OFFLINE APPROACH FOR HIGHER ORDER CONCENTRATION MOMENTS

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Abstract: We developed a fluctuating plume model able to evaluate all the higher concentration moments only requiring the knowledge of the first one. The simple algorithm used to calculate the meander centroid component is independent of the method used to obtain the mean concentration field and makes the computational time lower than most meandering plume model versions. Thus it is especially suitable for practical applications.

Key words: *Fluctuating plume model, Concentration fluctuations, Urban canopy*.

INTRODUCTION

Modelling concentration fluctuations is fundamental to a great number of practical applications such as prediction of air pollution, determination of reaction rates in turbulent chemical reactors and analysis of turbulent combustion. In this work we present an offline approach able to evaluate the concentration field of passive and reactive scalars from their mean concentration field. This method is based on the assumption (Gifford, 1959) that the total plume dispersion can be split into two independent components, the meandering barycentre and the relative dispersion. While the meandering motion of the plume centroid has to be modelled, the relative dispersion, taking into account the turbulent mixing and scalar dissipation, can be simply parameterized. The barycentre probability density function is obtained (Cassiani and Giostra, 2002) by applying a linear compression to a previously evaluated or measured mean concentration field. Then it is coupled with a Gamma distribution that parameterizes the mixing around the centroid and it is integrated to provide, in principle, the whole concentration probability density function. Being independent of the method used to obtain the mean concentration field this approach is an ideal offline tool to predict second and higher order concentration moments. The model adaptability to different kinds of turbulence is shown by comparing its results first with analytical predictions present in the literature for homogeneous isotropic turbulence and then with a dispersion experiment in a canopy generated boundary layer. The simplicity of the numerical algorithm used to calculate the meandering centroid component makes the model very fast and suitable for practical applications.

FLUCTATING PLUME MODEL FORMULATION

In the fluctuating plume approach the absolute dispersion can be divided into two statistically independent parts, the meandering motion of the barycentre and the relative diffusion around it. Following Gifford (1959) the concentration PDF can be written as:

$$p_c(c;t,y,z)=\int_0^H\int_{-\infty}^{\infty}p_{cr}\left(c;t,y,z,y_m,z_m\right)p_m\left(t,y_m,z_m\right)dy_m\,dz_m \tag{1}$$

where $p_c(c;t,y,z)$ is the concentration probability density function (PDF), p_m is the centroid position PDF, p_{cr} is the relative concentration PDF and H is the characteristic vertical length scale. Using equation (1) and the definition of statistical moment we have:

$$\langle c^n(t,y,z)\rangle=\int_0^{\infty}c^n p_c\,dc=\int_0^H\int_{-\infty}^{\infty}\left[\int_0^{\infty}c^n p_{cr}\,dc\right]p_m\,dy_m\,dz_m=\int_0^H\int_{-\infty}^{\infty}\langle c_r^n\rangle p_m\,dy_m\,dz_m \tag{2}$$

where $\langle c^n\rangle$ and $\langle c_r^n\rangle$ are the n-order moments of the absolute and relative concentration, respectively.

Equation (2) summarizes the idea of the fluctuating plume stating that the concentration field can be evaluated through two different contributions, the meandering of the plume centroid that has to be simulated in a fixed coordinate system relative to the source, and the relative concentration statistics that has to be parameterized on a local reference frame around the barycentre. We assume statistical independence between vertical and lateral diffusion, so that we can factorize both the meander and the relative concentration PDFs.

EVALUATING PLUME CENTROID STATISTIC.

The recent versions of fluctuating plume model are coupled with a Lagrangian Stochastic Model for the particle trajectories. Our choice of Cassiani and Giostra (2002) approach to evaluate the meandering barycentre part removes the need for the knowledge of the trajectories, requiring only a mean field concentration input and thus relaxing the need for Lagrangian modelling. We neglect the along wind dispersion, so that, apart from the normalisation factor, the crosswind-integrated concentration $\langle c_y \rangle$ corresponds to the PDF for the vertical position p_z :

