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Comparison of monitored air quality data with the predictions of ADMS-3

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Abstract

Version 3 of CERC's Air Dispersion Modelling System has been used to construct a model of air quality in the lower Trent Valley, UK, in order to test the predictions against field measurements. The area is predominantly agricultural, however there are also three large coal fired power stations. There are no other significant sources of SO_2 close enough to affect the area significantly. Four continuous air quality monitoring stations are operated around the lower Trent Valley, and a further six SO_2 bubbler sites measure daily averages.

The predictions of a model of the air quality in the lower Trent Valley for 1998 are compared with the measured values of SO_2 at all the specific monitoring sites, and some analysis has been made of the sensitivity of the model to individual input meteorological parameters. A brief comparison was also made with the USEPA model AERMOD.

The results of ADMS-3 for long term statistics, in particular the 99.9^{th} percentile, are good when the complexity of the model is considered. The predictions are also stable to small perturbations in the input data set, suggesting a generally robust model formulation. By contrast, when individual hours are considered the prediction accuracy is significantly poorer, and a large variation can be induced from small perturbations to the input meteorology.

The predictions of ADMS-3 and AERMOD agree quite well for concentrations up to about the 99^{th} percentile. Above this the behaviour of the two models diverges rapidly, with large over-predictions from AERMOD, and moderate under-predictions from ADMS-3 above about the 99.9^{th} percentile.

It is concluded that the predictions of ADMS-3 are broadly representative for long-term statistics, but the model is less successful when predicting individual hours.

Air Pollution VIII, C.A. Brebbia, H. Power & J.W.S Longhurst (Editors)

1 Introduction

Cambridge Environmental Research Consultants have recently released version 3 of the atmospheric dispersion model ADMS. The model is a new generation dispersion model, and has been developed in conjunction with the UK Meteorological Office. The Environment Agency for England and Wales use the model, as do many UK companies and Government Organisations. The model uses boundary layer height and Monin-Obukhov length to describe turbulence in the atmosphere, and uses a skewed Gaussian distribution to represent the plume concentration profile under convective conditions. Plume rise is modelled by solving the full conservation equations, rather than via empirical relations.

This report describes a study carried out to compare the predictions of ADMS-3 with monitored data from the lower Trent Valley. A variety of model configurations were used to predict ground level concentrations in the lower Trent Valley, and statistical tests were applied to compare the results with monitored data.

2 Method

2.1 Study area

The area used for this study is the Lower Trent Valley, which is a low-lying rural area on the Nottinghamshire Lincolnshire border in Eastern England, south of the Humber Estuary. There are three large coal fired power stations on the west bank of the river, but land-use is predominantly for agriculture. Lincoln is the largest settlement in the area, and is on a hill to the east of the river. Other urban areas in the area are Gainsborough, Newark and Retford.

Air quality monitoring has been carried out in the area since the late 1960s. Early instrumentation was of the SO_2 bubbler type, which recorded daily averages. Some of these still operate in a network of six sites. Modern continuous monitors were introduced from the early 1980s onwards. Such instrumentation has a much higher capital cost, but gives a much better measurement of short-term SO_2 concentrations. There are four automatic monitoring sites containing such instrumentation, located to the north, south, east and west of the group of power stations. These monitoring sites are run under the auspices of the Joint Environmental Programme (JEP) of National Power, PowerGen and TXU Europe Power (formerly Eastern Generation).

There are three power stations in the lower Trent Valley. High Marnham is a 1000MW power station operated by TXU-EP. Emissions from the five units are via shared ducting to two stacks, each 137m tall. This is the oldest power station in the area, but is still operating at over 30% load factor. Cottam Power Station is a 2000MW station operated by PowerGen. It has a single 198m stack, which contains a separate flue for each of the four units. This arrangement is generally found to lead to the best dispersion of the plume, especially if not all the units are operating. West Burton Power Station, operated by TXU-EP, is also a 2000MW station, but is of a slightly older design. There are two 183m tall stacks, each of

Air Pollution VIII, C.A. Brebbia, H. Power & J.W.S Longhurst (Editors)

which is associated with two units. This does not give as good plume dispersion as a single stack because the heat capacity of each emission is smaller, leading to less buoyancy. There is also reduced emission velocity when only one of the two units associated with a stack is operating.

