1.5 LAGRANGIAN STOCHASTIC MODELING OF CONCENTRATION FLUCTUATIONS IN ATMOSPHERIC FLOWS

M. Cassiani [a,*], P. Franzese [b], J. D. Albertson [a] and A. Radicchi [c]

a)Department of Civil and Environmental Engineering, Duke University, Durham, North Carolina 27705
b)School of Computational Sciences, George Mason University, Fairfax, Virginia 22030
c)Facoltà di Scienze Ambientali, Università di Urbino "Carlo Bo", Urbino, 61029, Italy

1. INTRODUCTION

A Lagrangian stochastic probability density function (LS-PDF) model has been used to predict statistics and PDF of concentration generated by continuous releases of substances in the atmospheric boundary layer. In the past years much research has been devoted to model the mean concentration field of substances released in the atmospheric boundary. Nevertheless, several applications require the estimates of higher order moments of concentration, or even the PDF of concentration.

The LS-PDF approach has been originally developed to study complex reacting systems in chemical and combustion engineering (Pope, 1985, 2000, Fox 2003) and only recently adapted and applied to atmospheric dispersion (Gonzalez, 1997; Luhar and Sawford 2005 a, b; Cassiani, Franzese, and Giostra (CFG) 2005, a, b, Cassiani, Radicchi and Alberston (CRA) 2005). The strength of this approach is in the ability to deal exactly (i.e. no closure is needed) with any non-linear function of concentration (e.g., chemical reactions, biological processes).

In the LS-PDF approach, an ensemble of particles representing the true fluid particles moves according to a system of differential equations. Each particle carries its own concentration vector. Upon averaging, the ensemble of particle gives all the statistical characteristics of the scalar field.

2. EQUATIONS

This approach is based on the following transport equation for the joint PDF of turbulent velocity and concentration $f_{fU} = f(\mathbf{V}, \mathrm{y}; \mathbf{x}, t)$, which is derived directly from the Navier-Stokes and scalar transport equations (Pope, 2000):

$$\begin{aligned}&\frac{\partial f_{fU}}{\partial t} + V_i \frac{\partial f_{fU}}{\partial x_i} - \frac{1}{r}\frac{\partial \langle p \rangle}{\partial x_i}\frac{\partial f_{fU}}{\partial V_i} + \frac{\partial}{\partial y_a}\left[f_{fU} S_a(\mathrm{y})\right] = \\ &-\frac{\partial}{\partial V_i}\left(f_{fU}\left\langle n\nabla^2 U_i - \frac{1}{r}\frac{\partial p'}{\partial x_i}\middle| \mathbf{U}=\mathbf{V}, \mathrm{f}=\mathrm{y}\right\rangle\right) \\ &-\frac{\partial}{\partial y_a}\left(f_{fU}\left\langle \Gamma\nabla^2 f_a \middle| \mathbf{U}=\mathbf{V}, \mathrm{f}=\mathrm{y}\right\rangle\right)\end{aligned} \qquad (1)$$

Angle brackets denote ensemble average and therefore $\langle \bullet | \bullet \rangle$ is a conditional expectation. n is the viscosity of the fluid, Γ the molecular diffusivity of the scalar, y_a represents the sample space variable for the concentration f_a of the chemical species a, and $\mathbf{V}$ is the sample space variable for the velocity vector $\mathbf{U}$. S_a is the source-sink term associated with emission and chemical transformation of scalars. The terms on the left hand side are closed. On the right hand side, the first term represents the effect of viscous stresses and fluctuating pressure gradient and the second term (the conditional Laplacian) describes the dissipative effects of turbulence and molecular diffusivity on concentration fluctuations.

Equation (1) is usually solved using a system of ordinary and stochastic differential equations (e.g. Pope 2000; Heinz 2003):

$$\begin{aligned}du_i^* &= a_i(\mathbf{X}^*, \mathbf{u}^*, t)dt + b_{ij}(\mathbf{X}^*, t)dz_j \\ dX_i^* &= \left(u_i^* + \langle U_i^* \rangle\right)dt \\ df_a^* &= j_a(f_a^*, \mathbf{X}^*, \mathbf{u}^*, t)dt + S_a(\mathrm{f}^*, \mathbf{X}^*, \mathbf{U}^*, t)dt\end{aligned} \qquad (2)$$

where the asterisk denotes modelled quantities. $\langle \mathbf{U}^* \rangle$ and $\mathbf{u}^*$ are the modelled mean and fluctuating particle velocity respectively and $\mathbf{X}^*$ is the position vector. ϕ^* is the concentration associated with the particle. dz_j indicates a vector of independent Wiener processes. The term