$$p_z(t, z) = \frac{\langle c_y(t, z) \rangle}{\int_0^H \langle c_y(t, z) \rangle dz} = \frac{\int_{-\infty}^{\infty} c(t, y, z) dy}{\int_0^H \left[\int_{-\infty}^{\infty} c(t, y, z) dy \right] dz} \tag{3}$$

where the double integral at denominator represents the normalisation coefficient. Luhar et al.(2000) derive the trajectory of the instantaneous plume centre of mass $z_m(t)$ from the particle trajectory $z(t)$ generated by a single particle Lagrangian stochastic model using the linear transformation:

$$z_m(t) = \frac{\sigma_z^2 - \sigma_{zr}^2}{\sigma_z^2} (z(t) - \langle z(t) \rangle) + \langle z(t) \rangle \tag{4}$$

where σ_z^2 and σ_{zr}^2 are respectively the absolute and relative vertical position's variances. We use the same linear transformation but applied to the points of the calculation grid instead of Lagrangian trajectories. It is trivial to show that a relation between the PDFs of two stochastic processes linearly related such as $z_m(t)$ and $z(t)$ is given by $p_z \Delta z = p_{zm} \Delta z_m$. This is a compression of the PDF $(\sigma_{zr} < \sigma_z)$ that reduces the variance conserving at the same time all the other scaled moments. Hence the resulting form of PDF is $p_{zm} = 0$ out the compressed concentration field and $p_{zm} = p_z \Delta z / \Delta z_m = p_z \sigma_z^2 / (\sigma_z^2 - \sigma_{zr}^2)$ in it. The relative position variance has to be parameterised. We propose a form similar to Mortarini et al. (2009) given by:

$$\sigma_{zr}^2 = \frac{\alpha_N g\varepsilon (t + t_s)^3}{\left[1 + \alpha_D (g\varepsilon t^3)^{2/3} \right]^{3/2}} \tag{5}$$

where g is the one-dimensional Richardson constant, ε is the dissipation rate of turbulent kinetic energy (TKE), t_s accounts for a finite initial source size and the parameters α_N and α_D are introduced to set the contribution of two different behaviours for small and large time. In fact the expression corresponds to the inertial range relative dispersion formulation at small time, and tends to Taylor's limit at large time, accounting also for the boundaries' effect that reduces the vertical spreading.

PARAMETERISATION FOR THE RELATIVE CONCENTRATION.

Following Luhar et al. (2000) and Mortarini et al. (2009) the relative concentration PDF can be represented as function of the Gamma distribution:

$$p_{cr}(c; x, z, z_m) = \frac{\lambda^\lambda}{\langle c_r \rangle \Gamma(\lambda)} \left(\frac{c}{\langle c_r \rangle} \right)^{\lambda - 1} \exp\left(-\frac{\lambda c}{\langle c_r \rangle} \right) \tag{6}$$

where $\langle c_r \rangle$ is the mean relative concentration, $\Gamma(\lambda)$ is the Gamma function of $\lambda = 1 / i_{cr}^2$ and $i_{cr} = \sigma_{cr} / \langle c_r \rangle$ is the relative concentration fluctuation intensity. This PDF has the following property:

$$\langle c_r^n \rangle = \int_{-\infty}^{\infty} c^n p_{cr} dc = \frac{\Gamma(n + \lambda)}{\lambda^n \Gamma(\lambda)} \langle c_r \rangle^n \tag{7}$$

Being the nth-order moment proportional to the first moment to the nth power, an expression for the mean relative concentration is needed. We consider the expression $\langle c_{zr} \rangle = p_{zr} Q / U$, where p_{zr} is relative position PDF, Q is the release of material per unit of time e U is the mean wind. Although it is possible to use a simple reflected Gaussian form (Franzese, 2003) for p_{zr} , a skewed PDF obtained as the sum of two reflected Gaussian PDFs (Luhar, 2000; Dosio and Vila-Guerau de Arellano, 2006) was found to provide better overall agreement with the experiments, especially for highly asymmetrical turbulence. The relative concentration fluctuations intensity i_{cr} can be expressed as proposed by Gailis et al. (2007) and Ferrero et al. (2012):

$$i_{cr}^2 = (1 + i_{cr0}^2) (\langle c_r \rangle / \langle c_{r0} \rangle)^{-\zeta} - 1 \tag{8}$$

where i_{cr0} is the i_{cr} 's minimum, $\langle c_{r0} \rangle$ is the $\langle c_r \rangle$'s maximum and ζ shape parameter within the interval (0,1). The values are chosen to have the best agreement with experimental data. As far as we know, in literature it is one of the few prescribed forms dependent on height, taking into account the conservation of TKE dissipation in the vortex scale reduction close to the boundaries.