For the purposes of this exercise, only the SO_2 emissions from the three power stations have been modelled. Other sources of SO_2 in the area have been identified from the National Atmospheric Emissions Inventory (NETCEN [1]), and the Inventory of Sources and Releases (Environment Agency [2]). The emissions were very small in comparison with power station emissions, and so non power station emissions are being treated as background. This does not imply that non power station sources could not lead to exceedences of air quality standards. However the location of such sources in relation to the monitoring sites and power stations means that most exceedences can be related to the most likely source by referring to wind direction measurements. The British Sugar factory at Newark is an exception to this, but is known to operate for only a few months per year, and has emissions of only 37t SO_2 per annum (cf 44,600t, 112,800t and 110,400t for High Marnham, West Burton and Cottam power stations respectively. (Eastern Generation [3], PowerGen [4]).)

Background values of SO_2 are used to represent the contributions from all sources other than power stations. The wind direction used in the model determines which site represents the upwind SO_2 concentration for every hour of monitored data. This value can then be subtracted from the ground level concentrations for the downwind site to give a value representing the contribution from the power stations only. This method could lead to discrepancies if either site is being affected by a very local source, so results are also compared with raw ground level concentrations and downwind concentrations with no upwind correction. Good vertical mixing is required for power station plumes to mix down to ground level, and background concentrations of SO_2 are generally low under such meteorological conditions.

2.2 Model set up

The ADMS-3 model was set up to calculate ground level concentrations of SO_2 across a grid of 31x31 squares, centred on SK858731, which is the grid reference of the monitoring site at Thorney. The area covers 45x45km, reaching from south of Newark to north of Gainsborough, and west of Retford to east of Lincoln. In addition, specific receptor points were defined for each monitoring site, both continuous SO_2 and SO_2 bubbler types. Outputs were defined for 900s, 1h and 24h averaging periods. The time varying source strength option was used, to allow the actual emissions patterns from the stations to be represented, and so it was necessary to use sequential data from Waddington for meteorological input.

PowerGen's Energy Management Centre provided emissions data for Cottam, and the Environment Unit of TXU-EP provided similar information for High Marnham and West Burton. In addition to the mass emission of SO_2, it was also necessary to estimate volume flows or exit velocities. For simplicity these were

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taken as being proportional to load, and emission temperature was assumed constant. Although this does not fully represent the situation during start up, for the purposes of long term modelling it is assumed that such transient events have no significant effect. To represent the multiple flues at Cottam the emissions were categorised by the number of units running at any one time. The model assumed 4 co-located sources with four different stack diameters, appropriate to 1,2,3 or 4 units running simultaneously. The time varying file was then set up such that the SO_2 emissions and volumes for any given hour were associated with the source representing the number of units running during that hour.

There are no significant gradients in the vicinity of the Power Stations, which all lie below the 100m contour. Limited regions toward the south west of the study area reached about 130m, as do the Lincolnshire Wolds which are to the east of the study area. It is generally considered that there is no requirement to use the complex terrain module of ADMS-3 if there are no gradients greater than 10% within the output grid (CERC [5]), a condition that the study area satisfies. Meteorological data for the area was obtained from the UK Meteorological Office site at Waddington, just south of Lincoln on a low ridge.

Various options of the model were looked at to check their validity. Long term statistics are the model output most appropriate to regulatory matters, and were therefore the focus of the testing; however there are other features that could be very useful for the investigation of isolated incidents. Short term concentration modelled at the locations of the continuous monitoring sites was used to compare time series of ground level concentrations.

2.3 Validity tests

Basic regression analysis techniques were used to test the agreement between modelled and measured long-term statistics for each site, and also for comparing the distributions. Measured data was processed to provide a suitable data set for comparison with the model. Since the only sources in the model were the three power stations, it was apparent that non-zero ground level concentrations of SO_2 would only be predicted when sites were downwind (i.e. wind blowing from the power station(s) to the site). The wind data from the meteorology input to the model defined whether this was the case. The background concentration of SO_2 was also estimated based upon the measured value at the most upwind site (i.e. wind blowing from the site to the power station(s)), again defined from the input meteorology. A single upwind site was considered appropriate because the two other sites also available would be measuring air masses that would pass over neither the station nor the downwind site. This provides three versions of measured data:

- **Measured SO_2** is the continuously measured concentration values obtained at the measuring site.
- **Downwind SO_2** is the continuously measured concentration values for all hours when the site is downwind of the power station(s). All other hours are set to zero, to match the prediction from the model during those hours.

