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A NEW MODEL FOR ESTIMATING THE CONCETRATION STATISTICS IN A TURBULENT BOUNDARY LAYER

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Abstract: We study the reliability of the Lagrangian stochastic micromixing method in predicting higher-order statistics of the passive scalar concentration induced by an elevated source (of varying diameter) placed in a turbulent boundary layer. To that purpose, we analyse two different modelling approaches by testing their results against the wind-tunnel measurements discussed in Nironi et al (2015). The first is a probability density function micromixing model, which simulates the effects of the molecular diffusivity on the concentration fluctuations by taking into account the background particles. The second is a new model, named VPΓ, conceived in order to minimize the computational costs. This is based on the Volumetric Particle Approach providing estimates of the first two concentration moments with no need for the simulation of the background particles. In this second approach, higher order moments are computed based on the estimates of these two moments and under the assumption that the concentration probability density function is a Gamma distribution.

Key words: *Concentration statistics; Gamma distribution; Lagrangian stochastic modelling; Micromixing modelling*.

INTRODUCTION

Concentration fluctuations generated by the dispersion of a contaminant from a localized source in a turbulent flow characterize many processes. The full statistical characterization of this random field requires a multi-point, multi-time probability density function (PDF) of the concentration. This is as complicated as fully solving the turbulent flow and it is therefore unfeasible. More practically, we may search for the full statistical characterization of the fluctuations in any point of the field. Recent studies have proposed to extend the use of single-particle Lagrangian models (Thomson, 1987) in heuristic ways, to account for the evolution of the second moment of the concentration fluctuations (Cassiani, 2013). This is the case of the Volumetric Particle Approach (VPA) that can be viewed as a simplification of a "traditional" Lagrangian PDF micromixing method. This model is computationally efficient, since it decouples the evolution of the dispersing plume from the background and it requires simulating the trajectories of the marked particles originated at the source, only. The assumptions on the functional form of the PDF rely on experimental investigation presented in Nironi et al (2015) and supporting the existence of a universal function for the concentration PDF. Namely, the measurements show that the PDFs due to a point source in a turbulent boundary layer are modelled with good accuracy by a family of one-parameter Gamma distributions depending on a single parameter k, which is a function of the fluctuation intensity $i_c = \sigma_c/c_m$ (c_m and σ_c are the mean and the standard deviation of the concentration):

$$p(\chi) = \frac{k^k}{\Gamma(k)} \chi^{k-1} \exp(-k\chi) \tag{1}$$

where $k = i_c^2$, $\Gamma(k)$ is the Gamma function, and $\chi \equiv c/c_m$ (c is the sample space variable).

MODEL EQUATIONS

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

$$dU_i' = a_i(\mathbf{X}, \mathbf{U}', t)dt + b_{ij}(\mathbf{X}, \mathbf{U}', t)d\xi_j \tag{2}$$

$$dX_i = \left(< u_i > + U_i^{'} \right) dt \quad (3)$$

where a_i and b_i are the deterministic drift and the stochastic diffusive terms, respectively, U_i' is the Lagrangian velocity fluctuation, $<u_i>$ is the Eulerian mean velocity, $d\xi_j$ is an incremental Wiener process with zero mean and variance dt, and X_i is the particle position. The deterministic acceleration term a_i is obtained by imposing the well-mixed condition (Thomson, 1987). The stochastic diffusive term b_{ij} is defined as $b_{ij}=\delta_{ij} \sqrt{(C_0\varepsilon)}$, where δ_{ij} is the Kronecker delta, ε the mean turbulent kinetic energy dissipation rate, and C_0 is the Kolmogorov constant.

