EVALUATION OF A LAGRANGIAN MODEL FOR PREDICTING CONCENTRATION FLUCTUATIONS IN URBAN AREAS

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INTRODUCTION

The accurate prediction of concentration fluctuations in a dispersing plume is fundamental to estimating many of the plume's most important characteristics. Applications as varied as the formation of secondary pollutants via chemical reactions, the levels of individual exposure, the levels of odour nuisance and the likelihood of ignition of flammable gases all require knowledge of the fluctuations of pollutant concentration as well as its mean. The fluctuations are caused by two turbulent mechanisms: firstly, eddies smaller than the size of the plume entrain clean air into the plume leading to small scale concentration gradients in the plume; secondly, eddies larger than the plume will cause the whole plume to meander horizontally and vertically and give rise to fluctuations at a fixed point as the plume is advected over the receptor. Meandering is particularly significant in atmospheric flows where turbulent length scales are normally larger than the dimensions of the source. In urban areas, the dispersion of plumes is complicated by the effects of the densely-packed buildings which modify the background wind flow and also increase the small scale turbulence. The greatest level of fluctuations will be in the near source region where the dispersion of the plume is governed by the local flow pattern. Consequently, modelling the fluctuations in an urban area requires an accurate description of the in-street flow as well as a dispersion model that can account for the widespread inhomogeneities. In this study, we use a microscale, *k*-*ε* CFD model to predict the flow between buildings and then model concentration fluctuations by combining a 1-particle Lagrangian Stochastic model with mixing using the interaction by exchange with mean (IEM) mechanism. The motivation is to develop a practical model of predicting fluctuations in urban areas that is far less computationally expense than eddy-resolving models such as LES. First, the model is tested against data of a plume in open terrain to verify the model's performance in a simple case without buildings; then the model is used to predict concentration fluctuations from a line source in a street canyon and the results compared with wind tunnel data.

MODEL

The Lagrangian Stochastic (LS) with mixing model used here is similar to those employed in Cassiani et al. (2005). A 1-particle or marked particle model is used to track fluid particles through the domain while the concentration pdf evolves using a mixing model. Particles are initially spread randomly throughout the domain with velocities randomly selected from a Gaussian distribution about the mean. The particle velocities and position evolve using the LS model of Thomson (1987) that takes account of the inhomogeneity in the flow. Only particles that pass through the source are assigned a positive concentration. The concentration of particles then evolves through the IEM mixing scheme as follows:

$$\frac{dC_p}{dt} = -\frac{1}{t_m}(C_p - \langle C \rangle)$$

where C_p is the concentration of the particle, $\langle C \rangle$ is the mean concentration and t_m is the mixing timescale. Here we set t_m to be a function of the local turbulent kinetic energy k and dissipation rate ε, i.e. $t_m = \alpha k/\varepsilon$, where α is a tuneable constant. Particles are reflected off solid boundaries with no loss of concentration or momentum. In order to stop excessive computation of particle trajectories near solid boundaries, a virtual 'reflection level' z_{rfl} is imposed above the boundaries, off which the particles are reflected.

