

# Modelling the dispersion of a tracer gas in the wake of an isolated low-rise building

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**Abstract.** Mean concentrations of ammonia gas released as a tracer from an isolated low-rise building have been measured and predicted. Predictions were calculated using computational fluid dynamics (CFD) and two dispersion models: a diffusion model and a Lagrangian particle tracking technique. Explicit account was taken of the natural variation of wind direction by a technique based on the weighted summation of individual steady state wind direction results according to the probability density function of the wind direction. The results indicated that at distances  $>3$  building heights downstream the weighted predictions from either model are satisfactory but that in the near wake the diffusion model is less successful. Weighted solutions give significantly improved predictions over unweighted results. Lack of plume spread is identified as the main cause of inaccuracies in predictions and this is linked to inadequate resolution of flow features and mixing in the CFD model. Further work on non-steady state simulation of wake flows for dispersion studies is recommended.

**Key words:** computational fluid dynamics; dispersion; tracer gas; modelling; building wake.

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## 1. Introduction

The prediction of pollutant concentrations downwind of isolated structures is important in the evaluation of environmental hazard and also in the case of ammonia in the deposition and re-emission rates from plants and soils. This mechanism is particularly important in the near wake, which presents particular modelling difficulties because the currently used Gaussian and computational fluid dynamics (CFD) based scalar diffusion models are invalid in this region. It is also the region of maximum sensitivity to the detailed structure and variability of the approach flow.

The study described here was carried out with the objective of determining firstly whether a current Lagrangian stochastic model provides a more accurate simulation of dispersion in the near wake compared to a simple diffusion model, and secondly whether the variability of the approach flow was a significant factor in the accuracy of prediction of dispersion in this region, and if so, how to account for this in simulations. To test these hypotheses a number of simulation studies were undertaken in conjunction with experimental measurements of ammonia released from an isolated building. The building had previously been used for a study of wind effects which have been well documented (Robertson and Glass 1988, Hoxey *et al.* 1995, Richardson *et al.* 1995).

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## 2. Methodology

### 2.1. Experimental methodology

Fig. 1 shows the layout of the building, source and detection masts for the measurements of mean concentration of ammonia. Pure ammonia gas was released from a point source above the building ridge and denuder tubes used to collect samples at 5 heights on each of 3 masts downwind of the building, following the procedures of Ferm (1979). The denuder tubes consisted of a narrow glass tube, the internal surface of which was coated in oxalic acid. Through these tubes was drawn a continuous sample of the air from the sample position by means of a critical orifice (to maintain a constant flow rate) and a pump. The total sample volume was measured for each denuder by a total flow meter. Once analysed to ascertain the total amount of ammonia captured by the oxalic acid in each denuder, this was divided by the total sample volume to give a mean air concentration sampled over the period of the experiment. These measurements were undertaken throughout the summer of 1996 and data were collected for many mean wind directions in both wet and dry conditions. For this study, because of the significant effect of wet deposition of ammonia gas (Couling 1996) only data for dry conditions are considered. In addition, for modelling simplicity, only data with mean wind angle up to 20 degrees from the normal to the long face of the building are considered. Release rates of ammonia gas from the source were  $1.6 - 2.5 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$  with the exact rate being measured for each sample period of between 15 and 30 minutes.

Wind data were collected from a reference mast (height 2.5 m) using an ultrasonic anemometer, located approximately 5 building heights (25 m) upwind of the building. This gave three component wind data at a 20.83 Hz sampling frequency. These data were collected over the entire gas release period of each measurement and subsequently analysed for mean wind-speed, direction and wind variability over each experimental period. This final measure was calculated both as an overall variance statistic and in terms of sub-interval means within the sample period. The length of these sub-intervals, 1 minute, was chosen to remove the small scale gust fluctuations but reflect the mean wind direction variations over the time period important to the dispersion. This allowed 15 – 30 sub-intervals per sample period (of 15 – 30 minutes) from which a histogram of the distribution of wind

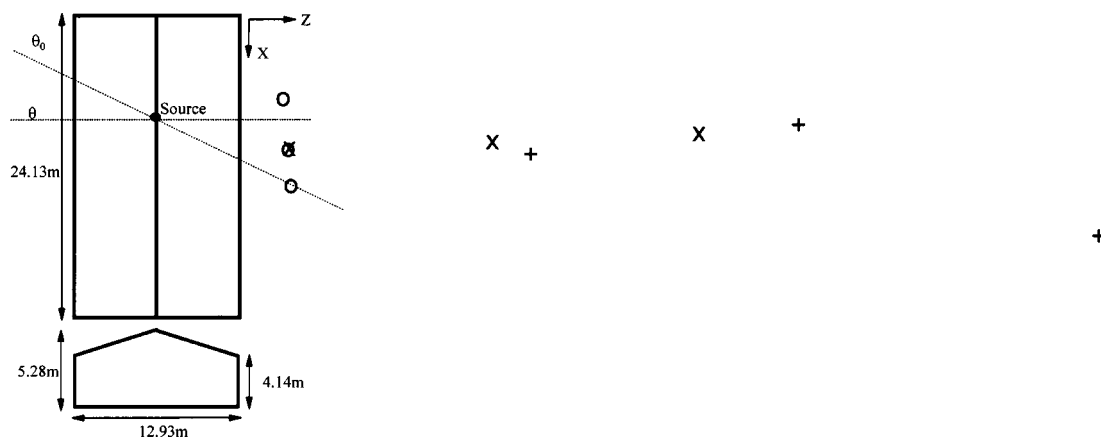


Fig. 1 Illustration of Silsoe Structures Building and position of measurement locations (Mast positions are shown as o for 26th July, x for 1st August and + for 21st August measurements)

direction could be constructed. A discussion of the effect of this choice is given in section 2.2.

