TURBULENT FLUCTUATIONS AND THEIR USE IN ESTIMATING COMPLIANCE WITH STANDARDS AND IN MODEL EVALUATION

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ABSTRACT
Turbulent fluctuations are important in dispersion problems where short time scale peak values can be critical. These situations include:

(i) releases of toxic, flammable or odourous substances where high short time scale impacts may be dangerous or cause a nuisance
(ii) estimating concentrations for regulatory purposes for comparison with limits based on a short time scale, such as the UK 15-minute or WHO 10-minute levels for SO_2
(iii) assessing the uncertainties in dispersion model predictions and aiding model comparison with measured data

The ADMS 3 dispersion model includes a module to calculate turbulent fluctuations which is based on a “two particle dispersion” concept but has much in common with Gifford’s meandering plume model. It has been used in critical applications where odour and exceedences of a regulatory value were the issues. In this paper the fluctuations model is described and each of the three applications is illustrated.

KEYWORDS
Turbulence, fluctuations, exceedences, correlations, clipped-normal distribution, ADMS.

INTRODUCTION

Most practical dispersion models used for regulatory purposes assume that the meteorological conditions are constant over the averaging period and calculate ensemble average concentrations. In practice, although the meteorological conditions may be constant, during the averaging period there will be short time scale variations due to boundary layer turbulence. The turbulent fluctuations will lead to variations in short term concentration.

Acknowledging the underestimate of short term peak concentrations if these fluctuations are ignored, modellers have adopted a variety of approaches. Factors are sometimes applied to convert between different averaging times. This is a rather crude approach as the factors may be based on monitored data that reflect contributions from many different sources and yet the factors may be applied to a single stack. The factors should be functions of the height of the source, the statistic in question, receptor height, distance of the receptor from the source and meteorology. In practice just one factor is often used to cover all cases. Other modellers account for a decreased averaging time by adjusting the amount of meandering of the wind direction. In the ADMS 3 dispersion model the fluctuations in concentration are calculated and the results presented in statistical terms: the standard deviation of concentration σ_c, short term percentile concentrations and the probability of exceeding threshold concentrations. For long term calculations, probability distributions calculated for individual meteorological conditions are combined to predict the expected number of exceedences of a threshold concentration during one year.

In many dispersion problems short term peak concentrations are of interest and it is critical to be able to estimate these short time scale variations, or fluctuations, in concentration. For instance, for inflammable, toxic or odorous substances, an hourly averaged concentration may be safe, but if a concentration, say 10 times higher, is exceeded over a short period during that hour, it may cause a nuisance, or be very dangerous, for instance causing ignition.

Fluctuations are also important when modelling for comparison with regulatory values based on short time scales, for example the UK 15-minute and WHO 10-minute concentration levels for SO_2. It should also be noted that fluctuations are not always negligible over a time scale of one hour, although this is commonly assumed.

Use of concentration fluctuations is also useful in model evaluation, for estimating the accuracy of modelled concentrations and for comparisons with field data. Short term percentile values can show the predicted range of concentrations.

This paper describes the ADMS 3 fluctuations module and then describes its use for each of the three applications: short term danger or nuisance, comparison with short term regulations and model evaluation.

THE ADMS FLUCTUATIONS MODULE

The ADMS fluctuations module (Thomson 1990, 1997 & CERC 1998,1999) calculates fluctuations in concentration due to boundary layer turbulence and plume 'meandering'. All other meteorological variables are assumed to be constant. The module takes as input the mean concentration profile and calculates the probability that the concentration averaged over T_{av} exceeds a threshold concentration $\hat{c}$, where T_{av}, the fluctuations averaging time, may range from 0 seconds to 1 hour. The module is based on a 'two particle dispersion' concept and uses an approximation introduced by Sawford (Sawford, 1983). For particles released from a source at time zero, Sawford argued that following a pair of particles backwards in time from time t to time zero the displacement of the centre of mass of particle pairs is close to Gaussian and independent of the particle separation, D. The mean concentration field $\bar{c}$ is calculated as usual and the concentration variance σ_c^2 is estimated using the Sawford approximation. Then exceedence probabilities are calculated by assuming a 'clipped-normal' probability distribution which can be calculated from $\bar{c}$ and σ_c:

$$P(\hat{c}) = \frac{1}{2}\left(1 - erf\left(\frac{\frac{\hat{c}}{s} - g}{\sqrt{2}}\right)\right) \qquad \text{Equation 4}$$

