H13-7

A FLUCTUATING PLUME MODEL FOR POLLUTANTS DISPERSION WITH CHEMICAL REACTIONS

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Abstract: A fluctuating plume model for pollutant dispersion is developed. The model is able to include chemical reactions, accounting for the segregation. The model is tested against measured data in wind tunnel experiment, where NO is emitted from a source in an environment of ozone. The results are presented in terms of the plume centreline dispersion and cross sections at different distances. It is shown that the agreement between predicted and measured values is satisfactory, notwithstanding the limitations due to the one-dimensional scheme adopted for the model.

Key words: *Fluctuating plume model, Segregation, Chemical reactions.*

INTRODUCTION

Lagrangian stochastic models (Thomson, 1987) are generally considered the more suitable tool to face many dispersion problems at different scales, including complex terrain and all stability conditions. Notably, these models are able to reproduce the short term dispersion in non-stationary conditions and peaks of concentration , which may play an important role in the modelling of flammable gas and chemical reactive pollutants. In particular, it is generally recognized that the segregation of the chemical reactants cannot be neglected in the short term concentration prediction (Garmory *et al*. 2006), when the chemical reactions take place before the pollutants are well mixed by the turbulence.

A correct description of this phenomenon needs the estimation of the concentration fluctuations. In the frame of the Lagrangian stochastic models the natural approach is the two-particles dispersion (Crone *et al*, 1999; van Dop, 2001). Unfortunately this kind of model can only be applied in homogeneous isotropic turbulence (Thomson, 1990) and this idealization strongly limits the application in real cases.

An interesting approach is the fluctuating plume model (Gifford, 1959), which is able to estimate the concentration fluctuations in non-homogeneous turbulence, like in the convective or canopy layers (Franzese, 2003, Mortarini *et al*, 2009). Recently we developed a Lagrangian stochastic one-particle model with chemical reactions (Alessandrini and Ferrero, 2009). In this model, the segregation coefficient, which depends on the covariance of the species concentrations, is calculated through a parameterisation. Despite the encouraging results yielded, this model cannot be considered generally applicable to any turbulence condition.

To overcome this limitation and to predict the reactive airborne elements concentration we followed an original approach: we re-wrote the fluctuating plume model using a bi-variate Gamma probability density function (Loàiciga and Leipnick, 2005), obtaining a new model able to simulate the simultaneous dispersion of two reactive species and to account for the segregation coefficient. The new model is used to reproduce a wind tunnel dispersion experiment of reacting non-premixed chemical species (Brown and Bilger, 1996). The results show a good agreement with the measured data.

THE MODEL

The basic fluctuating plume model used in this work was developed by us (Mortarini *et al*, 2009) following (Franzese, 2003). In this model we have introduced the simple chemical equation:

$$NO + O_3 \rightarrow NO_2 + O_2$$

which can be written in terms of the corresponding partial differential equations for the concentrations c_{NO}, c_{O3} and c_{NO2} In order to solve this equation in a discretised form we need to evaluate both the mean concentrations and the cross-correlations. This can be accomplished by solving the integrals in which their joint probability density function (PDF) appears. In the framework of the fluctuating plume model, the PDF can be split in the PDF of the position (y_m; z_m) of the plume centroid (barycentre), at a distance x from the source, and the concentration PDF relative to (y_m; z_m) in the reference frame moving with the cloud centroid, conditional to its location downwind. This is the basic assumption of the fluctuating plume dispersion model. Thus, evaluating the absolute concentration means to separately evaluate the PDF of the meandering and to find an expression for the concentration statistics in the barycentre system of reference. Far from the boundaries the movements of the barycentre on the y and z directions can be considered independent and then the barycentre PDF is given by the product of the two marginal distributions. Once these and the relative concentration PDFs are known, the moments of the concentration distribution can be calculated. The PDFs of the plume centroid position is evaluated using a single particle Lagrangian stochastic model, with a proper low-pass filter, in order to neglect the smallest eddies' scale. The relative concentration distributions is than parameterised assuming a bi-variate Gamma distribution (Loàiciga and Leipnick, 2005). This distribution has the property to yield to a recursive form for the higher order moments which can be expressed as a function of the first one. The assumption that the dispersions in the y- and z-directions develop independently enables us to decompose the mean relative concentration into separate lateral and vertical components. Furthermore we consider that each of these components possesses a self-similar Gaussian form in the relative frame of reference.

It should be stressed that the O_3 dispersion was simulated considering a fictitious species defined as the deficit of ozone background concentration (Alessandrini and Ferrero, 2009). As a matter of fact, the fluctuating plume accounts only for dispersion of pollutant contained in itself. Furthermore, this kind of model was used to simulate chemical reactions in atmosphere as never before.