## 2.2. Simulation methodology

A commercially available computational fluid dynamics (CFD) package [AEAT-CFDS CFX-4.1] was used as the basis for predicting the airflow around the building. The domain mesh used for these simulations was based on that used in previous studies of the wind loading on the Silsoe Structures Building (Richards and Hoxey 1992a). This grid had  $\approx 85\,000$  cells arranged in a domain  $264\text{ m} \times 252\text{ m} \times 85\text{ m}$  (11 building lengths  $\times$  21 building widths  $\times$  16 building heights) with a distribution of cells (geometric progression factor 1.41) such that the smallest ( $\approx 0.4\text{ m} \times 0.5\text{ m} \times 0.3\text{ m}$ ) were close to the building surface. This mesh was quite large in current building pressure loading simulation terms but was necessary for this study where a large domain was required. Further refinement would have increased typical run times significantly and was therefore not considered practical.

For the study the basic “ $k - \varepsilon$ ” turbulence model (Launder and Spalding 1974) was modified to include the modifications proposed by Tsuchiya *et al.* (1997) (the “MMK”  $k - \varepsilon$  model) for bluff body studies. In all simulations the Curvature Compensated Convective Transport (CCCT) differencing scheme (Gaskell and Lau 1988) was used for the velocity and turbulence quantities as this type of flux limited scheme has been suggested to be most appropriate for bluff body aerodynamics. Boundary conditions matching the roughness of the experimental site surface ( $z_0 = 0.01\text{ m}$ ) were also included. The inlet condition adopted for the atmospheric boundary layer (ABL) was developed in a separate simulation of flow over an infinite rough plate with roughness length equivalent to that found at the experimental site. This gave a logarithmic velocity profile which was self-sustaining over an empty fetch simulation and which closely matches the measured velocity profile at the experimental site (Hoxey and Richards 1992). The turbulent kinetic energy profile is under-predicted in this method, because of the normal problems associated with the  $k - \varepsilon$  turbulence model, and no changes were made to improve this agreement, such as altering  $C_\mu$ : (Richards and Hoxey 1992b). This was considered appropriate because normally studies of such dispersion problems would not involve alterations of the model parameters without detailed site information and that even then such changes are not advised when using CFD in order to preserve the generality of the model used. It has also been suggested (Richards and Hoxey 1992b) that there are physical reasons for this discrepancy in terms of the length scale composition of the turbulence of the ABL and that simulated by this type of model. From the experimental data collected, the mean reference wind speed was calculated as  $\approx 6\text{ ms}^{-1}$  at 50 m reference height for all of the cases considered in this study. This value was therefore used in the simulations to define the inlet boundary layer profile magnitude. This profile then remained constant for each simulation.

The dispersion modelling was undertaken using two methods. The first was a simple scalar field dispersion (i.e., scalar advection-diffusion) model, which is supplied within the CFD package (Patankar 1980, Launder 1996). This allows the simulation of the dispersion of a non-reactive neutrally buoyant gas and would be the standard approach used in conjunction with CFD. The non-reactive neutrally buoyant assumption is considered reasonable in this case because of the very dilute concentrations and short transit times of the gas within the domain associated with this study, although in reality the ground would not act as a simple boundary for ammonia. The second approach used a Lagrangian stochastic model (LSM) which is applied using the results of the CFD model as input. In principle, turbulent dispersion in the near-wake region is best predicted using a

Lagrangian stochastic model (LSM) because other techniques (e.g., Gaussian plume model or scalar advection-diffusion model) are either inappropriate or theoretically invalid in this region (Thomson 1987). However, further from the building relatively simple models (e.g., Gaussian plume models and advection-diffusion models) are appropriate. Indeed, in this region it can be shown that the LSM reduces to a diffusion equation. The basis of the LSM approach is to calculate the ensemble mean gas concentrations at any given location from the trajectories of thousands of simulated gas ‘particles’; each particle trajectory being modelled as a function of the mean flow streamlines plus a “random walk” turbulent element. Details of the numerical implementation of the model and its use with CFD can be found in Reynolds (1998a).

Currently, the ‘well-mixed condition’ (i.e., the requirement that the model give the correct steady state distribution of particles in phase space) constitutes the most rigorous theoretical framework for the formulation of Lagrangian stochastic models. In this study the simplest such model, due to Thomson (1987), which exactly satisfies the well-mixed condition for Gaussian turbulence, is adopted. It is appropriate to assume a Gaussian distribution for velocity for two reasons. First, only the first and second moments of the velocity distribution can be predicted by Reynolds Averaged Navier-Stokes Equation type CFD models. A Gaussian distribution is completely defined by its first two moments and moreover corresponds to maximising the uncertainty about the (non-predicted) higher order moments of the velocity distribution. Secondly, in highly inhomogeneous flows, the effects of the 3rd and higher order moments of the velocity distribution on particle dispersion are expected to be of secondary importance, compared with the effects of strong mean-streamline straining and large gradients in Reynolds stress (Reynolds 1997a). Thomson’s model, which describes the trajectory  $(\mathbf{x}, \mathbf{u})$  of a gas particle takes the form :

$$\begin{aligned} du_i &= a_i(\mathbf{x}, \mathbf{u}, t)dt + \sqrt{\frac{C_0 \varepsilon}{2}} dW_i \\ dx_i &= u_i dt \end{aligned} \quad (1)$$