$P(\hat{c})$ is the probability of exceeding the threshold concentration $\hat{c}$, ($\hat{c} \geq 0$) and σ and γ are parameters of the clipped-normal distribution, calculated from $\bar{c}$ and σ_c. $P(\hat{c}) = 1$ for $\hat{c} < 0$. Short term percentiles can be calculated by inverting the exceedence function $P(\hat{c})$.

Model output consists of the standard deviation of concentration σ_c, short term percentile concentrations and the probability of exceeding threshold concentrations. The ensemble mean of concentration to the power of p_{dose} may also be calculated. This quantity can be used in calculating the effect of exposure to toxic substances. For long term calculations, probability distributions calculated for individual meteorological conditions can be combined to predict the expected number of exceedences of a threshold concentration during one year.

The ADMS 3 fluctuations module has the capability to model anisotropic and multiple sources. Any source configuration is represented as a collection of point, crosswind line and crosswind-vertical area sources. Concentration covariances are calculated for each pair of sources and included in the overall concentration variance.

The model has been validated against field data (Mylne 1991, 1992, 1993, 1996) including LIDAR data (Carruthers et al, 1995) and against measurements from a pair of point sources (Davies et al, 1998).

The effect of modelling fluctuations can be to increase or decrease the predicted concentrations. Consider a set of ensemble mean concentrations calculated for a particular receptor point for a series of meteorological conditions. The thin line in Figure 1 shows the typical distribution of the non-zero ensemble mean concentrations. The bold line shows the distribution of concentrations including the effects of fluctuations. Note that there is a non-zero probability that the concentration will be zero when fluctuations are considered. For threshold concentrations greater than C_1, the fluctuations module will predict a higher number of exceedences of that threshold than would be predicted by the ensemble mean. However, for concentrations less than C_1 the effect of modelling fluctuations will be to decrease the predicted number of exceedences.

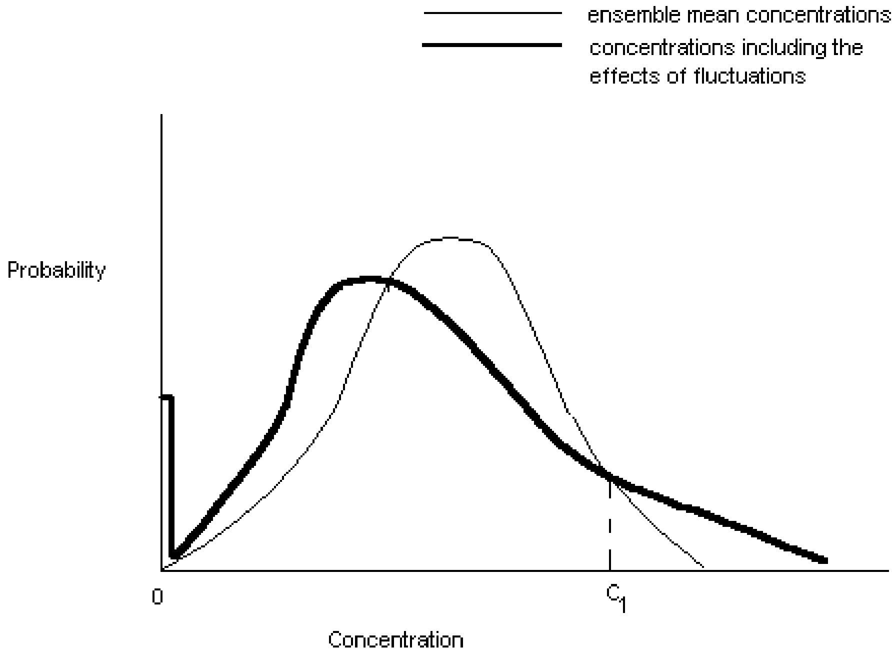


Fig. 1 Comparison of ensemble mean concentration distribution with the distribution of concentrations including the effects of fluctuations

APPLICATIONS OF THE ADMS 3 CONCENTRATION FLUCTUATIONS MODULE

The three sections following illustrate how consideration of fluctuations is important in applications where short term peak concentrations are the issue.