PDF Micromixing model

The PDF micromixing model (PMM) aims to solve a transport equation for the concentration PDF explicitly accounting for the dissipative effects of the molecular diffusivity (Pope, 1998). This approach simulates explicitly the micromixing process as given by a mass exchange between polluted fluid particles and 'clean' particles of ambient air. The simulation of the higher-order moments of the concentration field requires then the introduction of a Markovian state variable C representing the particle concentration and parametrized with the IECM model (Pope, 1998):

$$\frac{dC}{dt} = \frac{C - < C | \mathbf{X}, \mathbf{U} >}{\tau_m} \quad (4)$$

where $<C|\mathbf{X},\mathbf{U}>$ is the mean scalar concentration conditioned on the local position and velocity and τ_m represents the time scale of the local mixing, which is defined as a function of local velocity variance, mean turbulent kinetic energy dissipation rate, source size, and particle flight time (Cassiani et al, 2005).

The VPΓ model

This modelling approach is based on the use of the VPA model (Cassiani, 2013) and the assumption that the concentration PDF is given by a Gamma distribution. This approach simplifies the representation of the mixing phenomenon and it requires to simulate explicitly only the plume particles without taking into account the background particles. As a consequence of that, a considerable saving in the computational resources is achieved. To that purpose, the micromixing process is simulated as a change in a fictitious volume V_p associated with the plume particles. Since for a non-reactive the scalar mass of tracer m_p carried by a particle is conserved ($dm_p/dt=0$), we can compute the temporal evolution of the volume $V_p(t+dt)=V_p(t)C(t)/C(t+dt)$. The concentration C is modelled through Eq. 4, by implementing the Interaction by Exchange with the Mean (IEM) model (i.e. with Eq. 4 but adopting a unique velocity class, e.g. Pope, 2000). The computation of the moments of the concentration $<c^n>$ requires the spatial discretization of the computational domain:

$$< c^n > = \sum_{i=1}^{N_c} C_i^n \frac{V_{p,i}}{V_c} \quad (5)$$

where N_c is the particle number held in the generic cell of volume V_c. It is worth noting that the use of IEM model does not alter the mean concentration field in the VPA framework (Cassiani, 2013). The term $V_{p,i}/N_c$ can be seen as the probability that the particle i takes the concentration C_i. The approximations introduced in the VPA model provide reliable estimates of the mean and variance only. The higher-order statistics (n>2) are modelled by a family of one-parameter Gamma distributions (Eq. 1).

NUMERICAL CODE

The micromixing models - PMM and VPA - are implemented in a numerical code using a dynamical expanding grid to minimize the computational resources while maintaining a good accuracy of the numerical solutions (Cassiani et al, 2005). The following boundary conditions are imposed:

- at the top and lateral boundaries, the particle velocity and position are elastically reflected and the concentration is absorbed;
- at the ground, the particles are elastically reflected and they conserve their concentration;
- in the PMM model the source is represented by marking the particles with a normally distributed scalar concentration whereas in the VPA model we used a cylindrical top-hat distribution.

The PMM and VPA models require the setting of some free parameters, whose values are generally obtained by fitting the numerical estimates of the first and second-order concentration moments to the relative values provided by the experiments. These parameters are C_0, the initial source distribution σ_0, the Richardson-Obukhov constant C_r and the micromixing constant μ_t. The values adopted in the simulations are summarized in Table 1. The number of velocity classes used in the PMM model is 529 (23 for each of the two spatial directions).

Table 1. Model parameter values adopted in the simulations

C_0	σ_0	C_r	$\mu_{t,PMM}$	$\mu_{t,VPA}$
4.5	$\sqrt{(2/3)}d_s$	0.3	0.9	0.54

RESULTS

We simulated the dispersion of a passive scalar fluctuating plume in the neutral boundary layer and we compared the numerical results provided by the two micromixing models with the wind-tunnel measurements by Nironi et al (2015). We simulated the continuous releases emitted from an elevated source (z_s/δ=0.19) of varying diameter d_s: 1) ES 3 (d_s=0.00375δ), and 2) ES 6 (d_s=0.0075δ), where δ is the boundary layer thickness (equal to 0.8 m). The statistics of the velocity field required as input data for the Lagrangian stochastic models are: the mean longitudinal velocity (Fig. 1a), the standard deviation of the velocity components (Fig. 1b), and the turbulent kinetic energy dissipation rate (Fig. 1c).