RESULTS

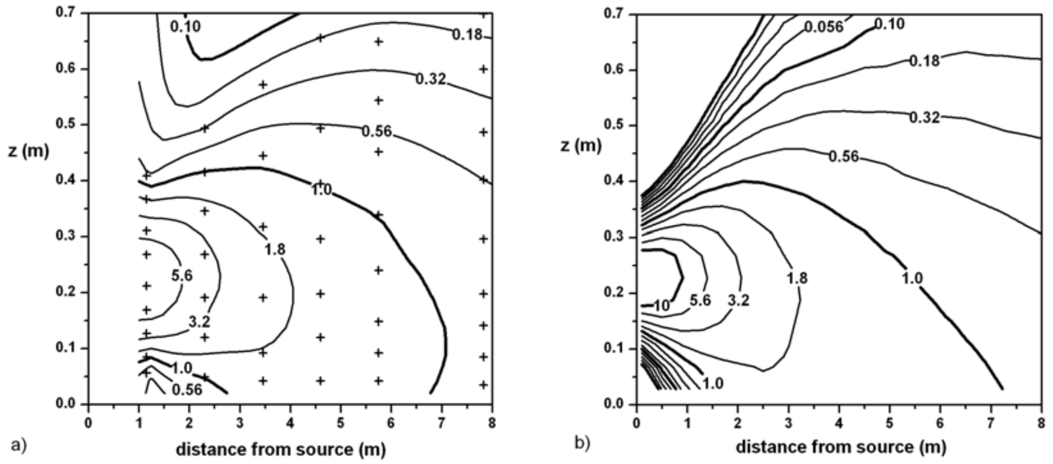

Fig. 1; Cross-sections of mean normalised concentration <C>/Q from a) Fackrell and Robins (1982) experiment and b) model.

Open Terrain

The model is first tested against the wind tunnel study of dispersion from an elevated point source by Fackrell and Robins (1982). The optimum model set-up was found with a Gaussian source distribution of σ_0 = 34mm (cf. experimental diameter of 8.5mm), constant c_0 = 5 and an IEM mixing timescale coefficient α = 0.75. The centre of the source was at a height of 0.228 m as in the experiment. The model domain was 8 m long by 0.88 m wide by 0.768 m high which was large enough to prevent concentration losses at the boundaries affecting the values on the cross-section through the plume centreline. The reflection level z_{rfl} was set at 0.008 m. 100,000 particle trajectories were tracked through the domain for 100s using a timestep of 0.2s. The model grid used to segregate particles for mixing had gridspacing of 0.4m, 0.08m and 0.04m in the *x, y* and *z* directions respectively.

Figure 1 shows the mean concentration <*C*> normalised by the emission rate *Q* from the experiment alongside the model simulation on the vertical cross-section through the plume centreline. In general, the agreement between model and experiment is good but there are some small differences. Model concentrations are lower in the top half of the domain than the experimental measurements, while at the lower boundary, the model plume reaches the surface slightly nearer the source than in the experiment, leading to higher concentrations in the model there. The model underestimates the vertical flux of tracer above the source level and overestimates the flux near the surface. This suggests the model does not fully capture the change in turbulence structure between the near surface region and at higher levels in the domain, i.e. larger eddies at higher levels are transporting more tracer away vertically in the experiment than the model, while near the surface, the model is transporting too much tracer towards the surface and so overestimating the size of eddies here. The differences between the model and the experiment are more marked in the comparison of fluctuation intensities σ_c/<*C*> in Figure 2. Both datasets show higher levels of intensity towards the edge of the plume in the top half of the domain but the model intensities are much higher than the experimental values. Some of this difference can be explained by the lower mean