SIMULATION AND RESULTS

For sake of comparison a wind tunnel experiment carried out by Brown and Bilger (1996) has been considered. In this experiment a NO point source emission was placed inside an airflow doped with a uniform O_3 concentration. The NO and O_3 concentrations were measured at different cross-flow sections along the plume centreline. Air doped with O_3 at 1 *ppm* entered the 2.8 *m* in diameter and 8 *m* long working section from upstream and crosses a turbulence generating grid made of square bars 65 *mm* X 65 *mm* and of pitch M = 320 *mm*. The nominal mean axial velocity of the flow (U) was 0.5 $m\ s^{-1}$ giving a Reynolds number Re = 10700. A point source, with a diameter of 31.5 *mm*, was located at the centre of the working section at a distance of 3M (0.96 *m*) from the inlet grid. Air doped with a NO concentration of 515 *ppm* was released by the point source at the same velocity U as the mean flow. Turbulence and concentration measurements were performed at different downwind distances from the point source (x/M = 7; 9; 12; 15; 17) along the flow on arcs concentric to the plume centreline. The measured turbulence was used as input of the dispersion model. First of all we compared the model results with the experimental data concerning the "frozen case". This means that the no- chemical scheme was activated and, consequently, only dispersion was reproduced. Figure 1 shows the comparison of the plume standard deviation, σ_m, (on the left) and the plume centreline concentrations (on the right). Note that the "frozen case" corresponds to the dispersion of a conserved scalar (NOx, in the present case). It can be observed that the agreement of measured and simulated σ_m is very satisfactory. As far as the centreline concentration is considered some caution has to be taken. As a matter of fact, our model is, in this version, one dimensional and clearly the comparison with the experiment cannot be correctly accomplished unless the concentration distribution is re-normalized. Thus we multiplied the centreline concentration given by the model by the normalization factor of the Gaussian distribution, in which the standard deviation was prescribed using the Taylor formula. In the right panel of figure 1 the results of the simulation are represented by the black circles while the solid line refers to the re-normalized concentrations, red circles are the experimental data. Even in this case the agreement can be considered satisfactory.

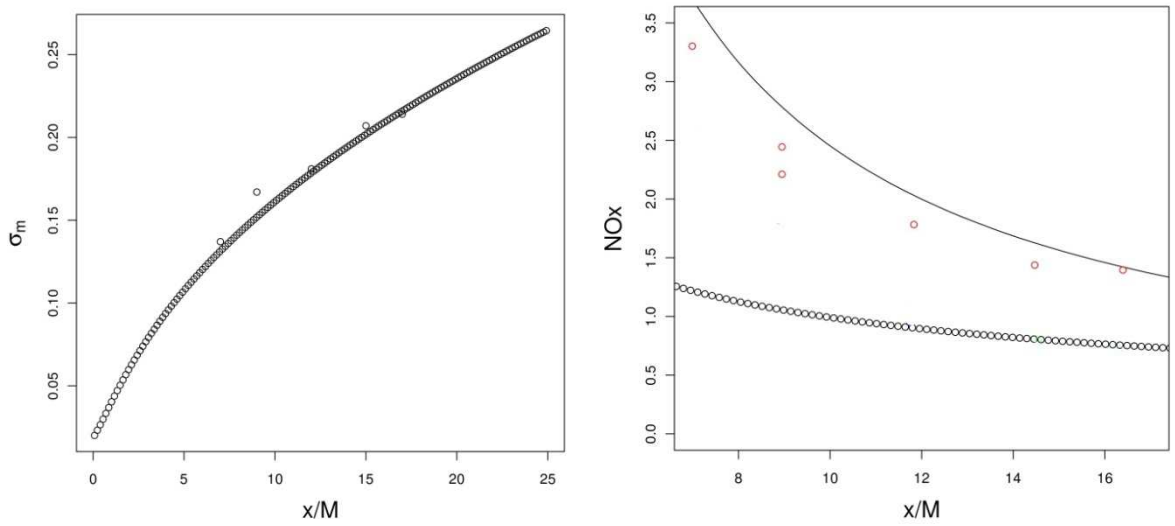

Figure 1. Frozen case: plume standard deviation (left), NOx concentration at the centreline as a function of the distance (right).

Figure 2 shows the comparison between simulated and measured NO concentrations at two sections whose distance from the source is respectively 7 and 17 turbulence scale M (the wind tunnel inlet grid mesh). In order to allow the comparison of the 1-D model with real data, the concentrations are normalised with the centreline values. The model behaves correctly well fitting the experimental data at both the distances.

