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STREET CANYON CONCENTRATION ESTIMATION COUPLING THE RANS MODEL MISKAM AND THE MICROMIXING LAGRANGIAN MODEL LAGFLUM

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Abstract: The stationary three-dimensional Lagrangian stochastic model LAGFLUM has been coupled with MISKAM to simulate numerically the higher statistical moments of concentration for a passive scalar in the 3D turbulent flow corresponding to MUST wind tunnel experiment. LAGFLUM is based on the coupling of a macromixing scheme founded on the well-mixed condition, while the micromixing scheme utilizes the IECM. The LAGFLUM input data have been obtained by using the output of the MISKAM model applied to the MUST experiment. The results show a reasonable agreement between simulated and measured statistical moments of concentration.

Key words: *concentration fluctuations, LAGFLUM, MISKAM, COST 732, MUST.*

INTRODUCTION

Street canyon concentration modelling represents a useful numerical tool for urban air quality management. The estimation of the mean concentration of traffic pollutants has been usually the main task of urban dispersion models. Nevertheless concentration fluctuations could be relevant at the micro-scale and are of primary importance for accidental releases. The Reynolds-Averaged-Navier-Stokes (RANS) meteorological model MISKAM (Microscale Flow and Dispersion) has been coupled with the micromixing Lagrangian dispersion model LAGFLUM (LAGrangian FLUctuation Model). This modelling system has been validated on the MUST (Mock Urban Setting Test) (Yee, E. and C.A. Biltoft, 2004) wind tunnel experiment by Bezpalcova, K. (2007) and Leitl, B. *et al.* (2007), where the dispersion of a passive tracer in a 3D stationary flow field, in presence of obstacles, was analysed.

The 3D stochastic model LAGFLUM, based on the coupling of a macromixing with a micromixing scheme, has been applied to determine the most significant statistical moments of concentration of a passive scalar. The macromixing scheme is founded on the well-mixed condition (Thomson, D.J., 1987), while the micromixing utilises the IECM (Interaction by Exchange with the Conditional Mean) (Pope, S.B., 1998). LAGFLUM can be easily coupled with common k-ε models, from which it carries out all the input data. In this work, the turbulent flow field used as input for LAGFLUM was obtained from MISKAM. It solves the Reynolds averaged Navier-Stokes equations with a modified k-ε turbulence closure in a non-uniform Cartesian grid. In particular mean velocities and turbulent kinetic energy evaluated with MISKAM, by modelling the MUST experiment, have been furnished to LAGFLUM. The next two sections describe MISKAM and LAGFLUM models, the successive one presents the main results of the concentration.

THE MISKAM MODEL

The flow field in this study is calculated using the MISKAM code. The MISKAM 3D RANS model is widely used in environmental assessment practice in Europe because of its simple model setup and the ability to gain results fast on personal computers. The model consists of a flow and a dispersion part: calculated flow fields serve as inputs for a Eulerian advective dispersion simulation. In this paper the MISKAM flow field results are used to drive the LAGFLUM code.

MISKAM model description

MISKAM solves the three-dimensional motion equations with Boussinessq-approximaton using the standard k-ε turbulence closure in which the production rates of turbulence kinetic energy and dissipation are replaced following suggestions by Kato, M and B.E. Launder (1993) and López, S.D. (2002). Grid type of Arakawa-C is used, with buildings represented as blockouts. The applied new version 6 introduced revised numerical schemes, with which high numerical diffusion of the upstream scheme used earlier could be avoided. A detailed description of the model can be found for example in Eichhorn, J. and A. Kniffka (2010). The model was extensively validated in the last years, comparison to simple geometries were performed by Eichhorn, J and A. Kniffka (2010) and by Olesen, H. *et al.* (2009). The implemented vegetation model was evaluated by Balczó, M. *et al.* (2009). The model also participated in several round tests of urban measurement datasets.

Flow simulation of the MUST case

The MUST was a full-scale wind and dispersion measurement campaign on an arrangement of 120 standard shipping containers in a Utah desert area. The MISKAM simulation of the MUST case was performed in the framework of the European COST Action 732 (Eichhorn, J. and M. Balczó, 2008). From several grids a fine one was selected as it gave the best agreement with wind tunnel data reported by Leitl, B. *et al.* (2007). The simulation domain is shown in Figure 1. Grid axes are parallel to the container walls, and wind direction is -45 degree.