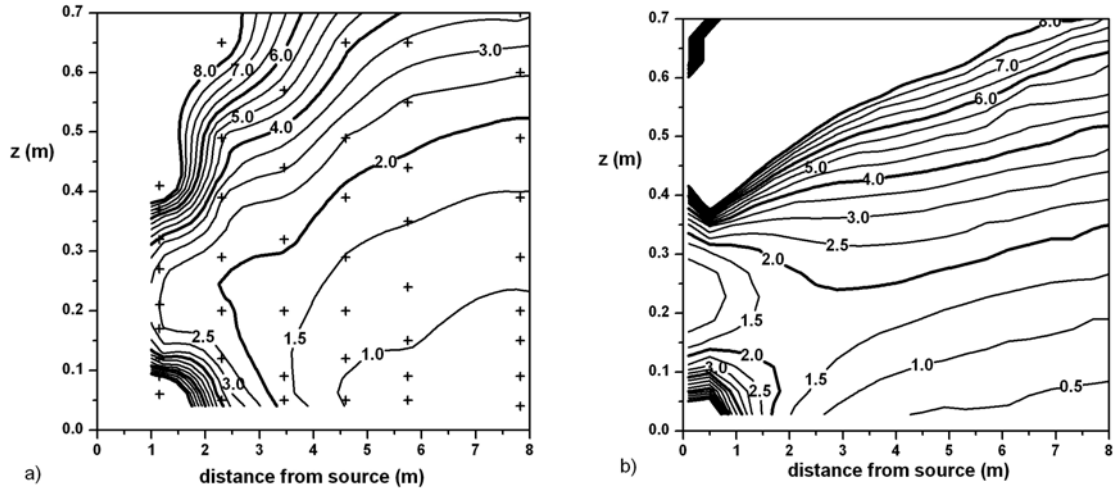

Fig. 2; Cross-sections of concentration intensity $\sigma_c/<C>$ from a) Fackrell and Robins (1982) experiment and b) model.

concentrations observed in the model at the top of the domain but the main factor is the reduced mixing in the model. Increasing the mixing, by reducing the coefficient α, can improve the model intensities at the top of the domain but only at the expense of making the intensities near the surface lower and further from the experimental results. The best comparison with model intensities was obtained with $\alpha = 0.75$.

The model does capture the effect of the lower boundary on the plume. The surface constrains the size of turbulent eddies in the flow above it, thereby reducing the meandering of the plume, while the increase in turbulent energy near the surface increases small scale mixing. Both these effects will tend to reduce the fluctuations near the surface. The results in Figure 2 show that the model is reproducing the low intensities at the surface well, although these low intensities are not penetrating as far into the flow as in the experiment. The effect of solid boundaries on the plume is crucial to modelling plume dispersion in urban areas, and here we have shown that a basic mixing model with simple reflection can capture the development of the fluctuation intensities at the surface reasonably well.

Street Canyon

The model is now tested against the wind tunnel data of Pavageau and Schatzmann (1999) who measured the concentration fluctuations in an idealised street canyon. A series of long, rectangular bars set at regularly-spaced intervals and perpendicular to the flow in the wind tunnel acted as a row of 2-dimensionsal buildings with street canyons between them. A continuous line source was set up in the nineteenth canyon downwind to simulate the pollution released from a steady stream of traffic. Measurements were made at 70 points in and above the test canyon using a high frequency, flame ionisation detector allowing cross-sections of the mean and fluctuating concentration to be constructed.

The flow field in the wind tunnel experiment was modelled using the k-ε, CFD model MISKAM Version 4.21 (Eichhorn 1996), which has been specifically written for flows in urban areas. RANS models like MISKAM are limited as they only produce a steady flow approximation to what is an essentially unsteady flow and so are not as physically correct as LES models that resolve the significant time-dependent eddies in the flow. The advantage of RANS models is that they are cheap to run, while they have shown good agreement with experimental data for flows around obstacles (Dixon and Tomlin, 2006). MISKAM is designed for full-scale simulations, so the wind tunnel experiment is reproduced at a scale one hundred times that in the wind tunnel, with a building height *H* of 6 m, inflow roughness of 17 cm and building and surface roughness of 5 cm. The inflow velocity profile was logarithmic with a value of 3 ms^{-1} imposed at a height of 3*H* i.e. the same value as the free-stream velocity in the wind tunnel. A reflection level z_{rfl} of 20 cm (0.0333*H*) was used at each side wall and the canyon floor. A top-hat distribution was used for the source and placed from the reflection level to a height of 40 cm (0.0667*H*). α was set to 0.75, the same as the optimum run in the open terrain simulations. The 2-dimensional model particle domain covered only the test canyon and 2 m above and 2m downstream. A grid with spacing of 0.25 m in the *x* and *z* directions was used to partition the particles for mixing. 20,000 particles were tracked through the domain over 5,000 seconds with a timestep of 0.1 s.