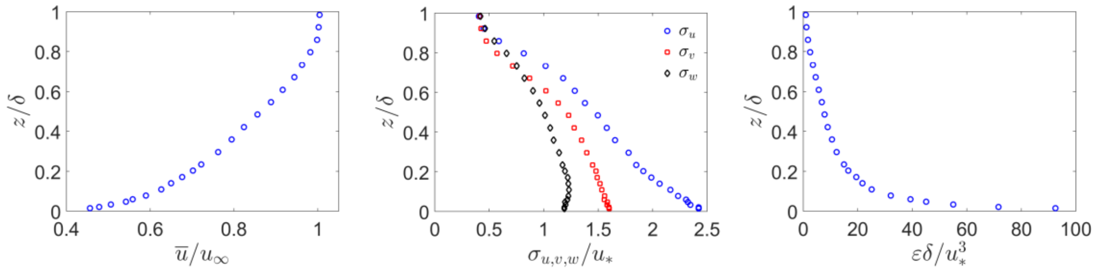

Figure 1. Vertical profiles of the velocity field imposed in the numerical simulations: a) mean longitudinal velocity, b) velocity fluctuations, c) turbulent kinetic energy dissipation rate. The velocity statistics are normalized using the free-stream velocity u_∞ and the friction velocity u_*. The ratio between the two is u_*/u_∞=0.037

Profile of concentration statistics

Firstly, the reliability of the model is evaluated by focusing on longitudinal profiles of the standard deviation, skewness, and the kurtosis at the source height z_s and at y=0. All the results presented in the paper were computed using 8×10^8 and 2×10^7 particles fort the PMM and the VPA model, respectively. This amount of particles was sufficient to get a satisfactory accuracy.

PMM model

The experimental data show that the source diameter has a significant influence on higher-order moments up to a distance of approximately x/δ=3.75 from the source (Figs. 2a-c), whereas its influence on the mean concentration is negligible (Fackrell and Robins, 1982; Nironi et al, 2015). The comparison between the measurements and the numerical results along the plume centreline in the x-direction shows two main features. First, the agreement between experimental and numerical profiles of i_c is very satisfactory in all the domain (Fig. 2a). Second, in the far field the model significantly overestimates the experimental values and predicts a spurious influence of the source size on Sk and Ku (Figs. 2b and c).

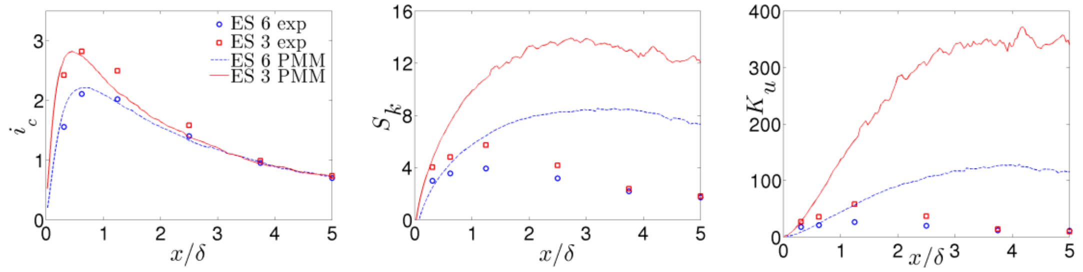

Figure 2. Results of the PMM model: longitudinal evolution of the concentration statistics: a) fluctuation intensity i_c, b) skewness Sk, c) kurtosis Ku

VPΓ model

This approach is based on the VPA model to compute the spatial distribution of the first two moments of the concentration field and on the assumption that the concentration PDF is a Gamma distribution, i.e. that the $Sk=2i_c$ and the $Ku=6(i_c)^2+3$.