TEST CASES.

We remark the independence of the presented model from the requested mean concentration field that can be obtained either from models or experiments. Hence it is possible to select the most suitable method to evaluate the mean field, as a simple and fast Gaussian model, or as a more complicated and efficient single particle model, depending on the class of turbulence investigated.

Homogeneous and isotropic turbulence: crosswind dispersion

The first step is the application of the model to the homogeneous and isotropic turbulence case. This is a first validation of the model and represents a good approximation for the crosswind direction even in more realistic kinds of turbulence. The mean and mean square concentration fields are investigated and compared with the theoretical predictions in the inertial subrange found in literature. Thomson (1990) obtained a theoretical prediction for the second-order moment developing a two particles model based on two Langevin equations for the particles separation and barycentre. Following Thomson (1990), Ferrero and Mortarini (2005) prescribe an analytical formula for the concentration fluctuations replacing the Gaussian distribution for a Richardson distribution in the separation PDF expression. An analytical solution for concentration moments can also be carried out from the equation (2) for the fluctuating plume models until the total and meander expansions are Gaussian and only for the case of not bounded variables, as shown by Luhar et al. (2000). The mean field required is obtained by the simplest single particle model wherein the velocity PDF can be considered Gaussian yielding a simple expression for the Langevin equation.

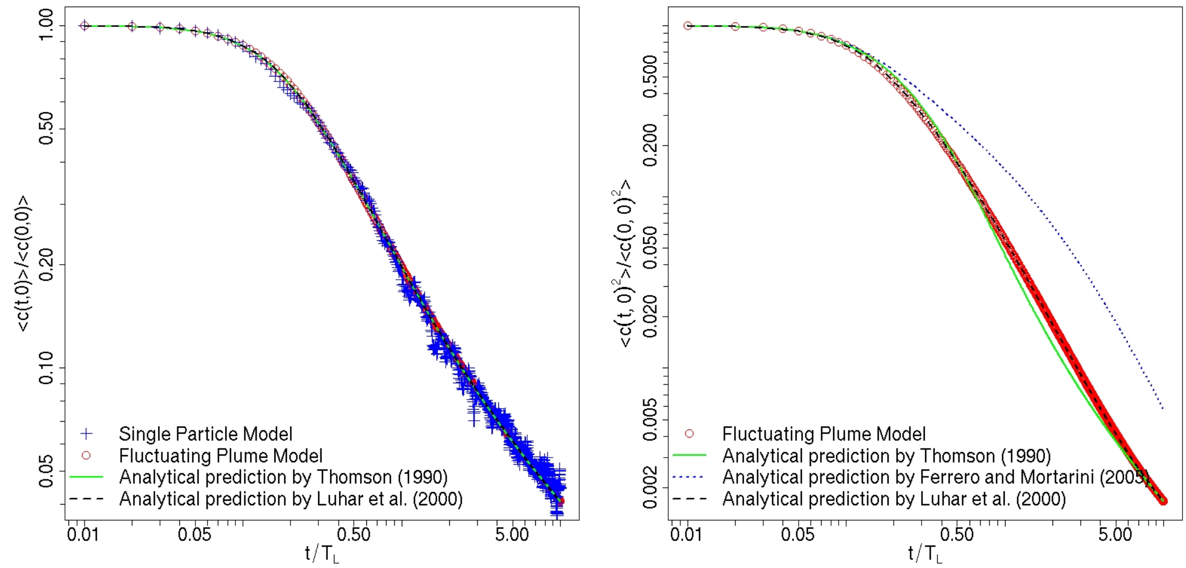

Figure 1: Non-dimensional mean (left) and standard deviation (right) concentration at centreline as function of non-dimensional time.