* Corresponding author address: Massimo Cassiani, Duke University, Dept of Civil and Environmental Engineering, 121 Hudson Hall, Box 90287, NC, 27708. e-mail: mcassian@duke.edu

j_a is the micromixing model of the chemical species a. This term models the conditional Laplacian in Eq. (1). We use the IECM model for j_a, as proposed by Fox (1996) and Pope (1998):

$$j_a = -\frac{1}{t_m}\left(y_a - \left\langle f_a^* \middle| \mathbf{u}^* = \mathbf{v}, \mathbf{X}^* = \mathbf{x} \right\rangle\right). \quad (3)$$

t_m defines the rate of relaxation of the concentration of a particle towards the local mean. It is related to the dissipation time scale of concentration variance, i.e. $t_m \approx t_f \equiv 2s_f^2 / e_f$, where s_f^2 is the scalar concentration variance and $e_f \equiv 2\mathrm{G}\left\langle \frac{\partial f}{x_i}\frac{\partial f}{x_i} \right\rangle$ is the mean scalar dissipation rate. Details on the parameterization of t_m in atmospheric turbulence are given in CFG (2005a) and CRA (2005). The diffusion coefficient b_{ij} and the drift coefficient a_i are obtained following Thomson (1987).

3. NUMERICAL METHODS

The equations are solved in parallel as this allows the treatment of potential chemical reactions in closed form. A grid is used to extract the statistics from the ensemble of particles. The grid should be refined enough to provide details of the field around the source. As a consequence, the computation is longer the smaller the source size, because a larger number of particles need to be simulated in order to have meaningful statistics at each grid point.

For emissions from a continuous point or line source Taylor's hypothesis (i.e., $X = \langle U \rangle t$) was used whenever possible to reduce the dimensionality of the problem.

3.1 Dynamical grid for a point source

The domain is reduced to two dimensions using Taylor hypothesis. Initially, a small grid is generated around the source. Then, the grid is advected with the mean flow and expands around the plume (Figure 1). During the expansion process the particle density is kept uniform (Figure 2). This is achieved by randomly sampling particles from the old domain and uniformly filling the new domain. The new particles carry zero concentration and their velocities are assigned ensuring the fulfilment of the well-mixed conditions.

3.2 Block-structured grid and particle splitting-erasing

When Taylor's hypothesis does not apply, this algorithm is used, aiming to the reduction of the memory requirements. This makes the practical application of 3-dimensional PDF IECM models possible.

The source is located in the most refined block of the grid (Figure 3). The number of particles in each cell is constant and independent of the cell size. To maintain a constant mass density the particles are split (when travelling from a coarse grid to a refined one) and erased (when travelling from a refined to a coarse grid). Each particle moves according to its own time step.

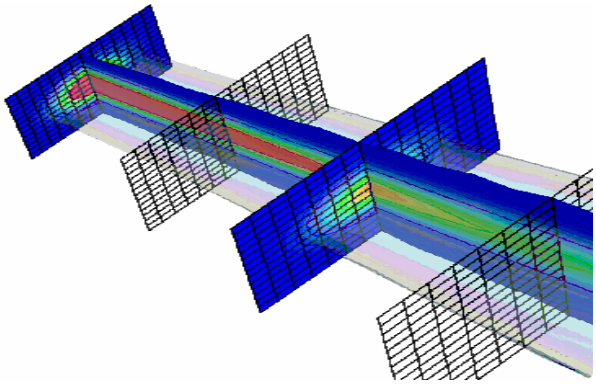

Figure 1. Dynamical grid expansion around the plume

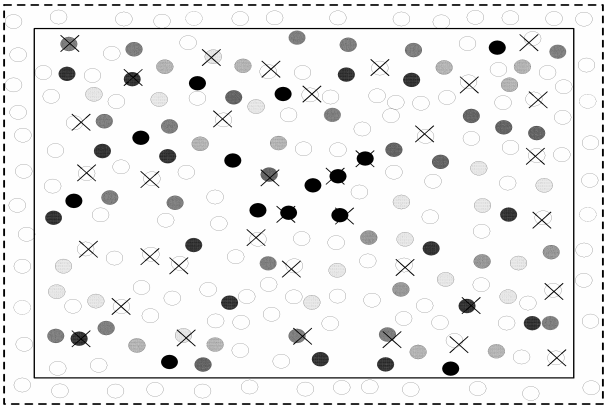

Figure 2. Sketch of the particle sampling and re-initialization. The new grid is indicated with the dashed line. Open circles are particles carrying zero concentration. Crosses indicate sampled particles.