Coupling technicalities

MISKAM simulation results of the variables k and the three components of the mean velocity vector $\overline{u},\overline{v},\overline{w}$, respectively along the x, y and z axis, from the denser simulation grid are linearly interpolated to the cell centres of the LAGFLUM grid. Variances of u, v and w were determined as 2/3 k. A problem emerges from the aligned positions of buildings in the different grids (Figure 2) which might cause deviations in the results near the container walls.

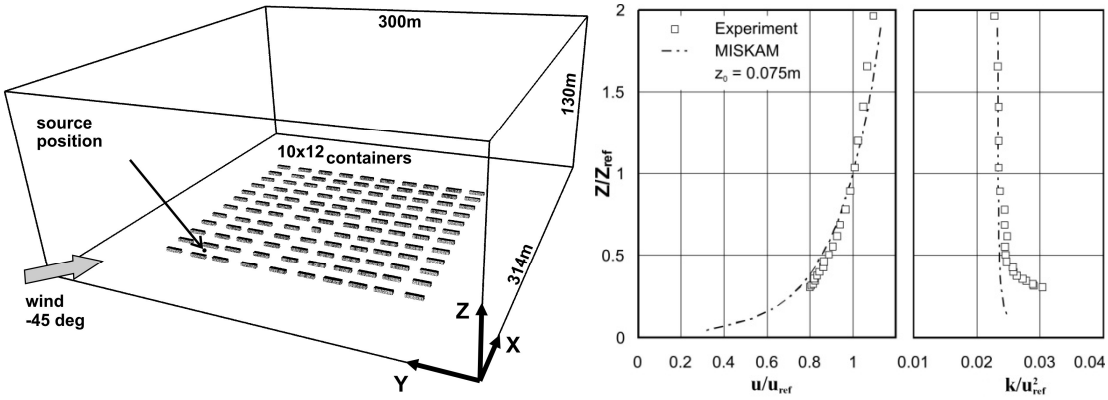

Figure 1. MISKAM domain of the MUST case (left); inlet boundary conditions (right).

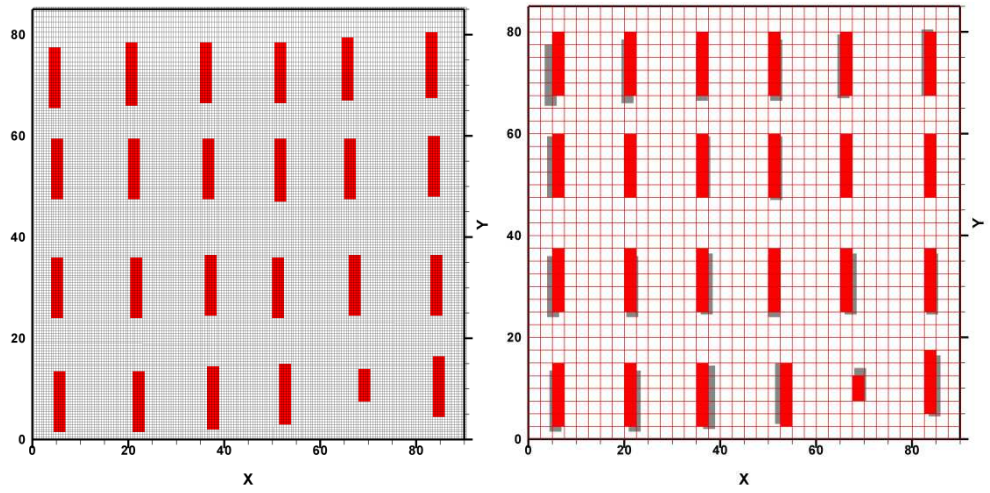

Figure 2. MISKAM grid (left); LAGFLUM grid with MISKAM (grey) and aligned (red) building positions.