Figure 1 shows that the model accurately reproduces the expected behaviours of mean and mean square dimensionless concentration at the centreline. In particular, the model coincides with the Luhar et al. (2000) analytical one; in fact, the coupling between the simple single particle model and the linear transformation of Luhar et al. (2000) ensures that the meandering PDF is Gaussian and hence the equivalence between the two methods . The mean field fits very well the Thomson (1990). About the second moment, the obtained results fit better the Thomson (1990) analytical prediction than the Ferrero and Mortarini (2005) one, probably because of the single particle model used to obtain the mean concentration field in this simulation. The slight overestimation between $t=T_L$ and $t=5\mathrm{T}_L$ of the model in respect to the Thomson (1990) checks the statement that in the intermediate subrange the separation PDF departs from the Gaussian distribution and approaches with the Richardson one (Ferrero and Mortarini, 2005).

Simulation in a canopy layer.

The interaction of the atmospheric flow with the buildings of an urban area generates a boundary layer with specific characteristics. The vertical structure of urban boundary layers comprises a roughness sub-layer near the ground and an inertial sub-layer above. In the lowest part of the roughness sub-layer, the buildings form a canopy. Difficulties arise in developing guidelines depend upon unique building arrangements and geometry.

Meteorological data in the urban boundary layer are not as available as from rural sites, hence we consider the control and repeatability of laboratory experiments. In particular we apply the fluctuating plume model to the Huq and Franzese (2013) laboratory experiment who has undertaken in a water tunnel at the Environmental Fluids Lab at the University of Delaware. They present measurements of turbulence, velocity and mean concentration of a passive scalar released from a continuous point source for three model urban canopies with different aspect ratios A_r (i.e. the ratio between the building height H_b and width w_b). The measurements for the canopy with $A_r=0.25$, which consists of a regular series of prisms, were taken by Macdonald and Ejim (2002), while the measurements with $A_r=1$ (arrays of cubes) and $A_r=3$ (arrays of tall prisms) are new. The building length in the along-wind direction B is constant. The velocity and scalar measurements were taken in the plane along the centreline of the canopy where the scalar source is located at ground level. All experiments simulate in-canopy dispersion in the near field, where the plume vertical dimension is smaller or comparable to the mean building height. Huq and Franzese (2013) use a simple vertically-reflected Gaussian model to approximate the mean concentration field:

$$\langle c(t,y,z)\rangle=\frac{Q}{U\,\pi\sigma_y\sigma_y}\exp\left(-\frac{y^2}{2\sigma_y^2}-\frac{z^2}{2\sigma_z^2}\right) \quad \textbf{(9)}$$

where $\sigma_y^2=\sigma_{y0}^2+\sigma_v^2 t^2$ and $\sigma_z^2=\sigma_{z0}^2+\sigma_w^2 t^2$. The values of quantities used in the Gaussian model and for scaling the data are summarized in the table (1), including the free-stream velocity U_∞ , the rooftop level wind speed U_∞ , source size $\sigma_{y0}=\sigma_{z0}=\sigma_0$, vertical and transverse velocity variance σ_v^2 and σ_w^2 , time scale T_y and T_z and length scale L_y and L_z .