Odour Nuisance

One area where short term concentrations averaged over a few seconds are of importance is odour modelling. The following example shows the use of the fluctuations module to assess odour nuisance from a flare stack. The stack details are given in Table 1. Concentrations were calculated with the stack located at (0,0), under convective, neutral and stable meteorological conditions with a wind from the west.

Stack parameter	Value
Stack height (m)	13
Stack diameter (m)	0.076
Exit velocity (m/s)	0.7
Release temperature (°C)	1000
Emission rate (OU m^3/s)	10000

Table 1. Flare stack details

Let us assume for the purpose of illustration, that concentrations above 2 odour units (OU) constitute an 'odour nuisance'. Figure 2 shows the hourly ensemble average concentration for each of the three meteorological conditions. Figure 3 shows the probability that the 1 minute average concentration exceeds 2 OU for each case, calculated using the fluctuations module. In neutral and stable conditions, the hourly ensemble mean concentration does not exceed 2 OU. However, the fluctuations module output indicates that there is a significant probability, of up to 0.2 (20%), that the 1 minute mean concentration will exceed this value. In convective conditions, there is a small region where the hourly ensemble mean concentration exceeds 2 OU (the 2 OU contour is shown in bold). The fluctuations module predicts that there is a much larger region where there is at least a 1% likelihood that the 1 minute mean concentration exceeds this value. However, note that the probability of exceeding 2 OU in the region where the ensemble mean concentration exceeds this value is approximately 12%. Here the ensemble mean approach suggests that the 2 OU level is exceeded during all of the hour, but the fluctuations approach suggests that the probability of 2 OU being exceeded during any one minute is only 12%, and hence that 2 OU is only exceeded for about 7 minutes in total during the hour.

Prediction of exceedences

The ADMS fluctuations module can also be used to predict the number of exceedences of limit values over longer periods. The following example illustrates the use of concentration fluctuations to calculate the expected number of exceedences of a limit value during a one-year period. The UK National Air Quality Strategy objective for SO_2 states that the 99.9th percentile of 15 minute mean concentrations should not exceed 100ppb (~270µg/m^3). Therefore, over the period of a year, there should be no more than 35 15-minute periods where the mean concentration exceeds 270µg/m^3. ADMS 3 was used to calculate ground level concentrations from a typical power station stack emitting SO_2. (Continuous operation was assumed, which is likely to produce a conservative result, i.e. an overestimate, depending on how it compares with the actual operating pattern.) The stack details are given in Table 2. One year of meteorological data (Birmingham, 1994) was used.

Stack parameter	Value
Stack height (m)	183
Stack diameter (m)	8.4
Exit velocity (m/s)	22.1
Release temperature (°C)	130
Emission rate (g/s SO_2)	2600

Table 2. Power station stack details

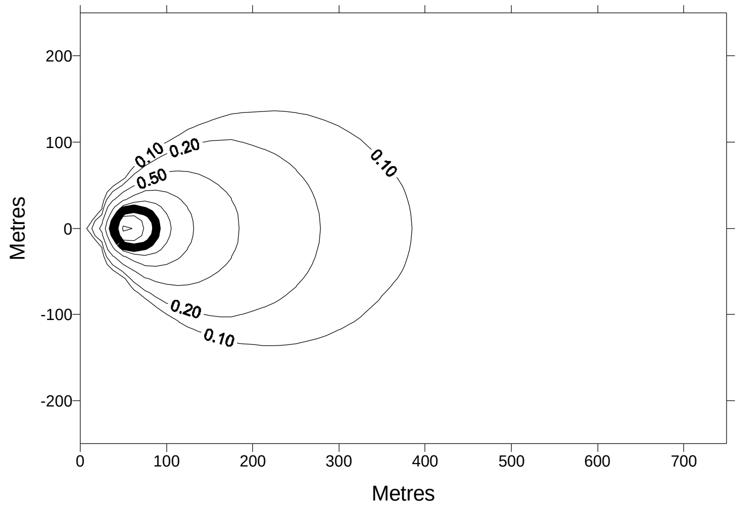
Two sets of results were calculated:

