Sensitivity analysis of a concentration fluctuation model to dissipation rate estimates

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Abstract: Lagrangian dispersion models require estimates of the local dissipation rate (ε) of turbulent kinetic energy (k). In this study, we evaluate the sensitivity of a Lagrangian model to different estimates of ε in simulating passive scalar dispersion in a turbulent boundary layer over a rough surface. Two different estimates of ε 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 allows us to discuss the performance of the model and to define its sensitivity to ε.

Keywords: LAGFLUM; environmental pollution; atmospheric dispersion; concentration fluctuations; Lagrangian dispersion models; micromixing; wind-tunnel experiment; dissipation rate.

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1 Introduction

The impact assessment of an accidental release of toxic or inflammable substances into the atmosphere would require the computation of the probability density function of their concentration (f_C) close to the source, or at least the estimation of the first moments of f_C – in practice we could refer to the mean and the variance.

Lagrangian micro-mixing modelling seems to provide a valid numerical tool in estimating concentration fluctuations. In this context, several dispersion phenomena have been studied: 1D scalar dispersion in grid turbulence from line or area sources (Sawford, 2004) and for multiple reacting pollutants (Sawford, 2006); 1D multiple scalar dispersion in convective boundary layers from area sources (Luhar and Sawford, 2005); 2D dispersion from point or line sources in neutral boundary layers (Cassiani et al., 2005a; Amicarelli et al., 2011), in convective boundary layers (Cassiani et al., 2005b), and from single or multiple sources in canopy turbulence (Cassiani et al., 2007; Dixon and Tomlin, 2007); 3D dispersion in canopy turbulence (Amicarelli et al., in press). These models usually require local estimates of k and its dissipation rate ε. Direct measurements of ε are not easy to achieve, even in laboratory experiments. Therefore, this quantity is usually estimated indirectly, assuming a series of simplifying assumptions. Several procedures have been adopted to obtain this input parameter, to

feed micro-mixing models. Sawford (2006) refers to analytical formulations; Luhar and Sawford (2005) and Cassiani et al. (2005a, 2005b) use some parameterisations derived from similarity theories; Dixon and Tomlin (2007) adopt estimations provided by k-ε schemes of Reynolds' average models; Cassiani et al. (2007) use equation (8), as discussed in the following.

In this paper, we test the sensitivity of LAGFLUM (LAGrangian FLUctuation Model; Sapienza University of Rome; Leuzzi et al., in press; Amicarelli et al., in press), a Lagrangian code integrating a macromixing and a micromixing scheme, to different approximations in the estimation of ε. These were derived using the meteorological measures obtained during a laboratory experiment simulating pollutant dispersion in a neutral atmospheric boundary layer (Salizzoni et al., 2008, 2009a). In the following paragraphs, capital letters refer to Lagrangian quantities. Eulerian averaged variables are indicated with small letters, whereas the apex indicates fluctuating quantities. Overbars denote time averaging and brackets ensemble averaging.

2 LAGFLUM: a Lagrangian model for concentration fluctuations

The numerical model LAGFLUM combines a macromixing and a micromixing Lagrangian scheme to compute the mean and the standard deviation of the concentration of a passive scalar. The mean concentration is estimated during the first computational phase by the macromixing scheme, while the concentration variance is obtained by the micromixing scheme in a second computational step using the already-computed mean concentrations.

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 (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 well-founded behaviour of the model in inhomogeneous turbulence. The macromixing scheme is based on the following set of stochastic equations (Thomson, 1987):

$$\mathrm{d}U_i = a_i\left(X,U,t\right)\mathrm{d}t + b_{ij}\left(X,U,t\right)\mathrm{d}\xi_j\,,\ \mathrm{d}X_i = U_i\mathrm{d}t, \tag{1}$$

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 (as used in Thomson, 1987). Here, the subscripts refer to the axis direction. The functions a_i and b_{ij} in stationary conditions can be calculated as follows:

$$a_i = -B_{ij}\left(V^{-1}\right)_{jk}\left(U_k - u_k\right) + \phi_i / g_a\,,\ 2B_{ij} = b_{ik}b_{jk} = \delta_{ij}C_0\varepsilon, \tag{2}$$

$$\frac{\phi_i}{g_a} = \frac{1}{2}\frac{\partial V_{il}}{\partial x_l} + u_l\frac{\partial u_i}{\partial x^l} + \left(\frac{1}{2}\left(\mathbf{V}^{-1}\right)_{lj}u_m\frac{\partial V_{il}}{\partial x_m} + \frac{\partial u_i}{\partial x_j}\right)\left(U_j - u_j\right) + \frac{1}{2}\left(\mathbf{V}^{-1}\right)_{lj}\frac{\partial V_{il}}{\partial x_k}\left(U_j - u_j\right)\left(U_k - u_k\right) \tag{3}$$

where u_i is the i-component of the mean velocity vector, C_0 is the Kolmogorov constant, assumed equal to 2 (according to Cassiani et al., 2007), g_a is the probability density function of the Eulerian velocity, δ_{ij} is the Kronecker delta, V_{ij} is the one-point velocity covariance matrix (whose elements are the velocity variances and co-variances), which is approximately diagonal. Einstein's notation is applied to all the subscripts but '$_i$'.