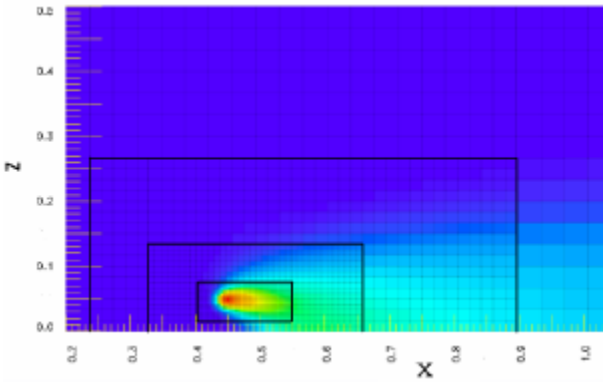

Figure 3. An example of Block structured grid for two-dimensional domain.

4. RESULTS

The predicted statistics and concentration PDF from releases by single source and multiple sources under different turbulent conditions are shown.

4.1. Dispersion in a CBL

Figure 4 shows the intensity of concentration fluctuations $s_f/\langle f \rangle$ obtained by the model and measured in the experiment of Hibberd et al. (2000) for a line source. X =(x/h) (w*/⟨U⟩) is the dimensionless downwind distance. *h* is the CBL height. w* is the convective velocity scale. The agreement is very good although some discrepancies arise far from the source. These are mainly due to the inability of the model to reproduce the air entrainment from outside the boundary layer. The air inflow feeds the concentration fluctuations causing the higher intensity observed in the experiment.

In figure 5 the cumulative distribution function (CDF) for a point source release in a CBL is simulated and compared with the experiments of Weil et al. (2002). The agreement is very good at both the downwind distances considered.

All the results shown for the CBL are obtained using the dynamical grid approach as described in CFG (2005b).

4.2. Dispersion in and above a Canopy layer

The model was applied to the completely different turbulent flow obtained in the wind tunnel experiments of Raupach et al. (1986), Coppin et al. (1986) and Legg et al. (1986) (see CRA 2005).

The releases were inside a canopy characterized by strong mean wind vertical gradient and along wind turbulence. Therefore, the Taylor hypothesis cannot be applied and we used the block- structured algorithm to fully account for wind shear effects.

We show some results from the simulation of the multiple line sources release of Coppin et al. (1986). The temperature was used as a passive tracer. $q_* = Q_s/(r_a C_p u_*)$ is the temperature scale, Q_s is the source strength, r_a the air density and u_* is the friction velocity.

The agreement between measured and simulated scalar standard deviation is very good. This can be appreciated in Figure 6, where the vertical profiles for two downwind distances are shown. $h_c = 0.06m$ is the canopy height, $h_s = 0.051m$ is the source height, and x_d is the downwind distance form the first source.

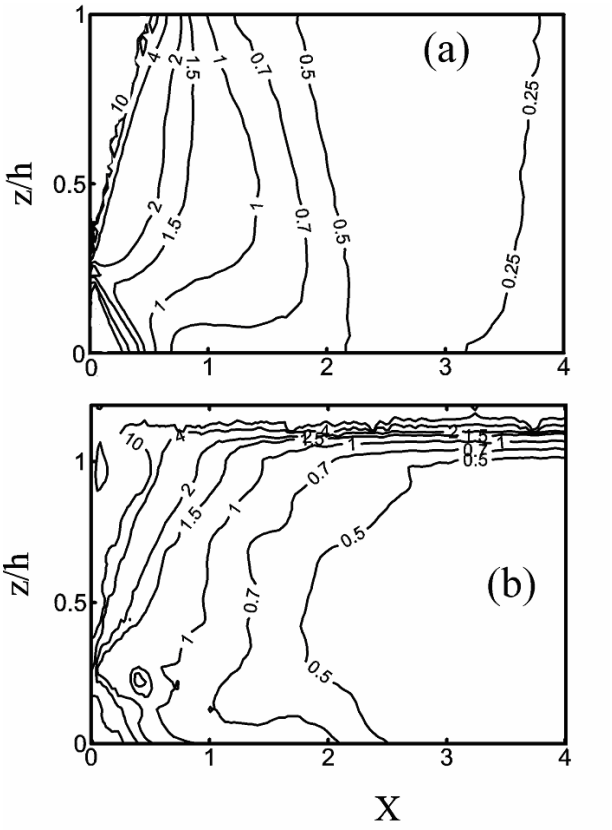

Figure 4. Contours of intensity of concentration fluctuations $s_f/\langle f \rangle$ for a crosswind line source at $z_s = 0.25h$. (a) Model simulation; (b) Hibberd (2000) measurements. X is the dimensionless distance and *h* the CBL height.