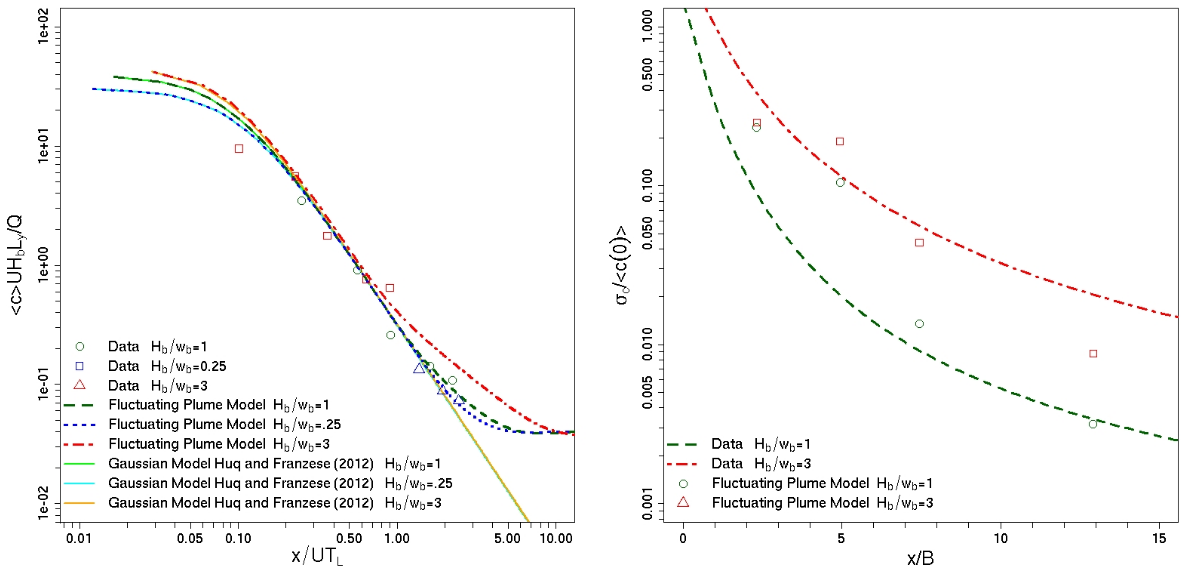

Figure 2: Non-dimensional mean (left) and root mean square (right) concentration at the ground, at centreline of the canopy as function of non-dimensional distances from the source.

The dimensionless mean concentration as a function of the scaled distance from the source is plotted in the figure 2 (left). The fluctuating plume agrees well with both Gaussian model and water tunnel data. The curves follow the -2 power law decay of concentration with distance from the source. The difference between the fluctuating plume and the Gaussian model in the far field is due to equation (9) containing only the near field (and not the far field) approximation of Taylor (1921). The evolution with the scaled distance from the source of the normalised standard deviation is plotted in the figure 2 (right). Again, the fluctuating plume fits well with the water tunnel data (personal communication, May 30, 2012). The use of the constant values (table 1) for the turbulence parameter instead of the measured profiles (Huq and Franzese, 2013) is a simplification for both the first and the second moment. In order to improve the comparison between the fluctuating plume and the experimental data, it would be possible to use as mean field input a single particle model instead of the Gaussian one, but it would mean the loss of the distinguished feature of the model, i.e. the simple and fast computation.

Table 1: Summary of experimental data and model parameters.

A_r	Q (cm^3s^{-1})	s_o (mm)	H_b (mm)	U_∞ (mms^{-1})	s_w (mm)	s_v (mm)	T_z (s)	T_y (s)	L_z (mm)	L_y (mm)	U_b (mms^{-1})	U (mms^{-1})
0.25	2.18	5	50	78	4.7	7.0	10.7	7.1	50	50.0	52	52
1	1.4	2	32	94	2.1	3.1	15.5	5.6	32	17.5	52	27
3	1.4	2	96	110	1.5	2.2	64.3	7.8	96	17.5	77	28

CONCLUSIONS.

The proposed fluctuating plume model includes the most favourable features of the existing versions, resulting versatile and simpler than the previous methods. The mean concentration field required by Cassiani and Giostra (2002) approach can be obtained either from models or from experiments, allowing to choose the most suitable method to evaluate the mean field, as a simple and fast model, e.g. a Gaussian model, or as a more complicated and efficient model, e.g. a single particle model, depending on the class of turbulence investigated. The parameterisation of relative motion is established on the analytical expressions producing the best agreement with the experimental data, e.g. the Gailis et al. (2007) height-dependent formula for the relative concentration fluctuations. The model can be easily adapted to different classes of turbulence modifying the parameterization of the relative contribution. After the validation in homogeneous and isotropic turbulence, the model was applied to a canopy layer and compared with a water tunnel data showing an overall good agreement. The low computational time demand coupled with the good efficiency makes the model suitable for practical applications considering that it is able to evaluate higher order concentration moments in few seconds on a standard computer. In fact, the evaluation of concentration fluctuations plays a crucial role in a great number of environmental issues: prediction of air pollution, simulation of chemical reactions of pollutants in the atmosphere, analysis of turbulent combustion and estimation of odour threshold.

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