where :

$$\begin{aligned} a_i &= \frac{-C_0 \varepsilon}{2} (\sigma^{-1})_{ik} (u_k - U_k) + \frac{1}{2} \frac{\partial \sigma_{il}}{\partial x_l} + \frac{\partial U_i}{\partial t} + U_l \frac{\partial U_i}{\partial x_l} \\ &+ \left( \frac{1}{2} (\sigma^{-1})_{lj} \left( \frac{\partial \sigma_{il}}{\partial t} + U_m \frac{\partial \sigma_{il}}{\partial x_m} \right) + \frac{\partial U_i}{\partial x_j} \right) (u_j - U_j) \\ &+ \frac{1}{2} (\sigma^{-1})_{lj} \frac{\partial \sigma_{il}}{\partial x_k} (u_j - U_j) (u_k - U_k) \end{aligned} \quad (2)$$

In Eq. (2) subscripts indicate the Cartesian components with implied summation. Here  $\varepsilon$  denotes the mean rate of dissipation of turbulent kinetic energy divided by fluid density,  $\sigma_{ij}$  are elements of the velocity covariance matrix (with inverse  $\sigma^{-1}$ ),  $U_i$  are components of the mean velocity and  $C_0$  is Kolmogorov’s constant. Note that this constant appears only in conjunction with the turbulent energy dissipation measure  $\varepsilon$ . The quantities  $dW_i$  are increments of a vector Wiener process with independent components :  $\langle dW_i \rangle = 0$ ,  $\langle dW_i^2 \rangle = dt$  where angular brackets denote an ensemble average.

There is considerable uncertainty about the value of the LSM model constant (Kolmogorov’s constant  $C_0$ ) (see Reynolds 1998b). This study has taken the value  $C_0 = 2$  which is at the lower end

of the range seen in previous studies (values in the range 2 to 7 have previously been accepted). Although this constant is supposedly universal, since it appears only in conjunction with  $\varepsilon$  in Eq. (2) it can be adjusted to compensate for shortcomings in the prediction of  $\varepsilon$ . It is the tendency of such turbulence models as used in this study to over-predict  $\varepsilon$  and therefore a lower value of  $C_0$  is warranted. However, the effect of explicit variations in  $C_0$  has not been addressed further in this study.

Previous studies of dispersion around buildings using this type of methodology have concentrated on the comparison of results from different LSM model implementations (Näslund *et al.* 1994), or comparison with other dispersion models and health risk analysis (i.e., the exceeding of exposure levels) (Lee and Näslund 1998) or have used experimental data rather than CFD as the basis for the flow field input to the LSM (Leuzzi and Monti 1998). These projects have illustrated the appropriateness of the LSM approach over other types of model but have also highlighted that small variations in the input flow field can significantly affect the predicted plume path (Lee and Näslund 1998). None of these studies, however, used full-scale data for validation of the results and therefore the question of wind variability during the experiments has not been addressed.

During the course of the experiments, the wind fluctuated in both strength and direction. Fluctuations in mean wind direction, unlike fluctuations in mean wind speed (which are assumed to move particles through the domain more or less rapidly but with the same trajectories), will be important in determining mean particle dispersion. Here, for simplicity, fluctuations in mean wind direction during the trajectories of individual particles are neglected. Therefore, in the numerical simulations only those fluctuations in mean wind direction that occur on time-scales greater than the particle transit times were taken into account. That is, the mean wind direction was effectively kept constant during the simulation of individual particle trajectories but varied between differing simulated particles.

This inclusion of wind direction fluctuations was achieved by predicting the mean concentration of ammonia for each of the nine wind directions  $[-20^\circ, -15^\circ \dots 15^\circ, 20^\circ]$  separately using a steady state simulation, and summing the results, with each concentration distribution weighted, by a factor  $p_\theta$ , according to the measured wind distribution. That is, the total mean concentration of ammonia is taken to be  $c(\mathbf{x}) = \sum p_\theta c_\theta(\mathbf{x})$  where  $\sum p_\theta = 1$ . When the wind direction (as measured by a one-minute mean) was predominantly between the angles of  $\theta = -20^\circ$  and  $\theta = +20^\circ$ , values for  $p_\theta$  could be estimated easily.

Two methods have been used to estimate the weights  $p_\theta$  from the measured distribution of wind direction. In the first, the nine wind directions considered in the simulations were used to reconstruct as accurately as possible the measured distribution (histogram) of mean wind direction. In the second, the weights  $p_\theta$  were chosen so that the first and second moments of the modelled distribution of mean wind direction corresponded to the first and second moments of the measured mean wind distribution. The extra degrees of freedom were removed by requiring that the uncertainty in the higher order moments is maximised (maximum entropy (ME)) i.e., the measured probability density function (pdf) is modelled as a normal distribution. This is considered appropriate because it yields the least biased choice for the pdf.

However, in some cases the measured wind direction was found to lie outside the range  $-20^\circ$  to  $+20^\circ$  for a significant period. In these cases, the distribution  $c_\theta(\mathbf{x})$  for angles  $\theta$  outside the range  $-20^\circ$  to  $+20^\circ$  was estimated from the symmetry of the distribution. Given that  $c_\theta(\mathbf{x})$  is approximately symmetric in  $\theta$  about the plane  $\theta = \theta_0$ , where  $\theta_0$  is the angle of the vector between the ammonia source and the point  $\mathbf{x}$  (Fig. 1). In this way, some angles outside the range  $-20^\circ$  to  $+20^\circ$  can be

mapped to an angle inside this range. Where this is not possible, the concentration  $c_\theta(\mathbf{x})$  was set to zero. Since such cases occur when  $\theta - \theta_0$  is large (i.e., the expected concentration will be small) this approximation is justified. When such a symmetry relation has been used, it is indicated in the results.