It is worth noting that the dissipation rate ε is assumed as an input of the model (together with the means and the standard deviations of velocity), and it is used to compute both the 'drift' term a_i and the stochastic term b_i (equations 1–3).

10^5 particles have been released, to calculate both the mean $<C|\boldsymbol{x}>$ and the conditional mean concentration $<C|\boldsymbol{U},\boldsymbol{x}>$. This represents the mean concentration of a sub-ensemble of virtual realisations of the dispersion phenomenon, approximately sharing the same instantaneous velocity field at a certain position (and time). This parameter is in some ways representative of a locally space-averaged concentration, related to an instantaneous plume. Then it rules the actual molecular diffusion fluxes, much better than the mean concentration. $<C|\boldsymbol{U},\boldsymbol{x}>$ is finally used to compute the instantaneous concentration C of each fluid particle, adopting the micromixing scheme IECM (Interaction by the Exchange with the Conditional Mean; Sawford, 2004(a); Pope, 1998):

$$\mathrm{d}C/\mathrm{dt} = -(C - < C \mid \boldsymbol{U},\boldsymbol{x} >) / t_m, \tag{4}$$

where t_m is the mixing time scale (using the formulation from Amicarelli et al., in press).

3 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 δ of the boundary layer was about 0.6 m, nearly 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 10,000 Hz, using a single X-probe. The passive tracer (ethane) was injected from an elevated line source, located at (x_s=0.03 m; z_s=3H=0.18 m). Its pollutant mass discharge (Q_s) is not available; nevertheless its value is not strictly necessary for this study, as the concentration measurements are scaled on Q_s (following a common practice – Franke et al., 2008 – which renders the concentration values non-dimensional). 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. (2009b, in press).

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), is dependent only on the vertical coordinate z, and is measured by hot wire anemometry. The mean longitudinal velocity $u(z)$ is instead well fitted within the surface boundary layer (SBL; 0.1<z'<0.2) by a logarithmic law:

$$u(z) = \frac{u_*}{k_v} \ln\left(\frac{z-d}{z_0}\right) \tag{5}$$

where k_v 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. Within the canyons, we assume a null velocity, which seems to be a simple approximation, but compatible with the rough spatial resolution needed. The profiles of the measured standard deviations of velocity are reported in Figure 2 (right). They are homogeneous within the SBL, which seems to lie in the zone H<z' <1.5–2H (this upper limit agreeing with Fischer et al. (2010) and Salizzoni et al. (2011)). Their canopy values (z'<1) are just a linear extrapolation of the above values, in agreement with the vertical evolution of the corresponding profiles of similar studies (Bezpalcova, 2007), related to neutral boundary layers within a regular canopy (no measured meteorological input for these regions were used). The peaks of σ_u and σ_w do not refer to the ground level, but to the obstacle tops. As we just wanted to process meteorological measurements to feed the dispersion model, analyse the effectiveness of this simplified procedure and avoid a CFD modelling of the main flow, we finally kept this 1D input (Salizzoni et al., 2008). Furthermore, we approximately neglect the correlation between the velocity components when applying the macro-mixing scheme.

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

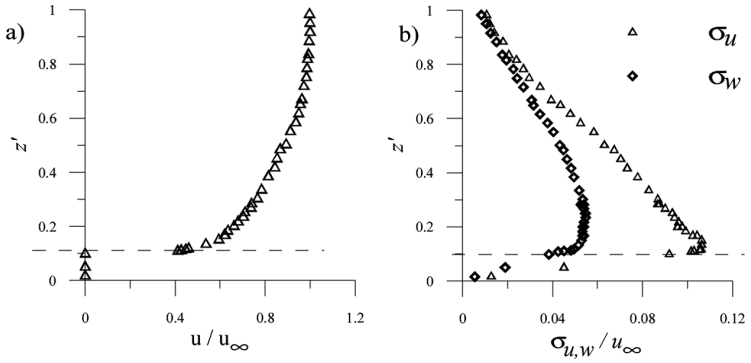
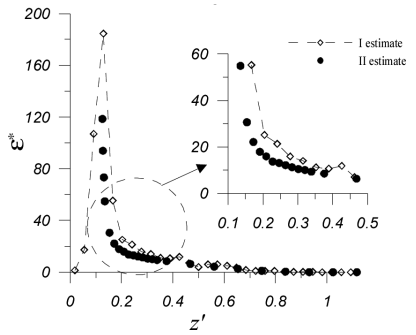