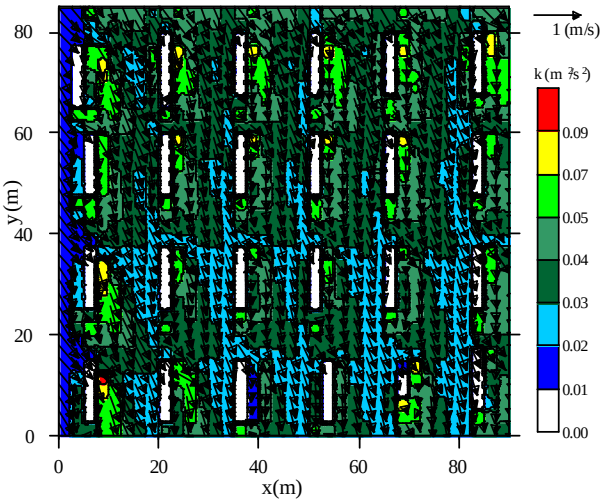

Figure 3. The horizontal wind speed (arrows) and turbulent kinetic energy k (colour map) at *z=H/2*.

Grid resolution is 0.5 x 0.5 x 0.5m in the region of the container blocks with a total number of 4.8 million (400 x 400 x 30) grid cells. The default boundary condition types of MISKAM are used: no-slip conditions were applied on the surfaces using wall functions, outflow boundaries had no-flux conditions. At the inlet boundaries a logarithmic profile was generated with an initial roughness length z_0. The reference velocity u_{ref} was set to 1 ms^{-1} at z_{ref} = 7.29 m. A good fit to wind tunnel data was

achieved using a higher roughness length z_0 than that in the original data set. On the top boundary constant variable values taken from the top of the inlet profile are prescribed.

Comparison of wind profiles at 18 tower locations in 498 measurement points gave a general good agreement with wind tunnel data. The model had however difficulties in resolving small-scale flow structures in the vicinity of containers (this would only be possible at higher grid resolution and eventually with another turbulence closure), and thus validation metrics were fair for variables of lateral and vertical wind velocity. Calculated hit rates for the mean velocity component U were 0.81 (excellent) while for W only 0.19 (poor). Turbulent kinetic energy k gave a hit rate value of 0.59 (nearly good). Hit rate values of above 0.66 might be seen as state-of-the-art. With these results however MISKAM 6 performed well in comparison to the range of microscale meteorological models investigated in COST 732. Figure 3 shows the fields of horizontal wind speed and k interpolated in LAGFLUM cells.

THE LAGFLUM MODEL

LAGFLUM utilises both macromixing and micromixing schemes. It calculates the mean concentration during the first phase (macromixing) of the model run, while the concentration variance is computed in the second phase (micromixing). The macromixing scheme is based on the so called "well-mixed" condition and describes the motion of fictitious trajectories of marked fluid particles. As pointed out by Pope, S.B. (1998), for high Reynolds numbers the mean of concentration and the mean conditioned on the velocity are unaffected by the value of molecular diffusivity. Therefore, polluted fluid particles, which do not exchange pollutant mass with the surrounding ones, can be utilised to estimate the averaged concentration. The well-mixed condition ensures a well-founded behaviour of the model also in inhomogeneous turbulence. The following set of stochastic differential equations have been integrated (hereinafter the Einstein notation applies):

$$dU_i = a_i(\boldsymbol{X},\boldsymbol{U},t)dt + b_{ij}(\boldsymbol{X},\boldsymbol{U},t)d\xi_j \tag{1}$$

$$dX_i = U_i dt \tag{2}$$

where U_i and X_i indicate the particle velocity and position respectively, the subscripts refer to the axis direction, and the $d\xi_j$ are the increments of independent Gaussian Wiener processes with mean zero and variance dt. The functions a_i and b_{ij} in stationary cases can be calculated as follows:

$$a_i = -B_{ij}\left(V^{-1}\right)_{jk}\left(U_k - \overline{u_k}\right) + \frac{\phi_i}{g_a} \tag{3}$$

$$2B_{ij} = b_{ik}b_{jk} = \delta_{ij}C_0\varepsilon \tag{4}$$

$$\frac{\phi_i}{g_a} = \frac{1}{2}\frac{\partial V_{il}}{\partial x_l} + \overline{u_l}\frac{\partial \overline{u_i}}{\partial x^l} + \left(\frac{1}{2}\left(V^{-1}\right)_j \overline{u_m}\frac{\partial V_{il}}{\partial x_m} + \frac{\partial \overline{u_i}}{\partial x_j}\right)\left(U_j - \overline{u_j}\right) + \frac{1}{2}\left(V^{-1}\right)_j \frac{\partial V_{il}}{\partial x_k}\left(U_j - \overline{u_j}\right)\left(U_k - \overline{u_k}\right) \tag{5}$$