The histogram of measured wind direction was constructed from the experimentally measured reference wind data sub-divided into discrete 1-minute periods and averaged. The validity of using the weighted steady state approach then depends on the variation time of these one-minute mean values being greater than the time of flight of simulated particles in the LSM (around 20 seconds in this case). Calculating the auto-correlation integral time scale for each data set can be used to assess this variability and for all the data considered here this criterion was satisfied, with auto-correlation time scales of up to 5 minutes.

The validity of using one-minute mean values to calculate the weighting function  $p_\theta$  was also investigated by calculating the weighting values for various averaging periods between 1 second and 5 minutes. This showed that the difference between the weighting values for alternative averaging periods was similar to that between the simple histogram and maximum entropy methods of calculating the weighting values for a given averaging period, so long as the averaging period was less than 1.5 minutes. For averaging periods greater than 1.5 minutes the weighting distribution became biased because of the small number of sub-intervals per run. One-minute mean values were therefore considered representative in this case.

### 3. Results

Mean concentrations of ammonia were measured at 5 points on each of 3 masts located in the wake of the building. Three different sets of mast locations have been considered. For each set of locations, measurements were made over a specific time period (run). In this way, each run had a different wind distribution, and so a different set of weights  $p_\theta$  were required for each.

The positions of the masts and the source are shown in Table 1. Fig. 1 illustrates the mast locations relative to the building. The mean and standard deviations of the wind distributions for each run are recorded in Table 2. The runs that have significant weights for wind directions outside the range of  $-20^\circ$  to  $+20^\circ$  and require the use of symmetry to determine  $c(\mathbf{x})$ , as described above, are indicated with an asterisk in Table 2. For each run the simulated and the experimental mean ammonia

Table 1 The positions of the masts and source for the measurements (see Fig. 1)

Set of Positions	July 26 <sup>th</sup>			August 1 <sup>st</sup>			August 21 <sup>st</sup>		
Mast	x/m	z/m	$\theta_0$	x/m	z/m	$\theta_0$	x/m	z/m	$\theta_0$
1	7.13	4.34	$-4.6^\circ$	10.33	4.34	$12.1^\circ$	10.64	23.53	$5.0^\circ$
2	10.33	4.33	$12.2^\circ$	10.20	20.83	$4.6^\circ$	9.38	44.26	$1.6^\circ$
3	13.18	4.41	$25.5^\circ$	9.69	37.62	$2.2^\circ$	17.24	68.01	$7.1^\circ$
Source	8.00	-6.47		8.00	-6.47		8.00	-6.47	

Table 2 Summary of the experimental wind distribution for each run considered

Experimental Date	July 26 <sup>th*</sup>	August 1 <sup>st</sup>	August 21 <sup>st*</sup>
Mean Wind Direction	$3.8^\circ$	$-3.7^\circ$	$8.5^\circ$
Standard Deviation of 1 minute means	$26.8^\circ$	$11.2^\circ$	$20.3^\circ$

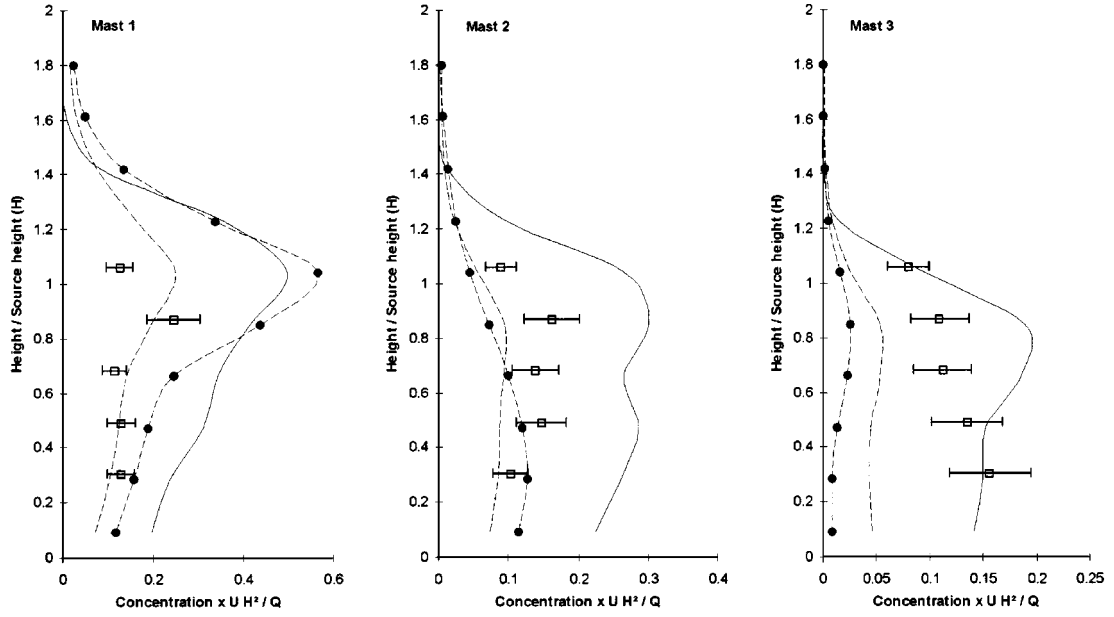


Fig. 2 Measured ( $\square$ ) and predicted mean ammonia concentrations for 26th July. Broken lines indicate the diffusion model and solid lines the LSM.  $\bullet$  = Unweighted scalar diffusion model

