluid particles. As pointed out by Pope, S. B. (1998), for high Reynolds numbers the mean concentration and the mean conditioned on the velocity are unaffected by the value of molecular diffusivity. Therefore, polluted fluid particles which do not exchange pollutant mass with the surrounding ones can be used to estimate the averaged concentrations. This condition ensures a well-founded behaviour of the model in inhomogeneous turbulence. The macromixing scheme is based on the following set of stochastic equations:

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

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

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

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

$$2B_{ij} = b_{ik}b_{jk} = \delta_{ij}C_0\varepsilon \quad (4)$$

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

where  $C_0$  is the Kolmogorov constant, assumed equal to 2 (according to Cassiani M. *et al.*, 2007a),  $g_a$  is the probability density function of the Eulerian velocity,  $\delta_{ij}$  is the Kronecker delta,  $V_{ij}$  is the one-point velocity covariance matrix, which we assume to be diagonal, and  $\varepsilon$  is the rate of dissipation of the turbulent kinetic energy.

One hundred thousand particles have been released, in order to calculate both the mean  $\langle C \rangle$  and the conditional mean concentration  $\langle C|U \rangle$ . This was then used to compute the instantaneous concentration  $C$  of each fluid particle with a micromixing scheme. The micromixing model adopted here is the IECM:

$$\frac{dC}{dt} = -\frac{C - \langle C|U \rangle}{t_m} \quad (7)$$

where  $t_m$  is the mixing time scale (Amicarelli *et al.* 2008).

**EXPERIMENTAL SET UP**

Experiments have been carried out at the reticulating wind tunnel of the Ecole Centrale de Lyon. An adiabatic atmospheric boundary layer was simulated by combining vortex generators at the beginning of the test section and wall roughness, which was made up by square bars placed normal to the wind and regularly spaced by a distance equal to the bars height  $H$ . The depth  $\delta$  of the boundary layer was about 0.6 m, about ten times the height of the bars  $H=0.06$  m. Velocity measurements were performed by hot-wire anemometry with a sampling frequency equal to 10000 Hz, using a single X-probe. The passive tracer (ethane) was injected from an elevated line source. Vertical profiles of instantaneous passive tracer concentration were measured with a Flame ionisation detector (FID) for increasing distances from the source, with a sampling frequency of about 500 Hz. Details on the experimental apparatus and a description of the dynamical condition of the boundary layer flow can be found in Salizzoni *et al.* (2008). Details on the passive tracer source and concentration measurements are given in Salizzoni *et al.* (2009, 2010).

The velocity profiles, as a function of the vertical coordinate  $z'=z/\delta$  used as an input for LAGFLUM are given in Figure 1. The mean velocity profile above the obstacles, i.e. ( $z'>0.1$ ), are dependent only on the vertical coordinate  $z$  (Salizzoni, 2008) and that is measured by hot wire anemometry. Within the cavity we assume a spatially averaged description of the flow along the  $x$  - axis and therefore  $u=0$  (Figure 1a).

The mean longitudinal velocity  $u(z)$  is well fitted in its lowest part ( $0 < z' < 0.3$ ) by a logarithmic law

$$u(z) = \frac{u_*}{K} \ln \left( \frac{z-d}{z_0} \right) \quad (8)$$

Where  $k$  is the Von Karman constant,  $u_*$  is the friction velocity,  $d$  is the displacement height and  $z_0$  is the roughness length. In our experiment we have  $u_*=0.33$  m/s,  $d=58$ mm and  $z_0=0.31$  mm.

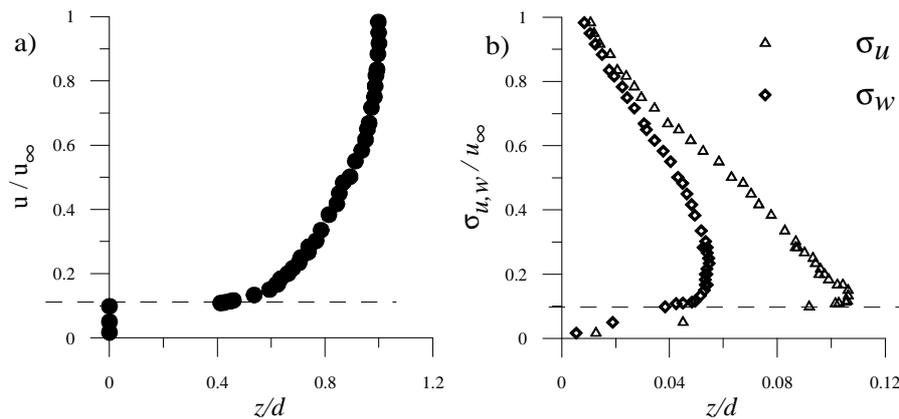


Figure 1. Vertical profile of non-dimensional a) mean longitudinal velocity and b) standard deviation of the longitudinal and vertical velocities. The dotted line indicates the obstacle height. See text for details.