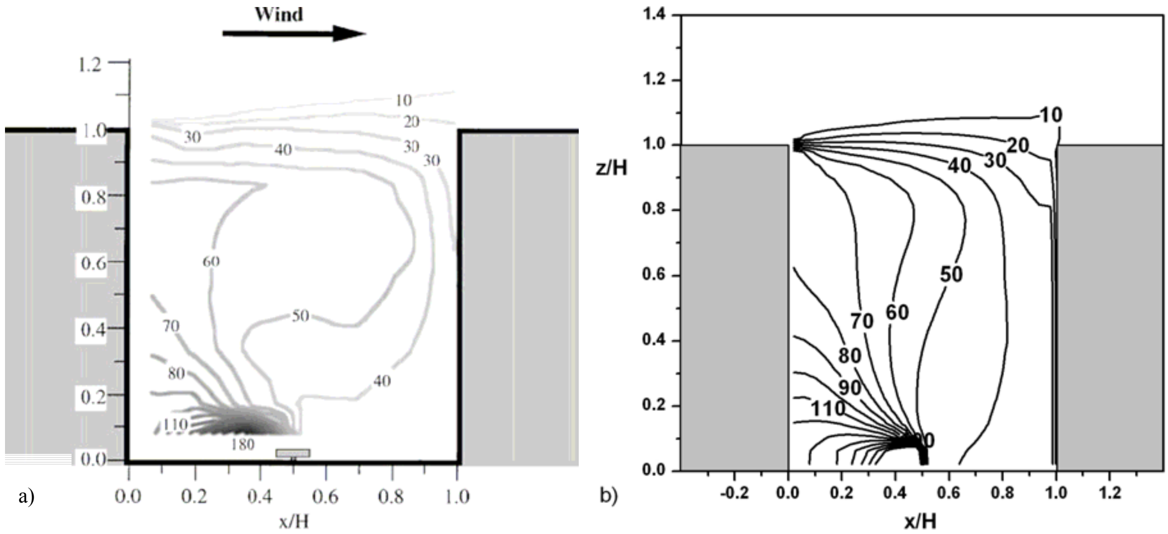

Fig. 3; Cross-sections of normalised mean concentration K from a) Pavageau and Schatzmann (1999) experiment and b) model.

Figure 3 shows the normalised mean concentrations *K* from the wind tunnel experiment and the model. *K* is defined as $K = \langle C \rangle U_{ref}HL/Q$ where $\langle C \rangle$ is the measured mean concentration, U_{ref} is the background flow velocity, *H* is the height of the obstacles and *Q/L* is the emission rate per unit length. The concentration is slightly higher in the model which is probably due to a reduced flux of concentration at roof level, otherwise the agreement is very good. The fluctuation intensities are shown in Figure 4 and the model captures the different intensity regions within the canyon. High levels of intensity occur downwind of the source which gradually reduces as the plume moves up the leeward wall. There is a region of low intensity in both experiment and model stretching from the upper part of the leeward wall to the bottom of the windward wall. The highest intensities occur in the shear layer at roof level. The experimental data shows the shear layer penetrates further into the canyon than in the model. Higher intensities also occur on the windward wall in the experiment reflecting the greater intrusion of clean air into the canyon.

CONCLUSIONS

This paper has detailed the development of a Lagrangian Stochastic model of dispersion with a mixing model to account for the dissipation of concentration fluctuations in an urban environment. The intention was to develop a model that can become a practical tool in predicting peak values of pollutants in cities on the street scale where dispersion is dominated