The model is able to simulate i_c in all the domain with good accuracy (Fig. 3a), and provides reliable estimates of the skewness and kurtosis (Figs. 3b and c). In doing this, the VPΓ model is able to reproduce correctly the effects of the source size, including its vanishing influence in the far field. Despite this general good agreement, it is still possible to detect some discrepancies between the two. For ES 3, the numerical solutions of i_c slightly underestimate the experiments in the near field, at $x/\delta=0.625$, and in the intermediate field, at $x/\delta=1.25$. The computed Sk and Ku of the ES 3 source overestimate the experimental values in the near filed and underestimate them in the far field. However, the relative error is limited (about 15% on the centreline). Some differences are also present in the near filed for the ES 6 source.

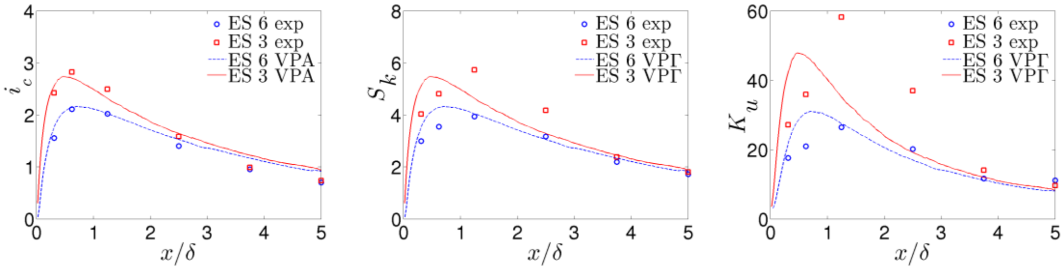

Figure 3. Results of the VPA model: longitudinal evolution of the concentration statistics: a) fluctuation intensity i_c, b) skewness *Sk*, c) kurtosis *Ku*

One-point concentration PDF

For the PMM model, the computation of the PDFs are obtained by collecting the concentration values carried by a large number of particles in a small control volume and organizing them according to their frequency. For the VPΓ model, the shape of the PDF is imposed to be that of a Gamma distribution, completely determined by c_m and σ_c (see Eq. 1). The PDFs are evaluated at $y=0$, $z=z_s$ and at varying distances from the release point. The PDFs are normalized with the local mean concentration. Note that the fluctuating plume considered here is characterized by a large intermittency in the near field, where the dispersion process is dominated by the meandering (Nironi et al, 2015). In particular, instantaneous concentration measurements show a majority of values very close to zero and few values marked by very high concentration. This implies that the concentration PDF assumes an exponential-like shape that both the models are able to reproduce (not shown here). Increasing the distance from the source, the influence of the meandering process becomes negligible, the intermittency at the plume centreline reduces and the form of the PDF shifts to a log-normal-like distribution (Nironi et al, 2015). In order to quantify the accuracy of the model, we also compute the relative errors $RE_{Sk}=|Sk_{mod}-Sk_{exp}|/|Sk_{exp}|$ and $RE_{Ku}=|Ku_{mod}-Ku_{exp}|/Ku_{exp}$, where Sk_{exp} and Ku_{exp} are the experimental values of skewness and kurtosis, respectively, and Sk_{mod} and Ku_{mod} are those estimated numerically. At $x/\delta=0.625$ for low values of χ we observe some differences between the experimental PDF and that evaluated with the PMM model (Fig. 4a). Note however that this disagreement does not preclude the model to correctly estimate the variance of the PDF (Fig. 2a). The relative errors for *Sk* and *Ku* are lower than 21% ($RE_{Sk,PMM}=0.206$ and $RE_{Ku,PMM}=0.143$, respectively). A similar behaviour is observed for the results of the VPΓ model, where $RE_{Sk,VP\Gamma}=0.208$ and $RE_{Ku,VP\Gamma}=0.457$, even the relative error of the kurtosis is slight larger than that of the PMM model. The low relative errors Re_{Ku} reveal that in the near field both models reproduces accurately the complete experimental PDF. In the far field the PMM and VPΓ behave differently (Fig. 4b). The form of the PDF computed with the PMM model suggests that, with respect to the experimental data, the large values of χ are overestimated and the low values are underestimated. The differences existing between the VPΓ solutions and the measurements are small and the reliability of the model is satisfactory. For the larger source the VPΓ relative errors are lower than 30% ($RE_{Sk,VP\Gamma}=0.062$ and $RE_{Ku,VP\Gamma}=0.282$), whereas the PMM model exceed 300% for the skewness and 900% for the kurtosis ($RE_{Sk,PMM}=3.262$ and $RE_{Ku,PMM}=9.343$). The experiments show that the two sources - ES 3 and ES 6 - induce the same concentration field at distances larger than $x/\delta=3.75$ from the release location. The VPΓ model reproduces this feature with good approximation (Fig. 3), whereas the solutions computed by the PMM model exhibit noticeable differences until x/δ=5.0 (Fig. 2).