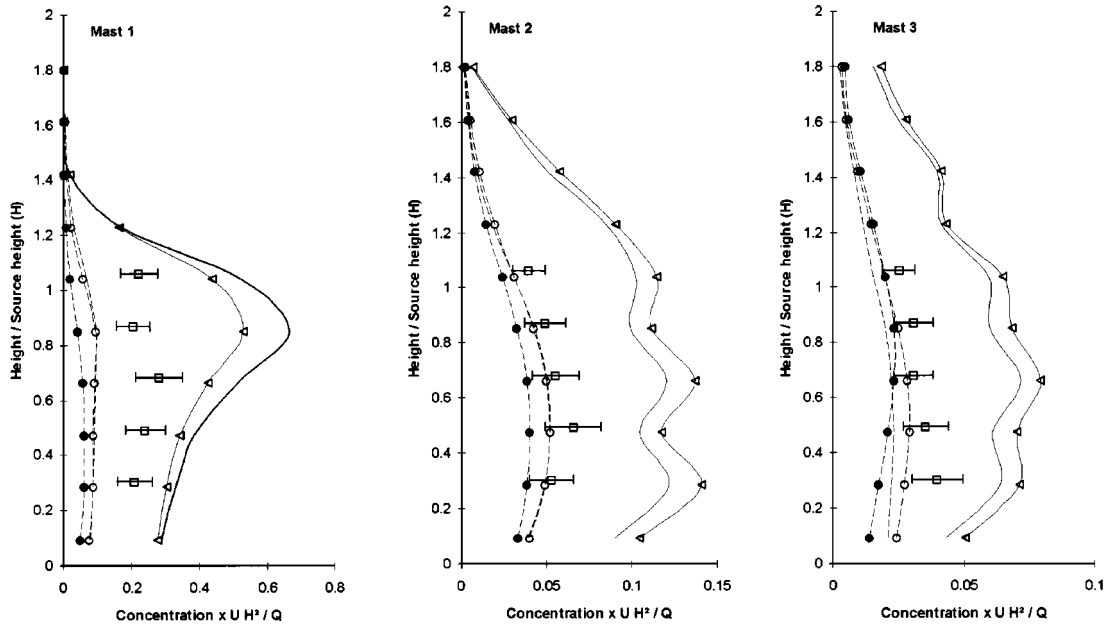


Fig. 3 Measured ( $\square$ ) and predicted mean ammonia concentrations for 1st August. Broken lines indicate the diffusion model and solid lines the LSM. Unfilled markers ( $\triangle$ ,  $\circ$ ) indicate the ME weighted predictions for both models.  $\bullet$  = Unweighted scalar diffusion model

concentrations are plotted for each mast to allow a comparison between simulation and measurement to be made. The ammonia flow rates in the measurements on each day were  $2.50 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$  for

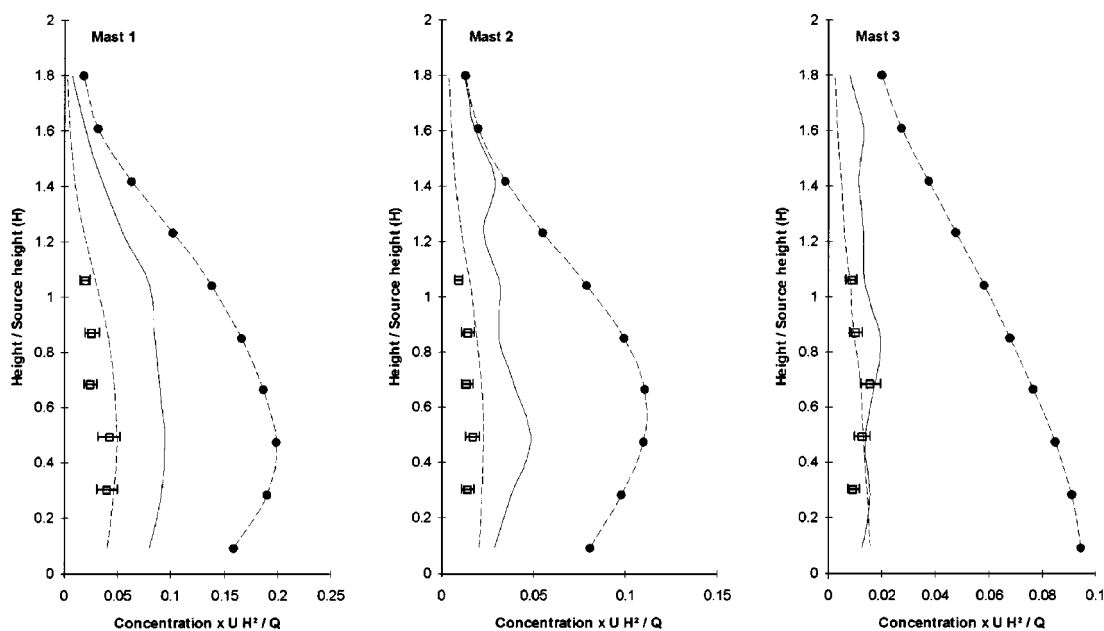


Fig. 4 Measured ( $\square$ ) and predicted mean ammonia concentrations for 21st August. Broken lines indicate the diffusion model and solid lines the LSM.  $\bullet$  = Unweighted scalar diffusion model