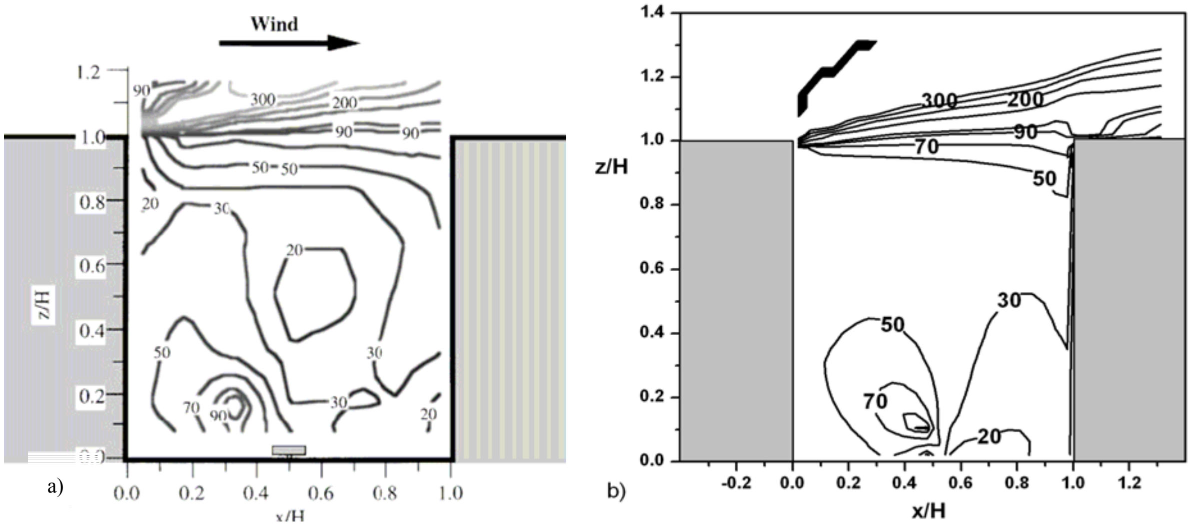

Fig. 4; Cross-sections of concentration intensity $\sigma_c/\langle C\rangle$ from a) Pavageau and Schatzmann (1999) experiment and b) model.

by the local flow pattern. Hence we have used an LS model that can be run using the flow fields from a steady-state, *k-ε* CFD model and the simple IEM mixing scheme so that computational expense is kept to a minimum. By choosing appropriate values for the source size and mixing timescale coefficient, the model has reproduced the mean concentration and fluctuation intensity from the open terrain experiment of Fackrell and Robins (1982) and the street canyon experiment of Pavageau and Schatzmann (1999) reasonably well. While the model results in the street canyon are encouraging, further tests are required in different and more realistic types of urban environments. However, there is a lack of wind tunnel and field studies of concentration fluctuations on the street scale at the present time. This is unfortunate because the street scale is where the pollutant concentrations will reach their highest levels and have their greatest impact and where models of concentration fluctuations will be most useful. As further experimental data becomes available, it will be possible to evaluate the range of models including RANS based and LES to assess the relative strengths and weaknesses of the different approaches. This will aid their application within real operational scenarios for the study of exposure peaks as well predicting secondary pollutant formation.

REFERENCES

Cassiani, M., P. Franzese, and U. Giostra, 2005: A PDF micromixing model of dispersion for atmospheric flow. Part 1: Development of the model, application to homogeneous turbulence and to neutral boundary layer. *Atmos. Environ.* **39**, 1457–1469.

Dixon, N.S., J.W.D. Boddy, R.J. Smalley and A.S. Tomlin, 2006: Evaluation of a turbulent flow and dispersion model in a typical street canyon in York, UK. *Atmos. Environ.* **40**, 958-972.

Eichhorn, J., 1996: Validation of a microscale pollutant dispersal model, *presented at the 21st International Meeting Air Pollution Modeling and its Application, Baltimore, 1995.*

Fackrell, J.E. and A.G. Robins, 1982: Concentration fluctuations and fluxes in plumes from point sources in a turbulent boundary layer. *Journal of Fluid Mechanics* **117**, 1–26.

Pavageau, M. and M. Schatzmann, 1999: Wind tunnel measurements of concentration fluctuations in an urban street canyon. *Atmos. Environ.* **33**, 3961–3971.

Thomson, D.J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *Journal of Fluid Mechanics* **180**, 529-556.