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- **Corrected SO_2** is the downwind SO_2 value with the upwind value for that hour subtracted from it, in order to estimate the contribution of the power stations only. Again all hours when the site is not downwind are set to zero. It is recognised that this is a very crude correction, and has generally not been used as the sole test against the predicted values.

Further tests involved generating a time series of SO_2 concentrations at each site. Simple regression analysis was less useful in this case, because the simplifying assumptions made by the model led to significant errors that did not appear in the ensemble statistics. A more qualitative approach to the validation was necessary because of time of flight and pollutant persistence considerations, as discussed below.

2.4 Sensitivity analyses

The atmospheric conditions can be characterised completely by three variables – boundary layer height, Monin-Obukhov length and wind speed. These parameters are always used by the model, and can either be input directly or calculated from other input parameters. Sensitivity analyses were carried out both on how sensitive the calculation of parameters is to the input data values of measured meteorological conditions, and also on the sensitivity of ground level concentrations to small changes in the same parameters.

The analysis involved applying a random function to all the meteorological file variables to simulate variation within the range of measurement accuracy. This was applied to both the input meteorology and the derived values as calculated by the model. The results were analysed against the basic model results using simple regression techniques to show how much effect small inaccuracies in meteorological estimates have on the calculated ground level concentrations. Work was also carried out to test the sensitivity to individual parameters, starting with the condition that led to the maximum ground level concentration, and changing each parameter in turn.

2.5 Comparison with AERMOD

The results from modelling the Trent Valley power stations using actual emissions within AERMOD are also presented here, to allow comparison to be made between the behaviour of the two models in relation to measured data.

3 Results and Discussions

3.1 Measured Concentrations of SO_2

Table 1 presents a series of statistics for measured concentrations of SO2 at the JEP monitoring sites in the lower Trent valley and the values of the same statistics predicted by ADMS-3. The table includes values based on the measured, downwind and corrected SO2 concentration as defined in 2.3 above.

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Table 1: Measured and Predicted Ground Level Concentrations of SO_2 at Monitoring Sites within the Trent Valley

Site	Statistic	Measured		Downwind	Corrected		Adms 3		AERMOD
		hr	15m	hr	hr	15m	hr	15m	hr
Thorney	Mean	5.1	5.2	2.31	1.23	1.23	3.31	3.41	1.2
	Max	298.3	363.7	298.3	294.4	359.8	174.0	213.9	336.0
	99.9%	187.1	197.1	145.2	122.1	161.9	131.8	168.7	242.6
	99%	64.4	72.5	53.3	41.6	44.6	81.5	92.8	80.6
Bottesford	Mean	3.9	3.9	0.45	0.32	0.32	0.76	0.77	0.4
	Max	159.2	183.1	159.2	147	182.6	117.1	191.1	193.5
	99.9%	67.8	77.6	47	46.1	50	79.50	117.5	97.9
	99%	27.5	27.6	10.2	8.2	6.9	26.84	23.23	27.8
Jenny Hurn	Mean	4	4	1.75	1.35	1.35	1.78	1.74	0.5
	Max	239.8	318.7	239.8	237.4	316.3	157.9	207.2	380.3
	99.9%	115.4	131.1	112.4	109.2	113.6	115.8	141.6	124.5
	99%	44.5	47.4	39.5	35.7	37.7	51.0	57.0	41.4
Grove	Mean	4.4	4.4	0.86	0.54	0.54	1.10	1.07	0.6
	Max	283.2	500.2	146.4	133.9	203.1	136.7	165.4	293.0
	99.9%	128	133.1	94	91.6	97.4	86.3	111.4	144.3
	99%	34.7	35.8	19	15.6	12.6	34.9	40.1	45.5