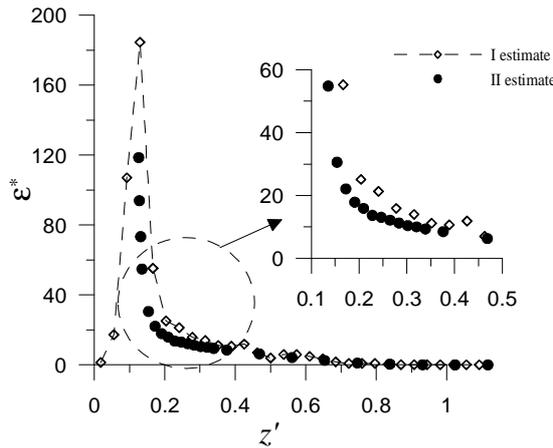


Figure 2. Comparison between two independent estimates of  $\epsilon^*$ , the non dimensional turbulent kinetic energy dissipation. *Estimate I* is obtained by mean of equation (9), *Estimate II* refers to equation (10). See text for details.

The profiles of the two estimates of the non dimensional t.k.e.  $\epsilon^* = \epsilon (\delta H) / U_\infty^3$  are given in Figure 2. The first estimate  $\epsilon_1$ , referred to as *I estimate*, is computed following Beljaars *et al.* (1987), Kitada (1987) and Detering and Etling (1985) as

$$\epsilon_1(z) = 0.3q \sqrt{\left(\frac{\partial u}{\partial z}\right)^2} \quad (9)$$

where  $q$  is the turbulent kinetic energy. The second estimate  $\epsilon_2$ , referred to as *II estimate*, is achieved evaluating the instantaneous velocity gradients of the horizontal velocity adopting Taylor’s hypothesis and assuming the local isotropy of the turbulent velocity field:

$$\epsilon_2(z) = v \frac{1}{u(z)} \overline{\left(\frac{\partial u'}{\partial t}\right)^2} \quad (10)$$

The values within the cavities, i.e.  $z' < 0.1$ , referred to as  $\epsilon_c$ , have been estimated as:

$$\epsilon_c(z) = \frac{2}{C_0 T_L} \frac{2}{3} q(z)$$

where  $T_L$  is the lagrangian time scale. This was roughly estimated as  $T_L = H/U_H$  being  $U_H$  the mean longitudinal velocity at roof level. The values of  $q(z)$  were inferred from PIV measurements performed by Salizzoni *et al.* (2009) which show that this variable is almost constant with height within the cavities.

Figure 2 shows that the main differences between the two estimates are completely concentrated in the lowest part of the boundary layer flow, i.e.  $z' < 0.4$  and can reach a difference of about 50% close to the top of the obstacles.

**COMPARISON BETWEEN EXPERIMENTAL AND NUMERICAL RESULTS**

The results provided by LAGFLUM with the two estimates of  $\epsilon$  have been compared to the experimental results. Figure 3 show vertical profiles of mean concentrations for increasing distances from the source. The profiles show that the differences in the estimates of  $\epsilon$  almost do not affect the simulated concentration values in most of the domain. Significant differences can be detected only at large distances from the source, when the plume begins interacting with the obstacles.

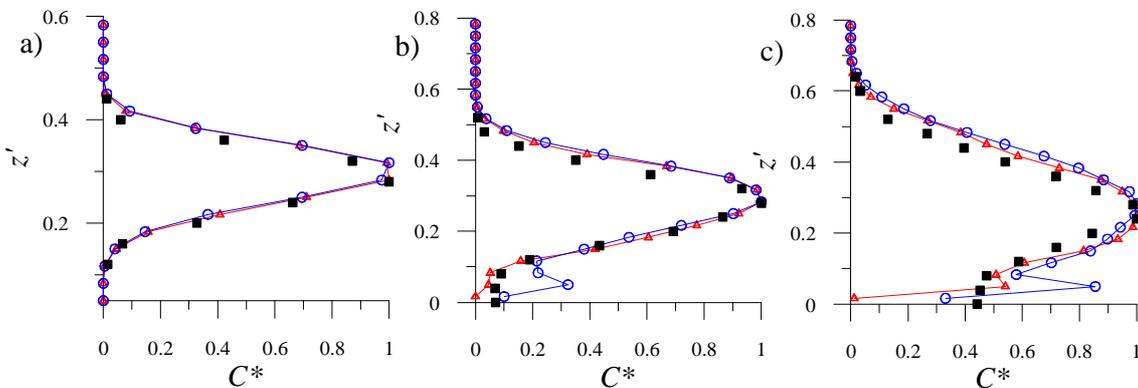


Figure 3. Vertical profiles of non dimensional mean concentration  $C^* = c/c_{max}$ . Comparison between experimental and numerical results obtained with the two independent estimates of  $\epsilon^*$  at different distances from the source. a)  $x/\delta = 0.975$ ; b)  $x/\delta = 1.1875$ ; c)  $x/\delta = 3.675$ . Squares: experiments; triangles: *Estimate I* - equation (10); circles: *Estimate I* - equation (11).