Figure 2 Comparison between two independent estimates of ε^*, the non-dimensional turbulent kinetic energy dissipation. *estimate I*: equation (6), *estimate II*: equation (7)



The profiles of the two estimates of the non-dimensional $\varepsilon^*=\varepsilon\,(\delta-H)/U_\infty^3$ are given in Figure 2. The first estimate, ε_1, referred to as *I estimate*, is computed following Beljaars et al. (1987), Kitada (1987) and Detering and Etling (1985) as:

$$\varepsilon_1(z) = 0.3k\sqrt{\left(\frac{\partial u}{\partial z}\right)^2}\,. \tag{6}$$

The second estimate, ε_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:

$$\varepsilon_2(z) = \nu\frac{1}{u(z)}\overline{\left(\frac{\partial u'}{\partial t}\right)^2} \tag{7}$$

where ν is the kinematic viscosity. The values within the cavities, i.e., $z'<0.1$, referred to as ε_c for both the simulations, have been estimated as a function of the integral Lagrangian time scale T_L (Thomson, 1987):

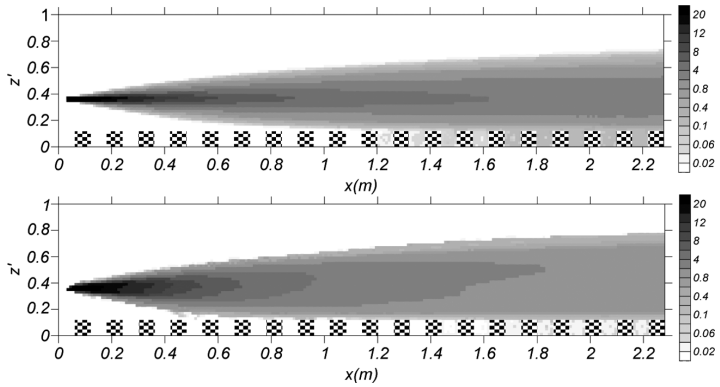
$$\varepsilon_c(z) = \frac{2}{C_0 T_L}\frac{2}{3}k(z) \tag{8}$$

We roughly assumed $T_L=H/U_H$. U_H being the mean longitudinal velocity at roof level. As no meteorological input inside the canopy has been used, we can just provide a very approximate estimation of ε in these regions, when using equation (8). Nevertheless, we obtain the same kind of evolution (ε growing with z; Figure 2, $z'<0.1$) as Cassiani et al. (2007), who analogously applied the same equation. In fact, the surface neutral boundary layer, characterised by a constant friction velocity and a hyperbolic evolution of ε (decreasing with z), just lies at $0.1<z'<0.2$, whilst the canyons do not refer to these evolutions. 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.

3 Comparison between experimental and numerical results

An example of the simulated fields of the mean and the standard deviation of concentration is shown in Figure 3. The height of the maximum of the mean concentration slightly slows down when increasing the distance from the source, because of its interaction with the canopy, whose overall effect is to confine the plume, increasing the mean concentrations in the lowest part of the domain. As the plume is entrained inside the canyons, a higher turbulent mixing in these confined zones decreases the gradient of the mean concentration and the absolute values of the concentration fluctuations. The standard deviation of concentration has then lower values inside the canyons and at their tops.

Figure 3 Simulated fields of the mean (up) and the standard deviation (down) of concentration (estimate I)



The low values of σ_C at the canopy top impose a sort of boundary condition for the upper domain, causing a corresponding reduction of the standard deviation of concentration all over the domain. These minima are even due to the direct interaction of the plume with the obstacle tops, which locally zeroes the mean concentration gradients and then the production rate of the concentration variance. The height related to the maximum value of the standard deviation along the vertical is then raised up, when increasing the distance from the source. In other words, the canopy acts like a sink for the concentration variance.

Numerical results obtained with the two estimates of ε have been compared to the experimental results. Figures 4 and 5 shows some vertical profiles of the mean and the standard deviation of concentration. In both cases, the main differences between experiments and simulations can be detected close to the obstacle tops and within the cavities. They are only due to the differences in the estimation of ε at the top of the canopy (and a few levels above it). At this level, in fact, the vertical turbulent fluxes of concentration are revealed to be sensitive to ε. These fluxes control the concentration values within the canopy. Further, this sensitivity of the numerical results to the input of the lowest part of the boundary layer points out a significant potential source of error, related to the simplifying assumptions adopted during the input processing.