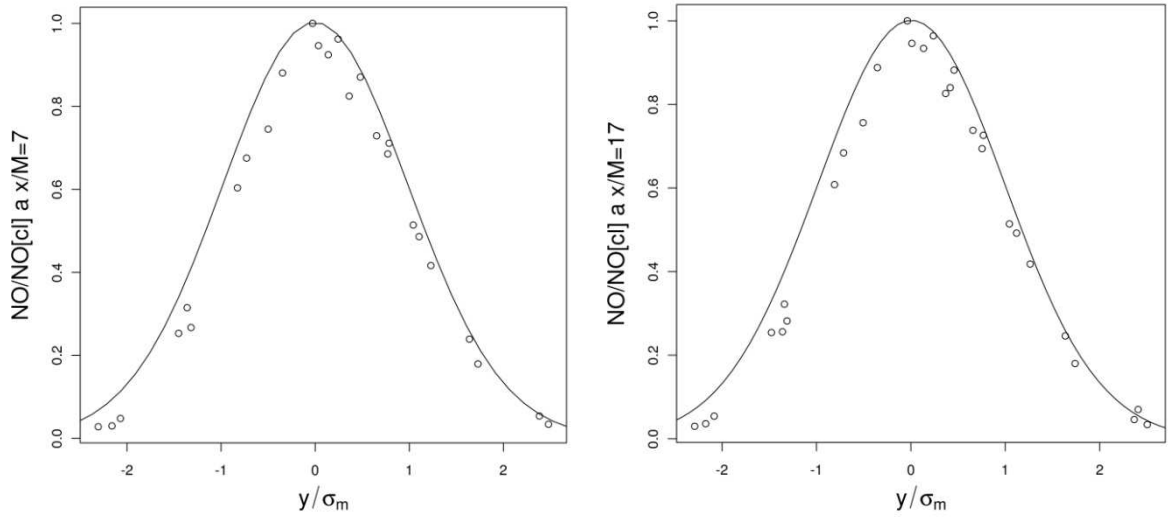

Figure 2. NO cross sections distribution at the two distances, lines: model, circles: experiment.

The second species considered is NO_2. The results are presented in figure 2. In this case the model underestimates the measured data at the first section (x/M=7). On the contrary, at the farthest distance a better agreement is found.

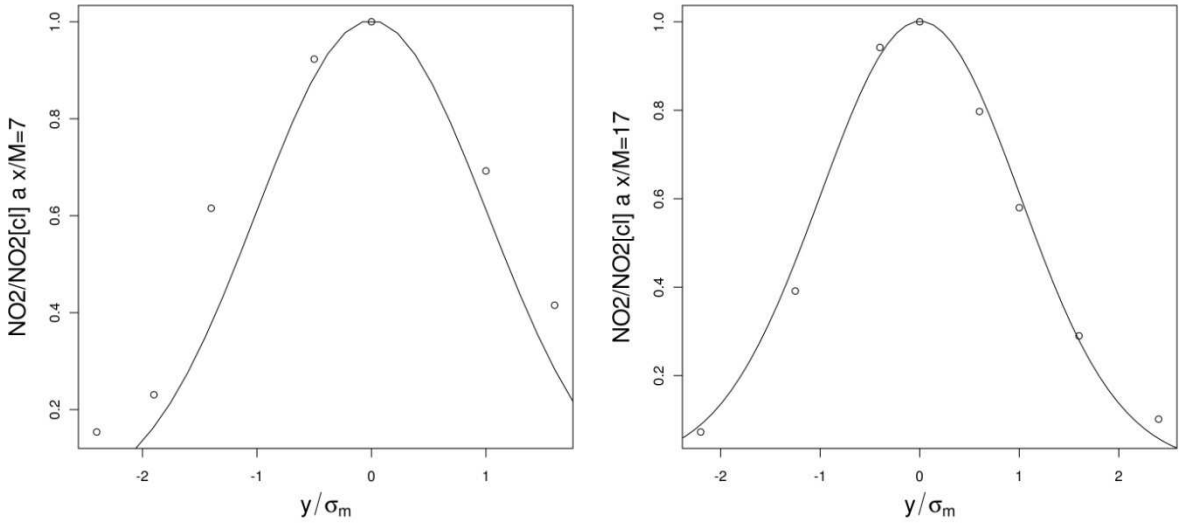

Figure 3. NO_2 cross sections distribution at the two distances, lines: model, circles: experiment.

Finally, results concerning the O_3 concentration are depicted in figure 4. The concentrations are normalised with the background ozone value. At x/M=7 the model overestimates the values at the plume edges and underestimates the centreline value. The agreement improves moving at further distances, where, except for the values close to the centreline, the data are well reproduced.