Similar conclusions can be drawn for the standard deviations profiles, which are shown in Figure 4. The calculated values of  $\sigma_c$  seem to be more sensitive to the input data of  $\varepsilon$ . However this increased dependence on  $\varepsilon$  does not lead to systematic differences which can be easily interpreted.

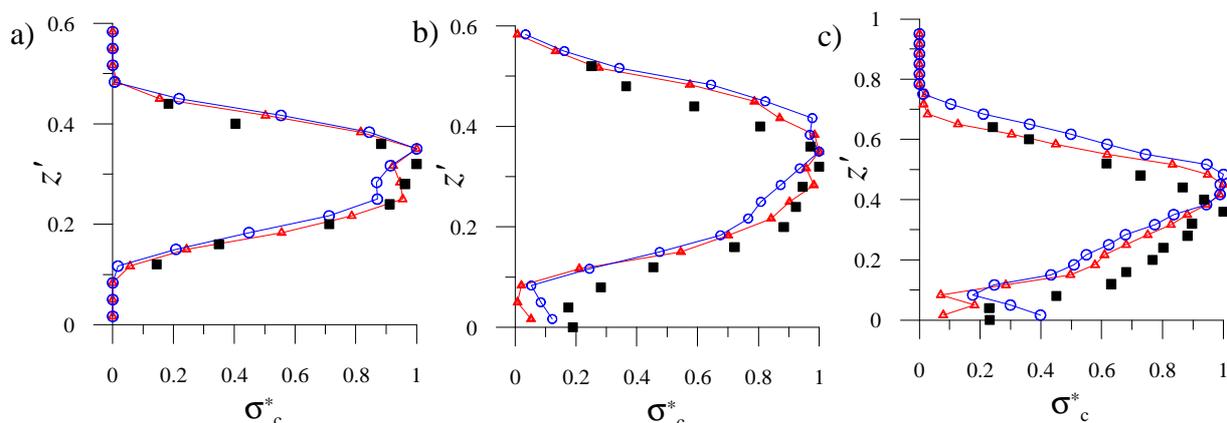


Figure 4: Vertical profiles of non dimensional standard deviation of the concentration  $\sigma_c^* = \sigma_c / \sigma_{c,max}$ . Comparison between experimental and numerical results obtained with the two independent estimates of  $\varepsilon^*$  at different distances from the source. a)  $x/\delta=0.975$ ; b)  $x/\delta=1.1875$ ; c)  $x/\delta=3.675$ . Squares: experiments; triangles: *Estimate 1* - equation (10); circles: *Estimate 1* - equation (11).

In order to evaluate the overall performances of the code LAGFLUM we have also estimated a series of statistical indicators and compared them with the reference values given by Franke *et al.* (2008). Namely these are the fractional bias (FB), the normalised mean square error (NMSE), the factor FAC 2, the geometric mean (MG) and the geometric variance (VG). The comparison in Table I shows that the model satisfies most of the requirements identified by Franke *et al.* (2008).

Table 1. Validation metrics for LAGFLUM's mean concentration results compared with the reference values given by Franke *et al.* (2008).

	FB	NMSE	FAC2 (%)	MG	VG
Franke <i>et al.</i> (2008)	$\pm 0.3$	4.0	50	$0.7 \div 1.3$	1.6
LAGFLUM	0.03	0.06	77	0.82	2.13

## CONCLUSIONS AND PERSPECTIVES

We have tested the model LAGFLUM against wind tunnel measurements in order to evaluate its sensitivity on the meteorological input, focusing on the estimate of the t.k.e dissipation  $\varepsilon$  in a simulated atmospheric boundary layer flow.

Results show that the approximate values of  $\varepsilon$  given by the k- $\varepsilon$  theory with time-averaged quantities do not differ significantly from that obtained by computing velocity gradients from instantaneous measurements, except in the lowest part of the boundary layer. In both cases the model agrees well with the experimental results in a large part of the domain. The main differences between experiments and simulations can be detected close to the obstacle top and within the cavities. These differences are certainly due to the rough description of the flow given in the cavities, which have therefore to be more accurate in order to improve the performances of the model. Furthermore, given the high sensitivity of the code to the dynamical conditions of the lowest part of the boundary layer, we believe that more instructive comparisons could be made considering the case of a ground level source.

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