C_0 is the Kolmogorov constant, assumed equal to 4, g_a is the probability density function of the Eulerian velocity $\overline{u_i}$ (corresponding to $\overline{u},\overline{v},\overline{w}$), δ_{ij} is the Kronecker delta and V_{ij} is the one-point velocity covariance matrix of the turbulence (due to lack of data this matrix has been considered diagonal) and ε is the rate of k. ε has been computed as a function of k (Stull, R.B., 1988):

$$\varepsilon = 0.3\,k\sqrt{\left(\frac{\partial \overline{u_i}}{\partial x_j}\right)^2} \tag{6}$$

Fifteen million particles have been released, in order to calculate both the mean $\bar{c}$ and conditional mean concentration $\langle c|\mathbf{U}\rangle$

In the second phase of the model run the IECM micromixing equation has been integrated. A large number of particles should be released all over the domain, uniformly distributed. Every particle should be initialized with the conditional mean concentration of the starting cell, in order to reproduce the motion of the whole fluid. Since the fluid motion has a predominant direction of motion, we can start the particles, in a more efficient way, only from the pollutant source and from the boundary of the plume. Sixty million particles have been released; they move according to the macromixing scheme (1,2) and exchange pollutant mass through the micromixing process. In this way all the particles (non conservative) have their own representative instantaneous concentration: their statistical computation in every cell of the domain gives, in theory, all the concentration moments. In practise the lower order moments are better simulated and we focus here on the mean, variance and skewness. The micromixing model adopted is the IECM:

$$\frac{dC}{dt} = -\frac{C - \langle c|\mathbf{U}\rangle}{t_m} \tag{7}$$

where C is the instantaneous particle concentration and t_m is the mixing time scale. Since the simulation represents a large number of realisations of the turbulent regime, the conditional mean in (7) is consistent with the particles exchanging pollutant mass only with the surrounding particles belonging to a similar realisation (i.e. with a similar velocity at the particle

location). The IECM scheme guarantees that the mean concentrations given by the macromixing model are unaffected by mixing, according to the balance equation for the pollutant mass. The mixing time scale is assigned consistently with the asymptotic mixing constraints (Cassiani, M. *et al.*, 2005):

$$t_m = \mu\left[1.225\frac{\sigma_0^{2/3}}{\varepsilon^{1/3}} + \sqrt{2T_L t_f}\right] \tag{8}$$

where μ=0.75 is the micromixing constant, $T_L = 4k/3C_0\varepsilon$ is the Lagrangian integral time scale, σ_0 is the source length scale and t_f is the mean flight time of the particles, calculated on each cell during the macromixing process. The numerical domain of (90*85*21 m^3) is divided into (36*34*42) cells with a horizontal spacing of dx=dy=2.5 m and a vertical one equal to dz=0.5 m. The pollutant source has been approximated with a continuous point emission. Furthermore, a geometrical reflection has been assumed for the particles hitting the ground or the obstacles.

RESULTS

The results of the numerical simulation have been compared with the wind tunnel measurements of concentration on the horizontal plane at half obstacle height (Figure 4). All the values of mean and standard deviation of the concentration have been normalized with the reference scale Q/H^2u_{ref}, where Q is the source mass rate.