	Measured (Daily)				ADMS 3				AERMOD			
Site	Ave	Max	99%	90%	Ave	Max	99%	90%	Ave	Max	99%	90%
Thorney	10.7	143	58.8	23.3	9.0	90	71.4	31.6	3.2	136.0	103.3	38.9
Gainsborough	8.4	72	36.8	15.2	8.7	76	67.0	32.3	8.0	118	70.5	28.5
Springthorpe	7	86	43.3	15.4	13.1	66	60.2	37.8	13.4	99	76.5	37.8
Carr Hill	7.7	60	36.9	18.3	2.8	62	40.8	9.2	3.7	104	49.7	16.8
Furze Hill	12.3	97	58.2	22.3	12.6	70	53.8	33.2	13.7	108	66.4	34.9
Egmanton	8.7	43	34.7	16.4	3.2	40	36.6	13.9	3.6	116	42.1	13.9

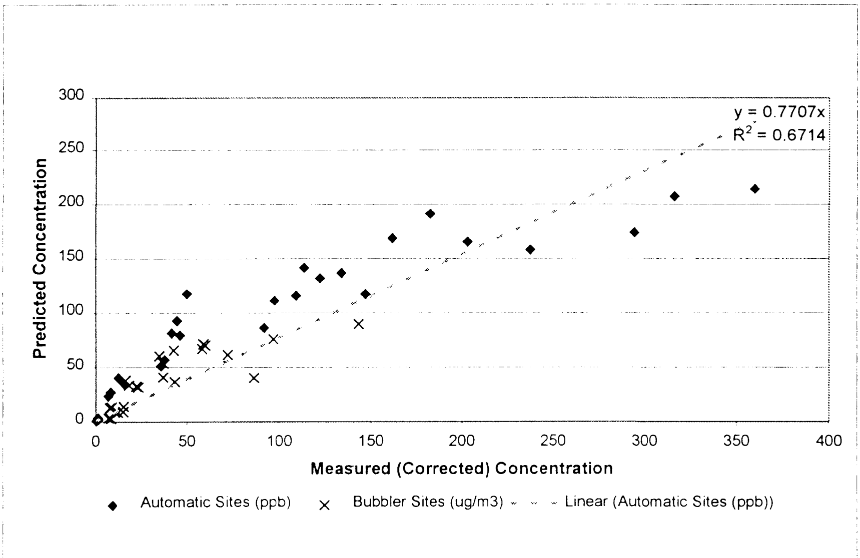

Figure 1: Ensemble plot of predicted against measured ('Corrected') concentrations as given in table 1

Figure 1 shows a scatter plot of these statistics for the continuous monitoring sites, with a regression line fitted to indicate how well the model is performing. The general performance of the model is good when used for long term statistical values, but there tends to be over-prediction at high percentiles, although the

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most extreme values, above about the 99.9th percentile of hourly values, show slight under-predictions. The long-term mean generally showed good agreement between measured and predicted values, with some exceptions. In particular, the bubbler sites to the west of the power stations showed large under-prediction of mean concentrations. This is probably because the western sites are downwind of power station plumes for a much smaller proportion of the year than those sites to the east, during which time they will measure background concentrations.

At Grove there is poor agreement between the model and the raw measurement of SO_2, but when an upwind correction is applied the agreement is much better. It is likely that other sources are present upwind of Grove, which is about 4km east of Retford, at the north-east of Grove village, but these will only affect the site when the plumes from local power stations do not. Small sources, such as domestic fuel burn, would be expected to have a very localised area of influence, and may be undetectable at a distance of over 0.5km. It is possible that Grove is the only automatic site that is significantly affected by local sources. Thorney is at the west side of a village (ie normally upwind), and in an area strongly influenced by all three power stations.