i) For each hour of met data, a 15 minute ensemble mean, without including the effects of fluctuations, was calculated.

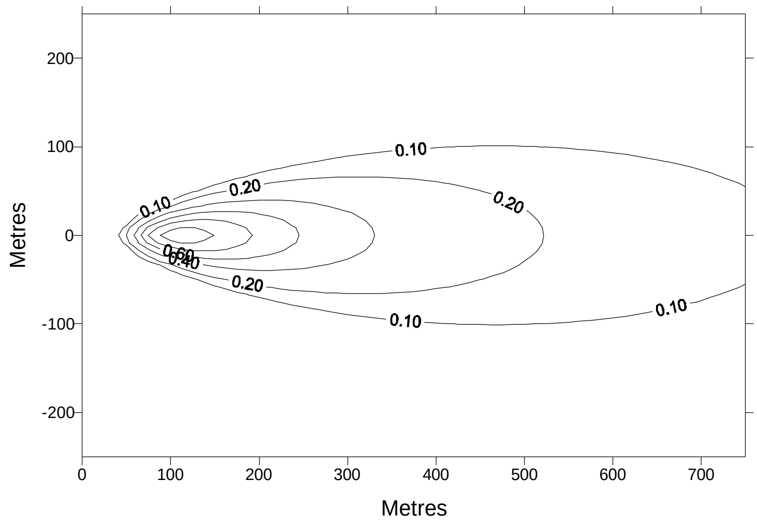
ii) For each hour of met data the fluctuations module was used to calculate the probability that the 15 minute mean concentration would exceed the limit value. The probability distributions for each hour of met data were combined to give the expected number of exceedences of the limit value over the year.

Figure 4 shows the number of exceedences of the limit value by the 15 minute ensemble mean. Contours of 1 and 5 exceedences are shown. The maximum value is 11 exceedences, well below the limit value of 35 exceedences.

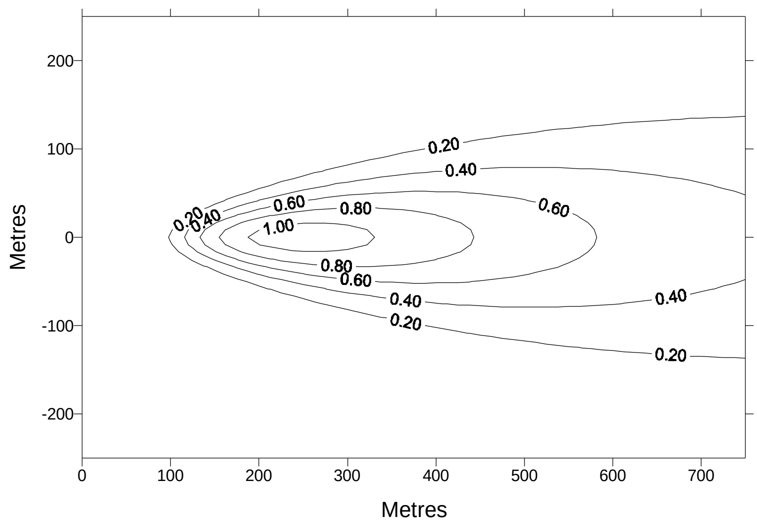
Figure 5 shows the expected number of exceedences of the limit value by the 15 minute average concentration taking into account the effects of concentration fluctuations. Contours of 5 to 85 exceedences are shown, with a contour interval of 10 exceedences. The maximum number of exceedences is 86. The 35 exceedences contour is shown in bold. In contrast with the ensemble mean exceedences, there is a significant area where the limit value is exceeded. Hence, in this case, neglecting fluctuations leads to underestimation of the short term impact of the release. Considering only the predicted ensemble mean concentrations, the stack would be expected to comply with the National Air Quality Strategy objective. However, accounting for turbulent fluctuations indicates that for some periods of time the stack would not comply with the standard over a large area.