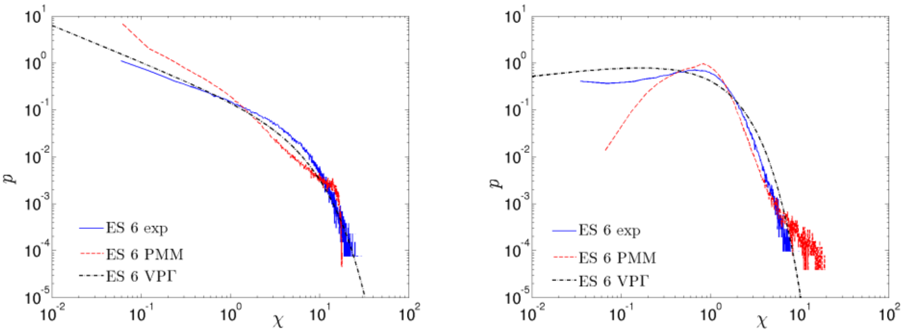

Figure 4. Concentration PDF of ES 6 source at y=0, z=z_S: a) x/δ=0.625, b) x/δ=5.0

DISCUSSION AND CONCLUSIONS

We have tested two micromixing model formulations, the PMM and the VPΓ model and we have investigated their ability in estimating the concentration statistics of a passive scalar emitted within a turbulent boundary layer. We simulated the dispersion of a fluctuating plume produced by a continuous release from two point sources of different diameter and we compared the results with the experimental data-set reported in Nironi et al (2015). The numerical solutions show that the PMM model is able to correctly simulate the concentration statistics in the near field, reproducing effects of the source size on the high-order moments. In the far field the PMM model clearly tends to overestimate the measurements, and the numerical profiles of *Sk* and *Ku* are still sensitive to the source size. This is markedly different from what is observed in the experiments (where the source size effects vanishes for x≥3.75δ). This behaviour can be reasonably attributed to the inability of the IECM model to correctly relax the concentration PDF form towards that of a Gaussian distribution in the absence of a relevant mean scalar gradient (see e.g. Pope, 2000,). Thus overestimating the occurrence of concentration values that are larger than the mean where the mean concentration gradients are weak. These limitations may be overcome by computing the high-order statistics using the mean and variance, both reliably modelled by the PMM, and assuming that the PDF is a Gamma distribution. We underline that the Gamma distribution hypothesis could be applied to any model being able to provide accurate estimates of the first two moments of the concentration, including e.g. the PMM model. Here we chose to calculate the first two concentration moments with the VPA model that is able to provide accurate solutions of mean and variance, requiring a number of particles that is significantly smaller than that needed by the PMM model, with a significant saving of memory and CPU time. The latter approach, referred to here as the VPΓ model, is then suitable for the simulation of dispersion phenomena for operational purposes.

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