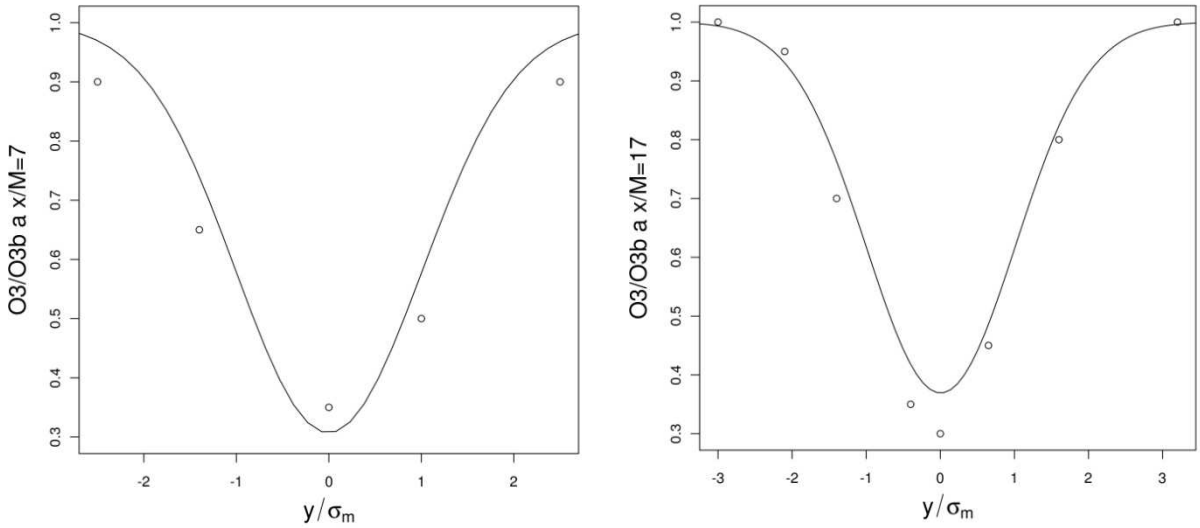

Figure 4. O_3 cross sections distribution at the two distances, lines: model, circles: experiment.

CONCLUDING REMARKS

A fluctuating plume model able to simulate the chemical reactions and accounting for the turbulence segregation effect is presented. In spite of its simple one-dimensional formulation the model performances are satisfactory both in the prediction of a conserved scalar dispersion and in the simulation of chemical reactions between reactive compounds. Further efforts need to be made in order to realize a two-dimensional model for real cases' simulation.

REFERENCES

Alessandrini, S. and Ferrero, E. (2009). A hybrid Lagrangian-Eulerian particle model for reacting pollutant dispersion in non-homogeneous non-isotropic turbulence. Physica A, 388, 1375-1387.

Brown, R. J. and Bilger, R. W. (1996). An experimental study of a reactive plume in grid turbulence. J. Fluid Mech., 312, 373-407.

Cassiani, M. and Giostra, U. (2002). A simple and fast model to compute concentration moments in a convective boundary layer. Atmos. Environ., 36, 4717-4724.

Crone, G., Dinar, N., van Dop, H., and L.Verwer, G. H. (1999). A Lagrangian approach for modelling turbulent transport and chemistry. Atmos. Environ, 33, 4919-4934.

Dosio, A. and Vilà-Guerau de Arellano, J. (2006). Statistics of absolute and relative dispersion in the atmospheric convective boundary

Franzese, P. (2003). Lagrangian stochastic modeling of a fluctuating plume in the convective boundary layer. Atmos. Environ., 37, 1691-1701.

Garmory, A., Richardson, E. S., and Mastorakos, E. (2006). Micromixing effects in a reacting plume by the stochastic fields method. Atmos. Environ., 40, 1078-1091.

Gifford, F. (1959). Statistical properties of a fluctuating plume dispersion model. Advances in Geophysics, 6, 117-137.

Loàiciga, H. A. and Leipnick, R. B. (2005). Correlated gamma variables in the analysis of microbial densities in water. Adv. Water Res., 28, 329-335.

Mortarini, L., Franzese, P., and Ferrero, E. (2009). A fluctuating plume model for concentration fluctuations in a plant canopy. Atmospheric Environment, 43, 4, 921-927.

Thomson, D. J. (1987). Criteria for the selection of stochastic models of particle trajectories in turbulent flows. J. Fluid Mech., 180, 529-556.

Thomson, D. J. (1990). A stochastic model for the motion of particle pairs in isotropic high Reynolds number, and its application to the problem of concentration variance. J. Fluid Mech., 210, 113-153.

van Dop, H. (2001). The evaluation of a Lagrangian model for turbulent transport and chemistry. Phys. Fluids, 13, 1331-1342.