Figure 4 Vertical profiles of the normalised mean concentrations $C^*=\langle c\rangle/\langle c\rangle_{max}$. Comparison between experimental and numerical results, at different distances from the source: (a) x/δ= 0.975; (b) x/δ= 1.1875 and (c) x/δ= 3.675. Squares: experiments; triangles: *Estimate I* (6); circles: *Estimate II* (7) (see online version for colours)

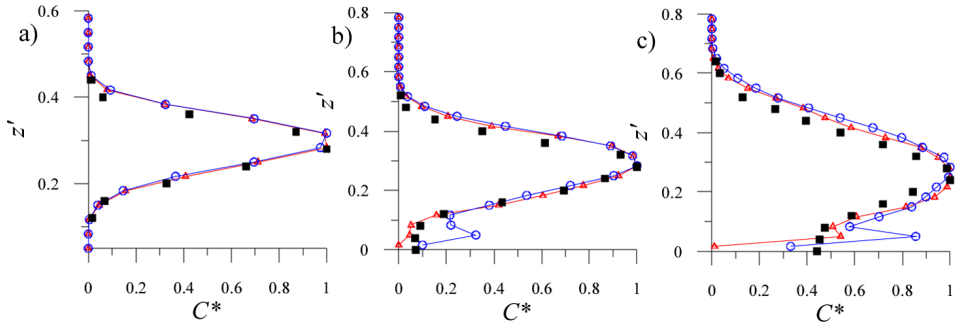
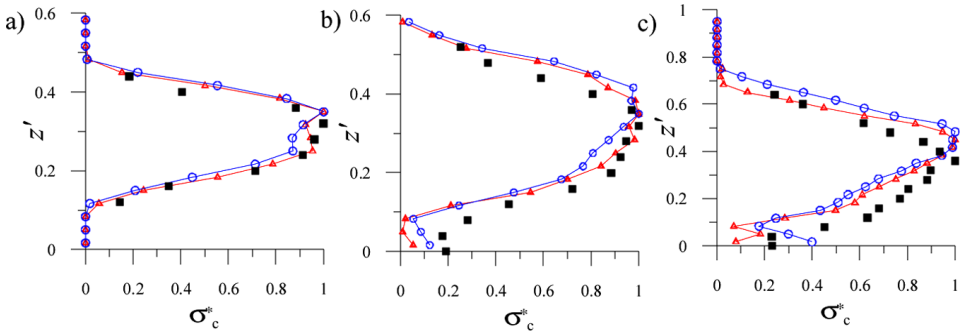


Figure 5 Vertical profiles of the normalised standard deviation of concentration (σ_c*= σ_c /$\sigma_{c\,max}$). Same legend as Figure 4 (see online version for colours)



To evaluate the overall performances of LAGFLUM, we have also estimated a series of statistical indicators and compared them with the references values given by Franke et al. (2008), defining the state of art for a pollutant dispersion model. Namely, these are the fractional bias (FB, the mean relative error); the Normalised Mean Square Error (NMSE); the factor FAC2 (the percentage of the simulated values lying between the 50% and the 200% of the corresponding measured values); the geometric mean (MG); and the Geometric Variance (VG) of the error. The comparison in Table 1 shows that the model satisfies most of the requirements identified by Franke et al. (2008). These overall metrics relate to estimation I (no relevant differences if compared to the ones obtained using estimation II, even because almost all the monitoring points lie above the canopy, where the simulations better agree). As no measurements of the absolute value of σ_C are available, we cannot finally compute the corresponding metrics.

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

	FB	*NMSE*	*FAC2* (%)	*MG*	*VG*
Franke et al. (2008)	± 0.3	4.0	50	0.7 ÷1.3	1.6
LAGFLUM	0.03	0.06	77	0.82	2.13

4 Conclusions and perspectives

We have tested the concentration fluctuation model LAGFLUM on a wind tunnel dataset, obtained from a 2D canopy neutral boundary layer flow. We have focused on the model sensitivity to the dissipation rate ε of the turbulent kinetic energy k. ε has been estimated using two alternative formulations, derived from simplified balance equations for k. The first (6) depends on the mean velocity gradient, the latter (7) on the time derivatives of the instantaneous velocities. These estimations usually agree, but at the top of the obstacles, where further investigation is needed. The results of the two corresponding simulations, in terms of mean and standard deviation of concentration, show their main differences inside the canyons. In these regions, in fact, the concentration statistics are ruled by the corresponding scalar turbulent fluxes at the top of the obstacles, which noticeably depend on ε. The results finally show how the standard deviation of

concentration is of the same order of magnitude as the mean, even in the presence of a canopy, which locally represents a sink for the concentration fluctuations.

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