i) Convective conditions

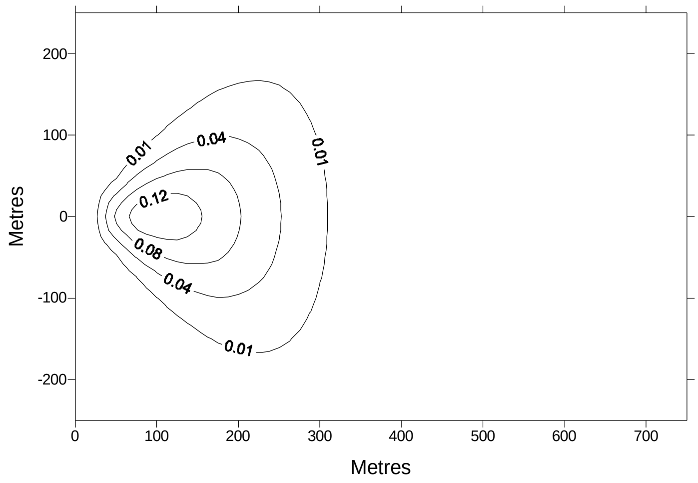


ii) Neutral conditions

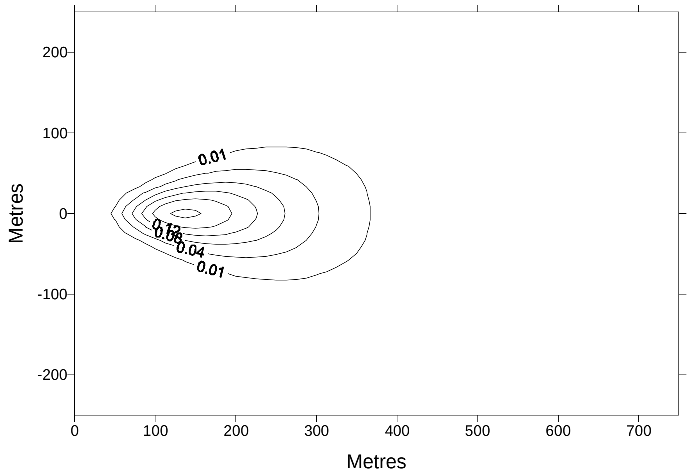


iii) Stable conditions

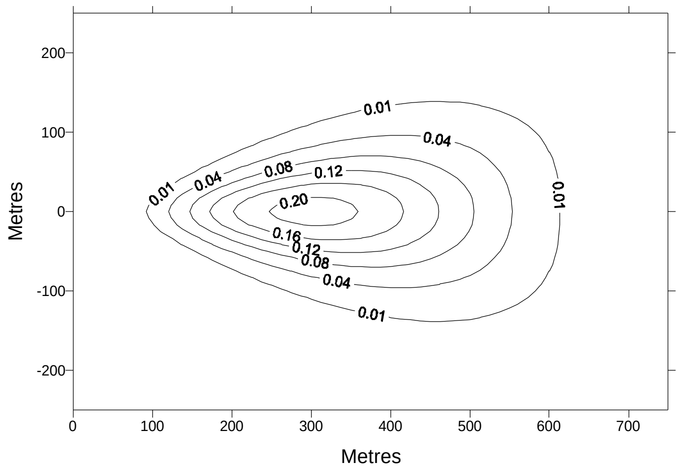
Fig. 2 Hourly average concentration from flare stack (OU) in convective, neutral and stable conditions



i) Convective conditions



ii) Neutral conditions



iii) Stable conditions

Fig. 3 Probability that the 1 minute average concentration from a flare stack exceeds 2 OU in convective, neutral and stable conditions

The ADMS fluctuations module has been used in studies for the UK Environment Agency, to predict the number of exceedences of the UK National Air Quality Strategy 15 minute objective for SO_2 due to a cement works stack (Carruthers et al, 1997), and to assess the impact of odorous emissions from a flare stack (Carruthers and Danskin, 1998).