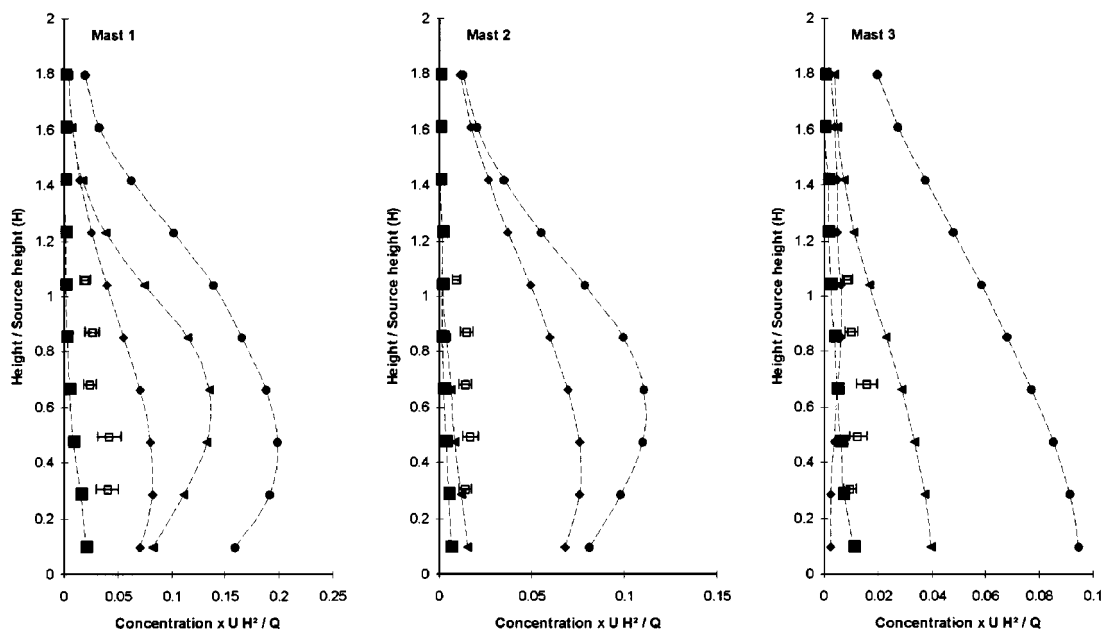


Fig. 5 Measured ( $\square$ ) and predicted mean ammonia concentrations for 21st August using a number of possible unweighted wind directions.  $\blacklozenge = 0^\circ$ ,  $\bullet = 5^\circ$ ,  $\blacktriangle = 10^\circ$  and  $\blacksquare = 15^\circ$

26th July,  $2.33 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$  for 1st August and  $1.67 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$  for 21st August.

The concentrations measured for each mast, compared with various model predictions, are

presented in Fig. 2 to 6. In these figures the vertical height of each measurement has been normalised by the source height ( $H = 5.28$  m) and the concentration values ( $C$ ) by  $UH^2/Q$  where  $U = 4.42$   $\text{ms}^{-1}$ , the mean wind speed at height  $H$  and  $Q$  is the source strength ( $\mu\text{gs}^{-1}$ ). Fig. 2 to 4 show the results for the simple histogram weighted LSM and scalar model as well as the unweighted scalar model results for each of the three experimental runs. All these results use the MMK model CFD flow fields as a basis. Fig. 3 also shows the ME weighted solutions for both the LSM and the scalar model. The unweighted results are those corresponding to the overall mean wind direction for the experimental period. This unweighted mean result is extremely sensitive to the wind direction and the position of the mast, giving concentration profiles which vary by an order of magnitude within a few degrees (Fig. 5) whichever type of dispersion model is used. This indicates the importance of accounting explicitly for the wind direction variations when calculating dispersion even using current scalar models.

