A fluctuating plume model for pollutants dispersion with chemical reactions

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Introduction

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. Recently we developed a Lagrangian stochastic one-particle model with chemical reactions (Alessandrini and Ferrero, 2009), where the segregation coefficient, depending on the covariance of the species concentrations, is calculated through a parameterisation. An alternative 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). To predict the reactive airborne compounds concentration we followed an original approach: we re-wrote the fluctuating plume model using a bi-variate probability density function, 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 model

In the basic fluctuating plume model we have introduced the simple chemical equation:

$$\mathbf{NO + O_3 \longrightarrow NO_2 + O_2}$$

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. The PDF is split in the PDF of the position $\mathbf{(y_m; z_m)}$ of the plume centroid (barycentre), at a distance x from the source, and the concentration PDF relative to $\mathbf{(y_m; z_m)}$ in the reference frame moving with the cloud centroid, conditional to its location downwind. 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 then parameterised assuming a bi-variate Gamma distribution (Loáiciga and Leipnick, 2005). We consider that the dispersion in each component possesses a self-similar Gaussian form in the relative frame of reference. The $\mathbf{O_3}$ dispersion was simulated considering a fictitious species defined as the *deficit of ozone background concentration* (Alessandrini and Ferrero, 2009).

Case study

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 $\mathbf{O_3}$ concentration. The **NO** and $\mathbf{O_3}$ concentrations were measured at different cross-flow sections along the plume centreline. Air doped with $\mathbf{O_3}$ 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 $\mathbf{s^{-1}}$ 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. The measured turbulence was used as input of the dispersion model.

References

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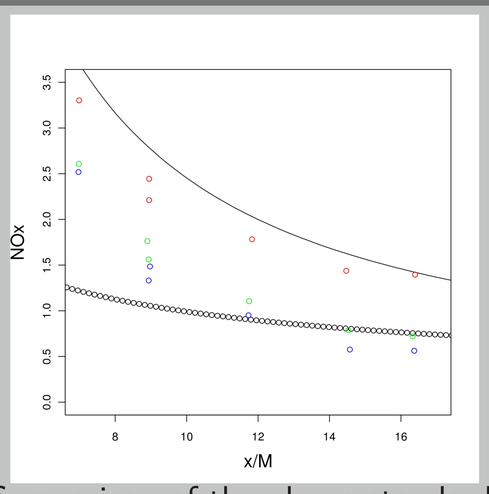
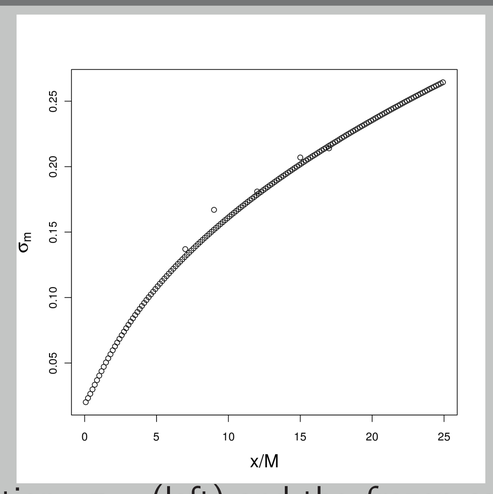
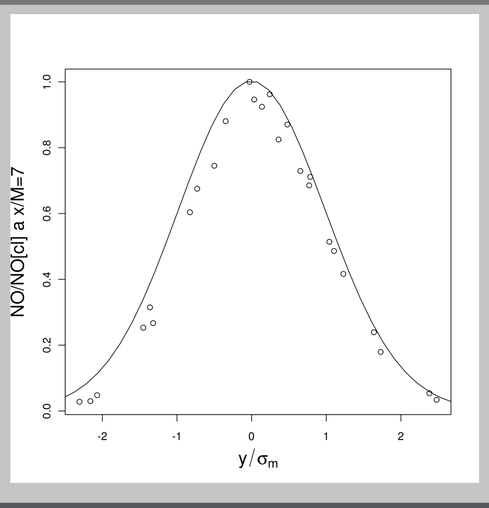
Results