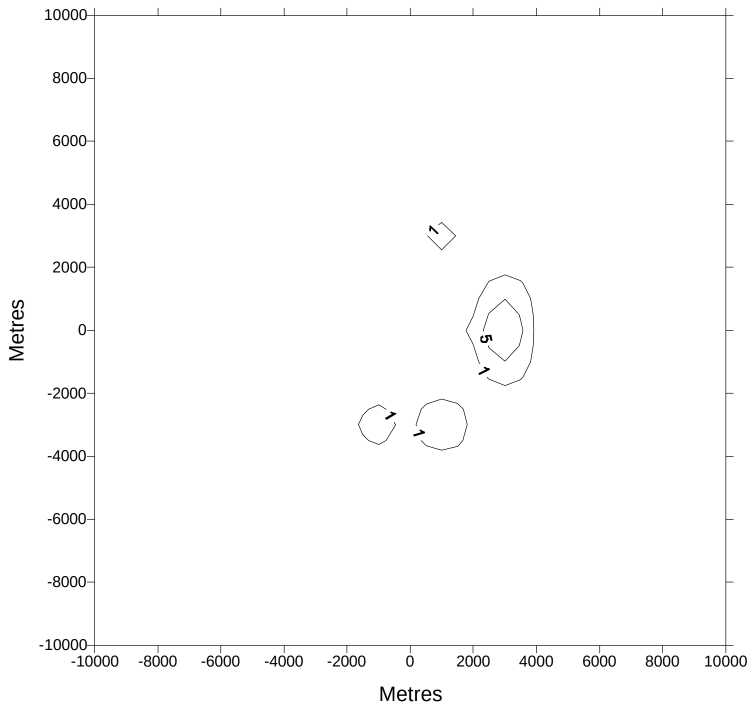


Fig. 4 Number of exceedences per year of 270µg/m^3 by the 15 minute ensemble mean.

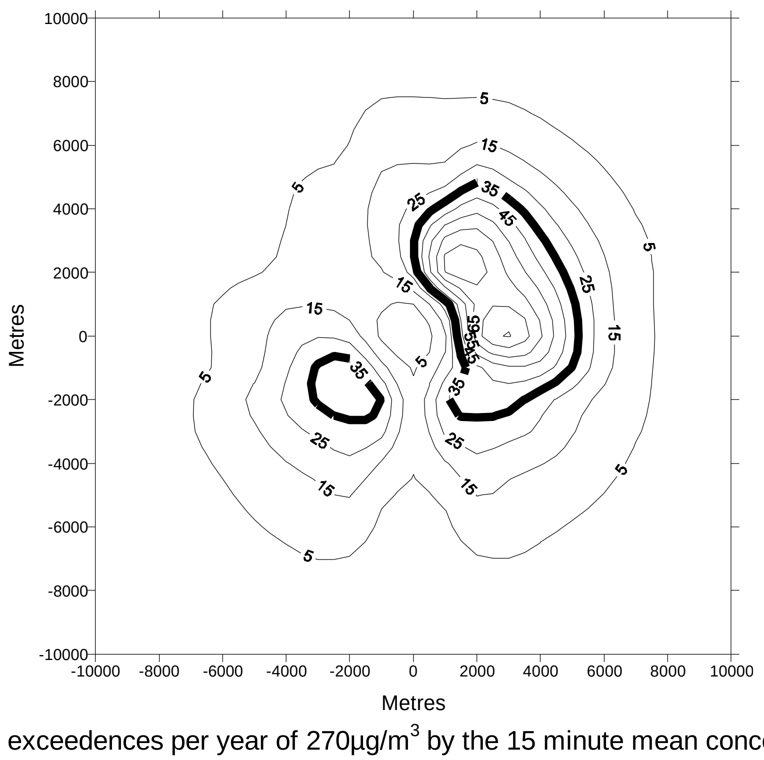


Fig. 5 Number of exceedences per year of 270µg/m^3 by the 15 minute mean concentration, including the effects of fluctuations. The bold contour corresponds to the limit value of 35 exceedences.