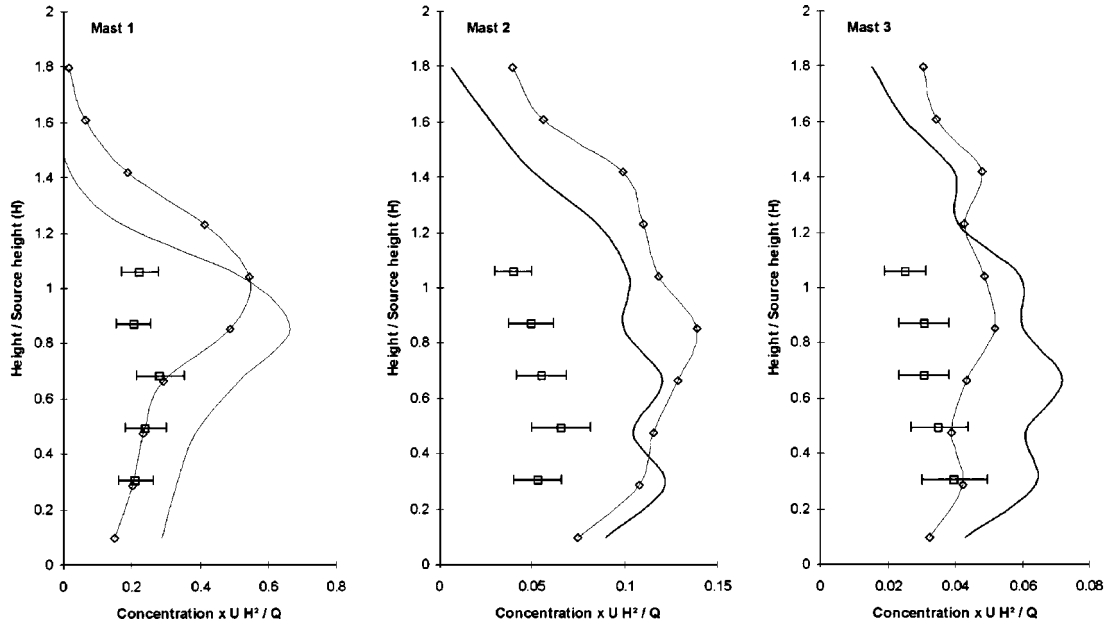


Fig. 6 Measured ( $\square$ ) and predicted mean ammonia concentrations for 1st August using the LSM with  $k-\epsilon$  ( $\diamond$ ) and MMK (unmarked) model flow fields

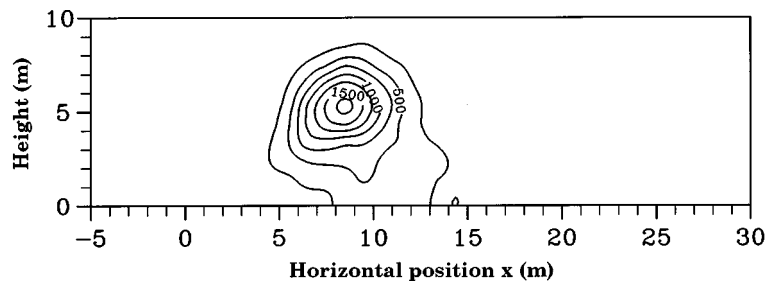


Fig. 7 A cross-section of the plume concentration (ppm) at  $z = 5.13$  m, for the case of  $\theta = 5^\circ$ , using the standard  $k-\epsilon$  model

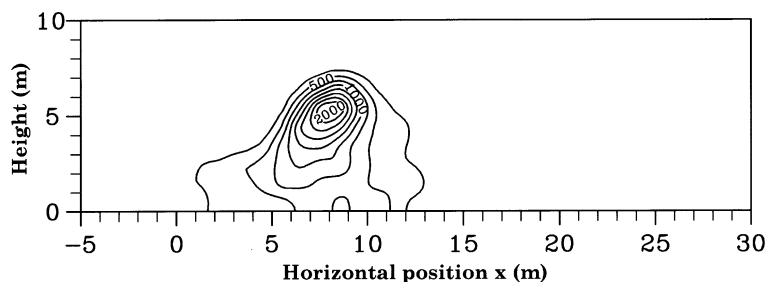


Fig. 8 A cross-section of the plume concentration (ppm) at  $z = 5.13$  m, for the case of  $\theta = 5^\circ$ , using the MMK  $k-\epsilon$  model

For the three cases considered in Fig. 2 to 4 it is apparent that the LSM tends to give higher mean concentrations than the scalar field model but that both models are more consistent with the measurements than are the unweighted predictions. The use of the ME weighting method (Fig. 3) compared to the simple histogram method does not seem to produce significant differences in profile shape, only small differences in magnitude.

The effect of using the MMK model flow fields is more significant. Fig. 6 shows the LSM results for the standard  $k-\epsilon$  and MMK model flow fields for one of the cases considered. It is apparent that the structure of the plume is significantly different in these two models. Fig. 7 and 8 show this difference more clearly as a cross section through the plume at a point downstream of the source for a single wind direction. The standard  $k-\epsilon$  model resulted in a plume that was basically circular in cross section whereas the MMK model gave a wider plume, especially in the region nearest the ground, which was less regular in shape. Two other points of note were that the plume peak concentration was higher with the MMK model and that in neither model did the plume extend above about 8 m.

#### 4. Discussion

The 1st August and 21st August experimental data sets (Fig. 3 and 4) show the reduction in ammonia concentration as a function of distance downwind of the source. This trend is also seen in the simulated results. The measurements indicate, however, that the ammonia concentration does not vary greatly with height. The simulated results show a similar effect at large distances from the building. Close to the building ( $z < 10$  m, i.e., all masts for 26th July and mast 1 for 1st August), the simulations predict a peak in ammonia concentration at a height of 4 to 5 metres. This is in contrast to the measured data, which shows only a small peak at 4 m on mast 1 on 26th July. Since there are no measurements beyond 5 m in height it is unclear if such a peak exists in reality above 5 m, though the available measurements show no evidence for it.

Although the simulated and measured mean ammonia concentrations are of the same order, there are some notable discrepancies. Fig. 4, for the 21st August results, shows that the magnitude of the mean concentration is over predicted by the LSM by as much as a factor of four for the case of mast 1. However, at larger distances, the extent of the over prediction diminishes, and the measured results for mast 3 are generally predicted correctly. The weighted scalar model appears to predict the correct concentrations for all three masts in this case but there are no high levels of ammonia in these measured data. The unweighted scalar model is obviously the least effective method in this case.

The 1st August case shows similar results when comparing the predictions and measurements, although there are generally higher levels of ammonia measured and predicted. Where the concentrations are lower, masts 2 and 3, the weighted scalar model appears to predict the levels better than the LSM. However, as one approaches the building the LSM results are more in line with the measurements. The comparison of the 26th July results is less obvious, since all the masts lie close to the building, but the general levels and trends again appear to be best predicted by the LSM. This is because the assumptions underlying the formulation of the scalar field model are invalidated in regions close to a source (i.e., when particle transit times  $t < T_L$  the integral Lagrangian time scale).