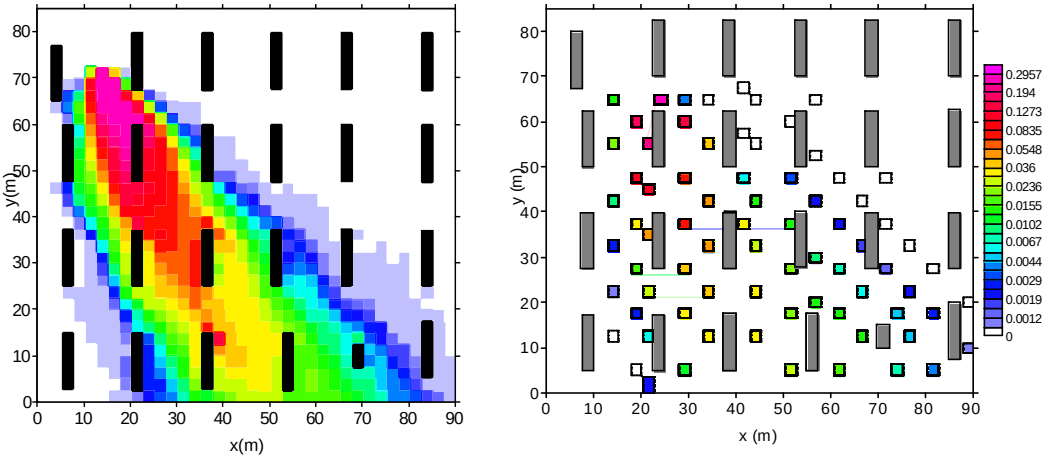

Figure 4. Comparisons between (left) the simulated normalized mean concentration and (right) the corresponding wind tunnel measures (squares) at z=H/2.

The centre of mass of the plume is not aligned with the wind speed reference direction, but it is rotated clockwise. In fact the obstacles channel the wind as it enters the array, due to their thin shape and the narrow canyons. However, as the distance from the source increases, the plume axis tends to the reference wind direction, because the pollutant flux from the zones above the array begins to be important. The comparison between numerical and experimental results shows a satisfying agreement. Both the plume shape and the concentration levels seem to be correctly reproduced, with the exclusion of a small underestimation of the pollutant dispersion across the plume axis. The standard deviations of the concentration are shown in Figure 5. In comparison to the mean, they show an accentuated channelling effect and a wider lateral spread of fluctuations in the neighbourhood of the source (Figure 5). Such behaviour is visible also in the measured data and confirms the good performances of the model, which seems to properly reproduce the dissipation of the concentration fluctuations along the particle trajectories. The agreement is further confirmed by the transversal profiles of the standard deviation of concentration reported in Figure 6a.

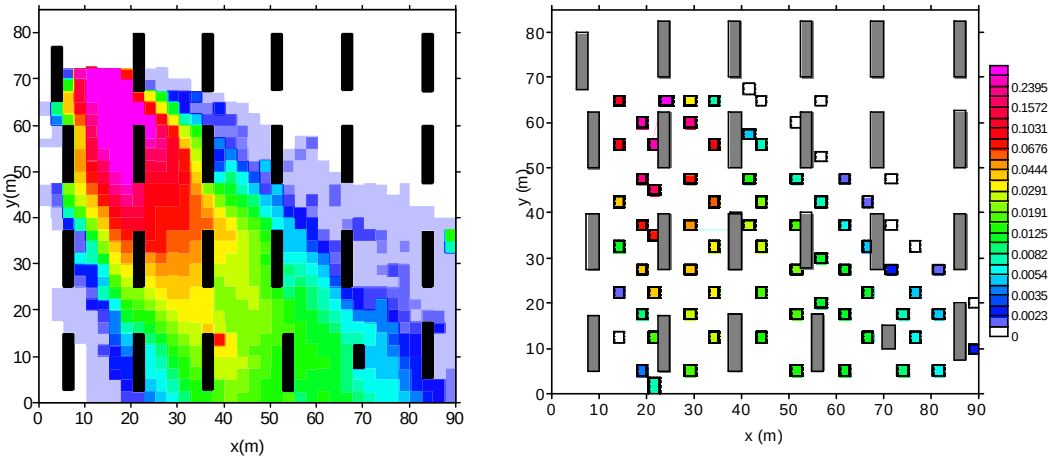

Figure 5. As in Figure 2, but for the normalized standard deviation of concentration.

Finally, Figure 6b shows the transversal profiles of the concentration skewness. A general overestimation with respect to the measurements occurs. However, as pointed out by Bezpalcova, K. (2007), discrepancies in the comparison of the higher moments of the concentration might be present, due to the different reference velocities used in the concentration normalization procedure (MISKAM utilizes a low reference velocity in order to approach the Reynolds number of the wind tunnel experiment).