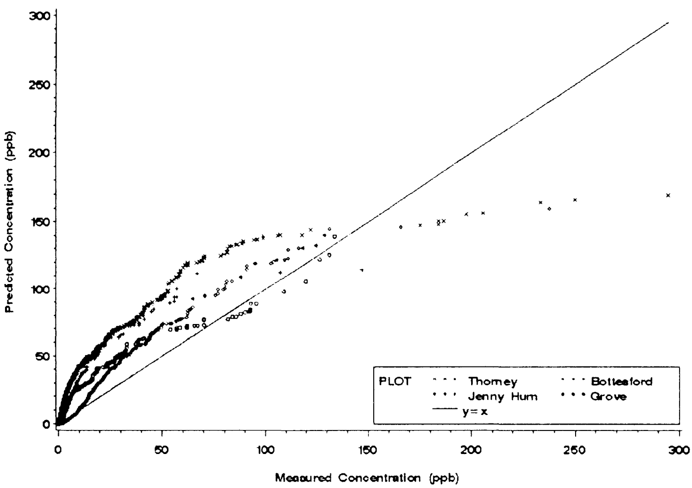

Figure 2: Comparison of predicted with measured (corrected) concentrations at the Lower Trent Valley continuous monitoring sites

Using the SAS® database engine it was possible to calculate all the percentiles of measured, downwind, corrected and predicted data at intervals of 0.01%. This gives a much finer resolution as shown in Figure 2. This was carried out for the four continuous monitoring sites, giving a consistent picture of how ADMS predictions match with measurements at each of the monitoring sites, illustrating the change from over- to under-prediction at around the 99.9th percentile. Note:

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Percentile calculations in ADMS-3 use a cumulative basis, leading to small differences between plotted and tabulated percentiles.

3.2 Patterns of predicted ground level concentrations

The pattern of ground level concentrations predicted in the lower Trent Valley is in line with what would be expected. Figure 3 shows a contour plot of the predicted 99.9th percentile ground level concentrations. A large area of the grid is predicted to experience 99.9th percentile ground level concentrations of SO_2 in excess of 100ppb for 1998. The monitoring sites, also shown, do not provide enough data to allow a mapping of the values, however reference to Table 1 shows how the values at those sites compare with the prediction.

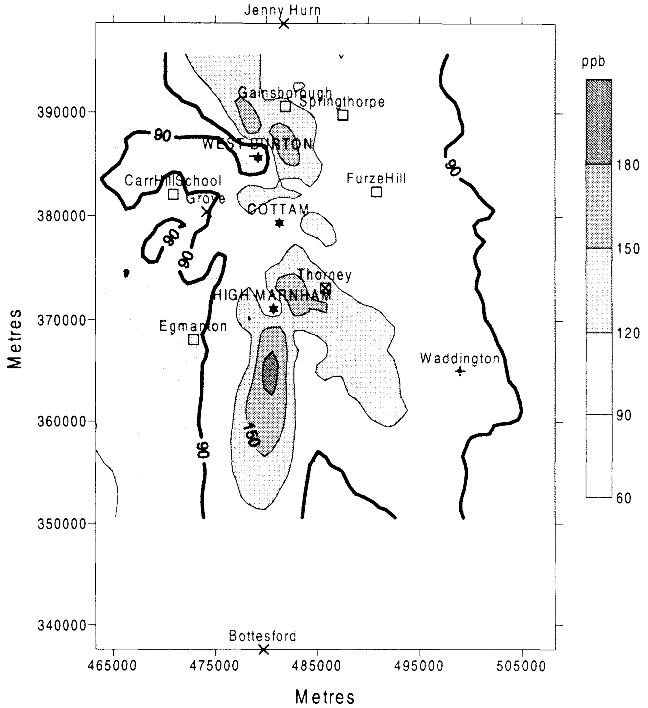

Figure 3: Contour plot of predicted ground level concentrations of SO_2 in the Lower Trent Valley

There is considerable interaction between the stations, especially at the high percentile values. Areas of increased concentration occur at various locations where two stations line up, and directly between stations. Thorney is in an area that is affected by the combined effects of West Burton and Cottam Power stations in a north westerly wind, and has measured peak hourly concentrations even higher than the predicted maximum.