These results seem to imply that the weighted scalar field model is no less accurate than the LSM, at least in regions of low concentration. However, considering that the scalar model systematically under-predicts the values in regions close to the building and that the individual scalar field solutions wildly under- and over-predict the concentrations for single wind directions (Fig. 5), then it must be concluded that there may be a more fundamental problem with this type of model. From the variability of the concentration field with single wind direction (Fig. 5), it would appear that the lateral spread of the plume is under predicted by the scalar model. This would give a narrow plume of high concentration which under-predicts the concentration when  $\theta_{\text{wind}} \neq \theta_{\text{mast}}$  and over predicts when  $\theta_{\text{wind}} = \theta_{\text{mast}}$  (see Table 1 for mast positions and angles). This is particularly true when using the standard  $k - \epsilon$  model flow field because of the reduced vertical spread of the plume (Fig. 7) when compared to the MMK model flow field plume (Fig. 8). This would be consistent with the idea that the isotropic eddy-viscosity approach to turbulence modelling is inappropriate in dispersion studies such as this, the lateral dispersion characteristics of the near ground plume being much greater than the vertical.

Fig. 3 for the 1st August run shows that there are only small differences between the simulated distributions calculated using the Simple Histogram and Maximum Entropy weighting methods, particularly at low heights. Therefore either method would seem acceptable. However, given the added assumption in the ME method of a Gaussian distribution of weights it would be more generally applicable to use the Simple Histogram method. This small variation in results also indicates that the predictions are insensitive to small changes in the weights  $p_\theta$ , so long as the overall mean and variance of the wind direction weights are kept constant. Since the effect of variations in the wind direction averaging period below 1.5 minutes was similar, in terms of the weighting function values, to the choice of weighting methodology this indicates that averaging period is also not a critical parameter in this case.

It is evident that with the MMK model there is a larger predicted mean concentration of ammonia close to the ground than there is with the standard  $k - \epsilon$  model. This is in line with the measurements, which show little indication of the concentration varying with height. Another feature of the results obtained with the MMK model is the rapid decline in concentration above 6 m height (Fig. 8). This indicates that, although dispersion downwards has increased, the dispersion upwards has decreased. With the MMK model, the plume cross-section loses some of its symmetry, and the position of the maximum concentration moves slightly (Fig. 7 and 8). It is evident that the dispersion close to the ground is larger for the MMK model, whereas close to the maximum it is not. In one case (Fig. 6, mast 3) the standard  $k - \epsilon$  model appears to give better agreement with the measured concentrations. However, the trends of concentration with height appear to be better predicted by the MMK based model even though the absolute concentration values are less good. This may be in line with the results of previous comparisons where the MMK model was found to better predict the trends of

distribution of turbulence than the standard  $k - \varepsilon$  model whilst under-predicting the absolute values (Quinn *et al.* 1998). This would lead to a more realistic plume shape but with higher peak concentrations than the standard  $k - \varepsilon$  model, as seen in Fig. 7 and 8.

The fluctuations in the wind direction over the course of the measurements require the use of many simulations, each performed for a different wind direction  $\theta$ . It is questionable whether the nine angles used are enough to describe the wind distribution properly. In addition, it has been assumed that each marked particle experiences a flow-field that does not change with time. In reality, time variation will occur for two reasons. First, for a constant wind direction, one would expect transient behaviour behind the obstacle. For example, vortex shedding by the building will give an increased lateral momentum transfer and hence enhanced dispersion. This is a potential reason for the over-prediction by the LSM technique in this case, which relies on the flow field for the advective component of dispersion. Secondly, fluctuations in oncoming wind direction occur. If these changes occur with a time-scale that is of the same order or less than the time of flight of a particle from the source to the mast, these factors are likely to be significant.

## 5. Conclusions

The dispersion of a point source of ammonia gas in the wake of a low-rise building has been predicted using a simple scalar (diffusion) model and Thomson's LSM. These models were used in conjunction with flow field data from a CFD model using the standard and a modified (MMK)  $k - \varepsilon$  turbulence model. In the building wake, at distances  $z > 3$  building heights, both models were successful in predicting correctly the mean ammonia concentration. However, even close to the building ( $z < 3$  building heights) the LSM was not found to be significantly better than the simple scalar diffusion model. This is presumably because of inadequacies in the predicted flow field, such as the lack of explicit resolution of time dependent features in the wake.

Significant improvements in predictions for mean concentration of ammonia were obtained when a partial account was taken of fluctuations in mean wind direction. The simulation agrees best with the experimental results when the masts do not lie in or near the centre of the plume. When the mean wind direction is such that the plume spends a considerable fraction of the time centred on a particular mast, the measured concentration of ammonia on the mast is over predicted substantially. This may in part be because the wind was described by only nine discrete directions and also because the model does not account for any structured mixing, e.g., by vortex shedding.

The standard and the MMK  $k - \varepsilon$  models also produced significantly different results. In particular, the extent of dispersion close to the ground is greater with the MMK model, and as a consequence the ammonia concentration varied less with increasing height and was thus more in line with the trends of the experimental results. However overall, the concentration levels were no better when using the MMK model than when using the standard  $k - \varepsilon$  model.

It is suggested that explicit modelling of wind direction fluctuations is essential to dispersion models of this type. Turbulence modelling has a significant effect on the predicted concentration field in the wake of buildings and until improvements in this modelling are made, the type of dispersion model used is of less significance.

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