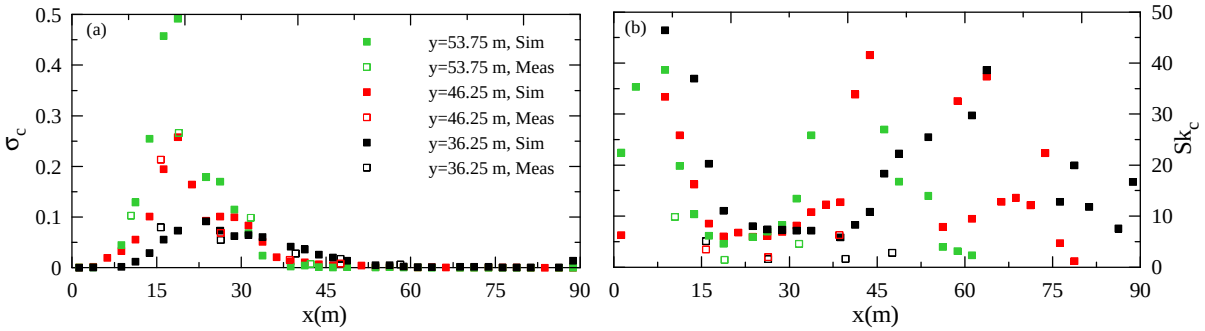

Figure 6. Comparison between simulated (full squares) and measured (open squares) standard deviation (a) and skewness (b) of the concentration.

CONCLUSIONS

The numerical 3D model LAGFLUM (LAGrangian FLUctuation Model) based on the "well mixed" macromixing scheme (Thomson, D J., 1987), and the IECM micromixing scheme (Pope, S.B., 1998) has been presented. The model has been applied to the wind tunnel experiment of Bezpalcova, K. (2007) and Leitl, B., *et al.*, (2007) on passive pollutant dispersion in presence of obstacles (MUST experiment). The LAGFLUM input data have been obtained by using the output of the MISKAM model applied to the MUST experiment. The simulated values of mean and variance of concentration show a reasonable agreement with the corresponding measurements; both shape and concentration levels are reproduced satisfactorily. The concentration skewness calculated by LAGFLUM has the same order of magnitude of the measured one. Since LAGFLUM can be easily coupled with common k-ε models, it seems to furnish a practical tool for the investigation of concentration fluctuations in very complex urban environments.

REFERENCES

Balczó, M., Gromke, C. and Ruck, B. 2009: Numerical modeling of flow and pollutant dispersion in street canyons with tree planting. *Meteorologische Zeitschrift*, **18** No. 2, 197-206.

Bezpalcova, K., 2007: Physical modelling of flow and diffusion in urban canopy, PhD thesis.

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

Eichhorn, J. and Balczó, M., 2008: Flow and dispersal simulations of the Mock Urban Setting Test. The 12th International Conference on Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes (HARMO12), Cavtat, Croatia, October 6-9, 2008. *Croatian Meteorol. J.*, **43**, 67-72.

Eichhorn, J. and Kniffka, A. 2010: The numerical flow model MISKAM: State of development and evaluation of the basic version. *Meteorologische Zeitschrift*, **19**, 81-90.

Kato, M. and Launder, B.E., 1993: The modelling of turbulent flow around stationary and vibrating square cylinders, Ninth Symposium on Turbulent Shear Flows, Kyoto, Japan, August 1993, 10.4.1–10.4.6.

Leitl, B., K. Bezpalcova and F. Harms, 2007: Wind tunnel modelling of the MUST experiment. Proceeding of the 11th International Conference on Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes, Cambridge 2-5 July 2007, **2**, 435-439.

López, S.D., 2002: Numerische Modellierung turbulenter Umströmungen von Gebäuden. PhD thesis, University of Bremen, Germany.

Olesen, H., Berkowicz, R., Ketzel, M., Løfstrøm, P., 2009: Validation of OML, AERMOD/PRIME and MISKAM using the Thompson wind-tunnel dataset for simple stack-building configurations. *Boundary-Layer Meteorol.*, **131**, 73-83.

Pope, S.B., 1998: The vanishing effect of molecular diffusivity on turbulent dispersion: implications for turbulent mixing and the scalar flux. *J. Fluid Mech.*, **359**, 299-312.

Stull, R.B., 1988: An Introduction to Boundary Layer Meteorology, Springer.

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

Yee, E. and Biltoft, C.A., 2004: Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. *Boundary-Layer Meteorol.*, **111**, 363–415.