Use in model evaluation

Since measured concentrations are subject to fluctuations, it is useful to be able to model concentration fluctuations when comparing measured and modelled concentrations for validation purposes. In the following example, the ADMS multiple source fluctuations module has been used to calculate the expected range of concentrations for a series of meteorological conditions, for comparison with measured concentration data. A study was undertaken for the UK Environment Agency of the emissions from two kiln stacks at a cement works (Carruthers et al, 1997). As part of this study, modelled concentrations were compared with monitored data obtained by the National Physical Laboratory (NPL). The measured values were 1 minute average concentrations, and meteorological data was supplied as 10 minute average values. 10 minute ensemble mean concentrations were calculated and the fluctuations module was then used to calculate the 95th and 5th percentile 1 minute mean concentrations. The original study used ADMS version 2; here the modelled concentrations have been recalculated using ADMS 3.

Figure 6 shows a time series of monitored versus measured data. The measured and predicted 10 minute average values agree fairly well. The 95th and 5th percentile 1 minute mean concentrations give a good indication of the range of the measured 1 minute average concentrations.

The emerging ASTM method for model evaluation (Irwin 1998) uses measured concentration values as part of a collection of values, some of which are generated by the boot-strapping statistical method. The model ensemble mean prediction is then compared with a mean of the range of values, measured and generated. The fluctuations model can be use to compare the model predicted range of values and the statistics of that range with the statistics of the measured and generated collection of values to provide further insight into the model performance.