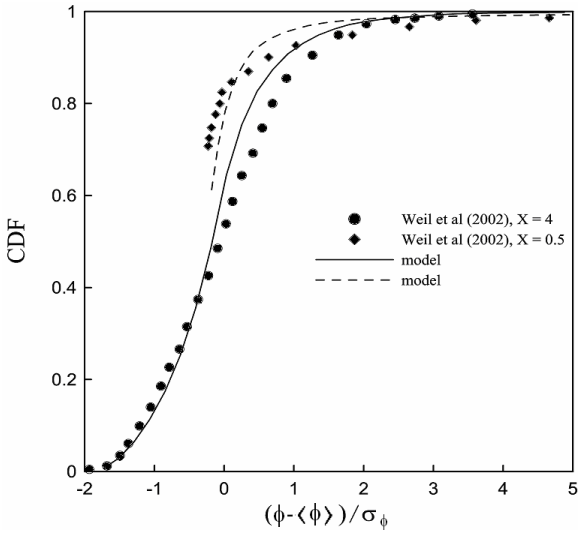

Figure 5. Measured and modelled cumulative distribution function (CDF) of concentration at two downwind distances from the source.

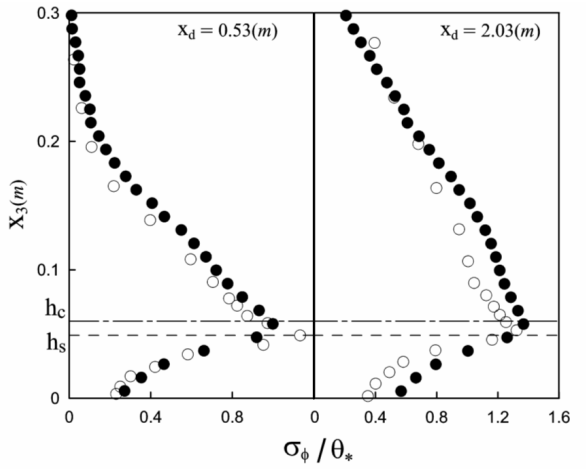

Figure 6. Measured (s_f,○) and modelled (s_{f^*},●) temperature standard deviation variance normalized with the temperature scale q_*. Multiple line sources experiments of Coppin et al. (1986).

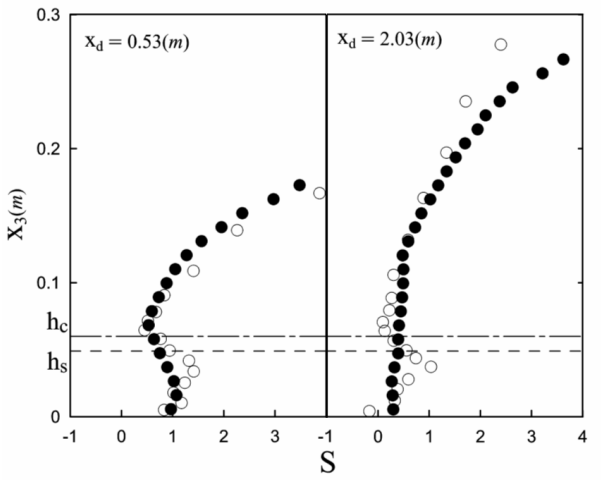

Figure 7. Measured (S,○) and modelled (S^*,●) temperature skewness. Multiple line sources experiment of Coppin et al. (1986).

In figure 7, the measured and modelled skewness of the scalar field are shown for the same downwind distances. The agreement is again very good although some discrepancies arise around the source level.

5. CONCLUSIONS

The LS-PDF modelling of dispersion proves to be a powerful tool when the knowledge of concentration fluctuations and higher moments of concentration is required.

The proposed approach can account for chemical reactions without any closure assumption. Coupling with tropospheric chemical models is also possible because of the low intrinsic dimension of such models (Loewe and Tomlin, 1999).

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