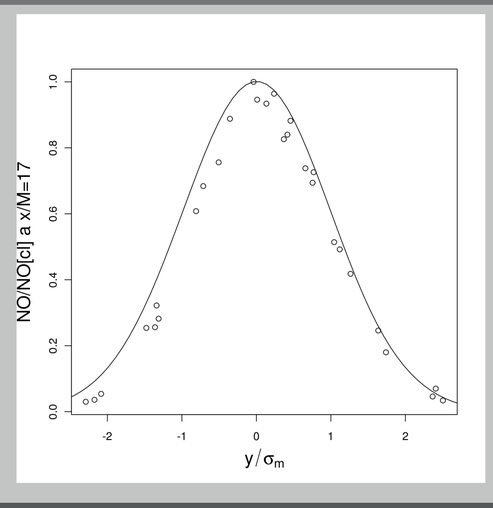




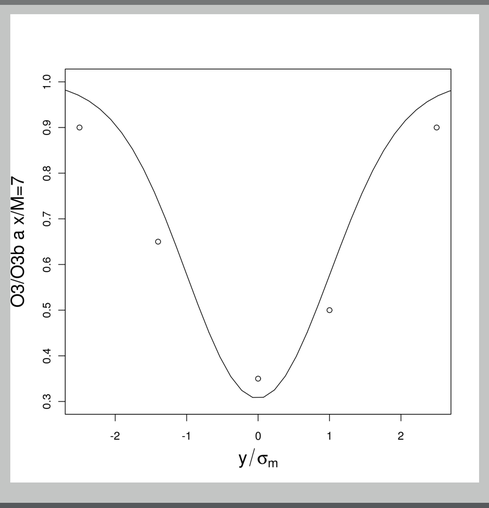
Comparison of the plume standard deviation, $\boldsymbol{\sigma_m}$, (left) and the *frozen case* plume centreline concentrations (right). The model is, in this version, one dimensional, thus the centreline concentration (black circles) is multiplied by the normalization factor of the Gaussian distribution (the solid line refers to the re-normalized concentrations) red circles are the experimental data.

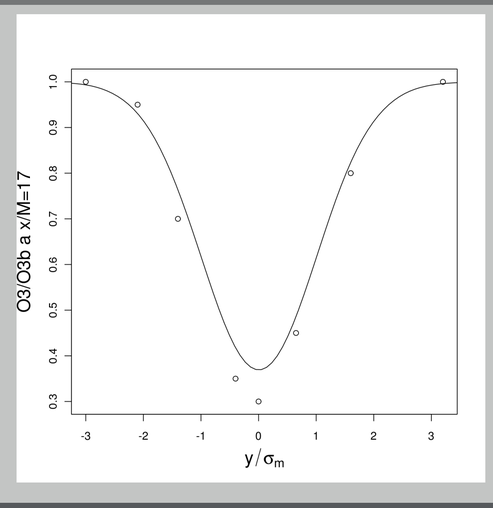
Results



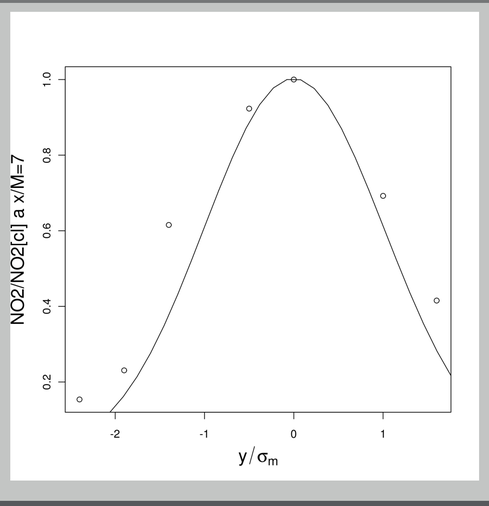


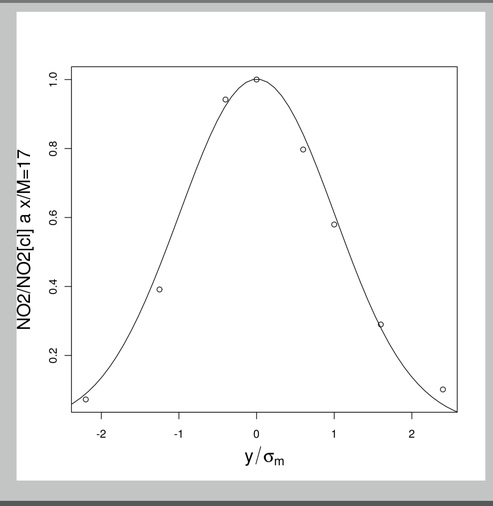
Results





Results





Conclusions

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 done in order to realize a two-dimensional model for real cases' simulation.

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