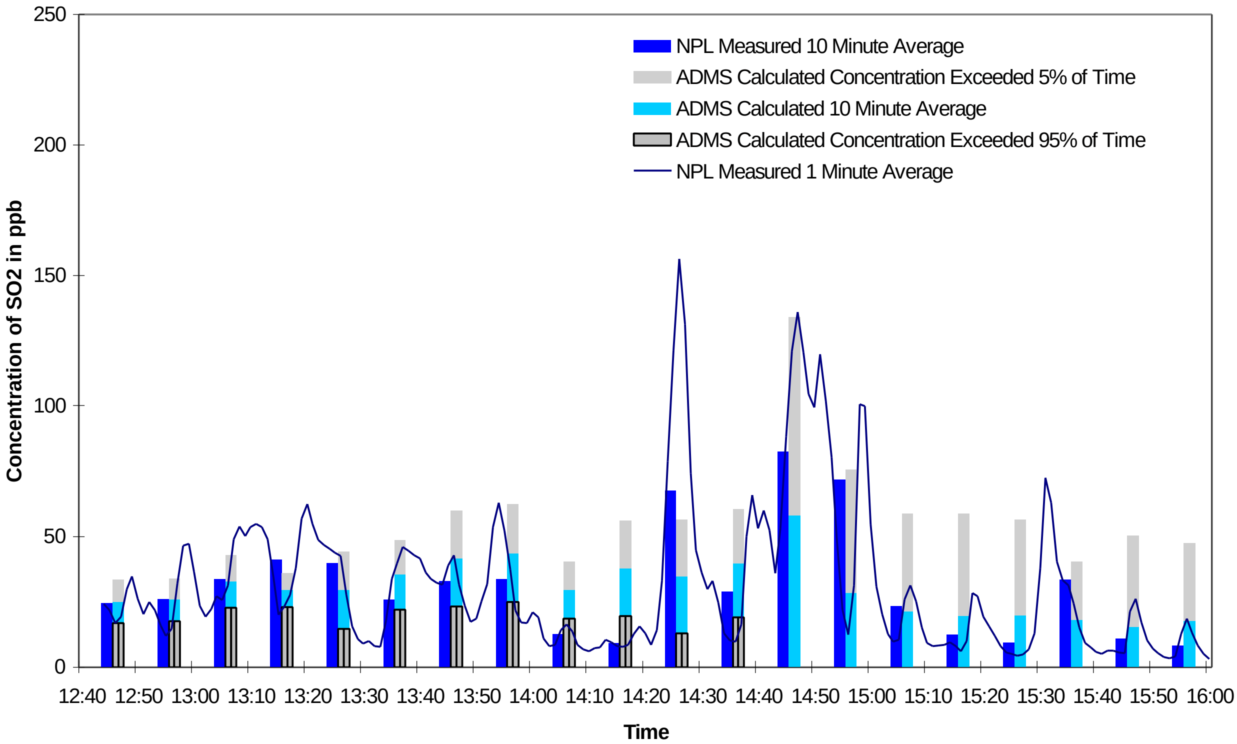


Fig. 6 Comparisons between NPL Measured Data and ADMS 3 Predictions for Cement Works. 10 minute mean averaging time - 1 minute fluctuations averaging time

CONCLUSION

There are many dispersion modelling scenarios in which short time scale peak concentrations are critical. Neglecting the effect of turbulent fluctuations in modelling can lead to the underestimation of these peak values and hence of the overall short term impact of a release. The fluctuations module of ADMS 3 calculates fluctuations in concentration due to boundary layer turbulence. Its practical application in assessing short term impacts for a variety of applications, including regulatory purposes and model evaluation has been demonstrated.

REFERENCES

Carruthers D. J., McKeown A. M., Ellis K. L. and McHugh C. A. (1997) *Air dispersion climate from the Castle Cement Works at Ribblesdale*. Environment Agency Report NW-7/97-20-BAZSQ

Carruthers D. J., Danskin A. (1998) *Dispersion Modelling Study of Odour Emissions from the Flare Stack at Petrus Oils Ltd*. CERC report.

Carruthers D. J., Edmunds H. A., Bennett M., Woods P. T., Milton M. J. T., Robinson R., Underwood B. Y. and Franklyn C. J. (1995) *Validation of the UK-ADMS Dispersion Model andAssessment of its Performance Relative to R-91 and ISC using Archived LIDAR Data*. Study commissioned by Her Majesty's Inspectorate of Pollution (published by Dept. of Environment). DoE/HMIP/RR/95/022

CERC (1998) *ADMS 2 Technical Specification.*

CERC (1999*) ADMS 3 Technical Specification*.

Davies B. M., Jones C. D., Manning A.J. and Thomson D. J. (1998) *Some field experiments on the interaction of plumes from two sources.* In preparation*.*

Irwin J. (1991) *Statistical evaluation of atmospheric dispersion models* Proc. Of 5th Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes. Pp46-53.

Mylne K. R. and Mason P. J. (1991) *Concentration fluctuation measurements in a dispersing plume at a range of up to 1000m* Quart. J. Royal Meteorological Soc. **117**, pp177-206.

Mylne K. R. (1992) Concentration fluctuation measurements in a plume dispersing from a stable surface layer Boundary Layer Meteorology, **60**, pp15-48.

Mylne K. R. (1993) *The vertical profile of concentration fluctuations in near-surface plumes*, Boundary Layer Meteorology, **65**, pp111-136.

Mylne K. R. and Davidson M. J. (1996) *Concentration fluctuation measurements in tracer plumes using high and low frequency response detectors*. Boundary Layer Meteorology, **79**, pp225-242.

Sawford B. L. (1983) *The effect of Gaussian particle-pair distribution functions on the statistical theory of concentration fluctuations in homogeneous turbulence*., Quart. J. Royal Meteorological Soc. **109**, pp339-354

Thomson D. J. (1990) *A stochastic model for the motion of particle pairs in isotropic high-Reynolds number turbulence and its application to the problem of concentration variance* J. Fluid Mechanics **210**, pp113-153

Thomson D. J. (1997) *The 'inertial-meander' sub-range of a dispersing plume* J. Applied Meteorology **36**, pp1046-1049