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For comparing predictions with the NAQS standards and objectives it is common to simply set the averaging time to 900s. This does not give the whole picture because the meteorology is still based upon hourly data. For this reason the 99.9th percentiles shown in Figure 3 are based upon the hourly averaged values. Close to the source the pattern of ground level concentrations will vary rapidly with time, so an hourly average in excess of 100ppb does not guarantee 4 fifteen-minute averages in excess of 100ppb. Similarly a fifteen-minute average over 100ppb can occur in an hour with an average concentration of as low as 50ppb (EPAQS [6]). In a recent trawl of JEP air quality data an example of a fifteen-minute exceedence in an hour with an average of only 30ppb was found. It has been suggested (Laxen [7]) that an equivalent to 100ppb at the 99.9th percentile of fifteen-minute averages is 90ppb as the 99.9th percentile of hourly averages (based on an empirical relationship between measured data averaged over those periods).

It should be noted that exceedences of the NAQS standard in 1998 should not be taken as failure to meet air quality objectives. Station management plans should ensure compliance with the NAQS objective by 2005.

3.3 Time series analyses

Time series of SO_2 concentrations over the entire square can be generated for up to 24 hours of sequential data, and for individual receptor points the sequential hourly ground level concentrations for the entire period of the meteorological data can be generated. Using these facilities it is possible to see how well the model operates when looking at individual episodes of poor air quality. Table 3 gives information about a selection of days on which above average SO_2 concentrations were measured at one or more sites, along with information about how well the model predicts these events. On most of the selected days the model successfully predicted an increased concentration at the site, but the time of the maximum concentration did not generally coincide with the time of the worst case measured value. There were also cases where the general variation of measured concentrations with time differed from the way the predictions suggested variation would occur. Note that there are also many cases of over-prediction, but the examples were found by searching the data for high measured concentrations.

Table 2: Measured & predicted SO_2 concentrations on selected days

Date	Site	Time(s)	Corrected SO_2	Predicted SO_2	Predicted Max
21/2	Thorney	13-16	294,250,233,198	77,75,76,82	94@18
10/3	Jenny Hurn	9-12	79,64,111,103	67,41,42,41	67@9
		17-20	88,91,109,57	0,0,0,42	
17/4	Thorney	6-9	51,94,118,122	0,0,8,19	106@10
21/4	Grove	20-22	126, 88,134	0,16,13	16@21
1/5	Bottesford	11-14	56,39,39,57	1,1,28,26	39@18
18/5	Grove	11-17	102,93,84,93,86,120,64	4,71,126,122,41,90,24	126@13
2/9	Bottesford	12-13	118,147	0,0	6@17

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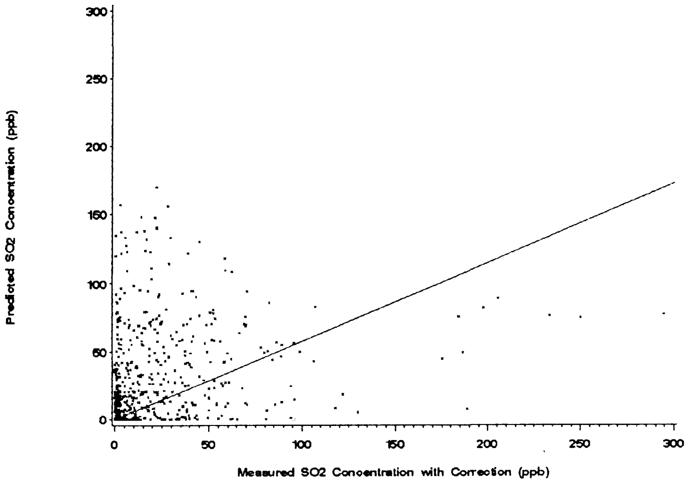

Figure 4: Scatter plot of hourly predictions versus measured (corrected) Concentration at Thorney

Figure 4 shows a scatter plot of time series results for Thorney, as an example of the lack of correspondence when the output for every hour is considered, rather than ensemble statistics as were discussed above. It is not surprising that ADMS-3 cannot accurately predict the hour by hour concentration at a given point, because of the necessary assumptions made to simplify the model, and the limitations in the accuracy of the data input to the model. The fact that higher concentrations are predicted on days when they occur indicates that the model has essentially the correct characteristics. Simplifications include:

- Meteorological conditions held constant for an hour – some can change on shorter timescales, especially during the morning and evening. This could lead to the model allowing the plume to be trapped under a boundary layer for a whole hour, when it would actually have risen above the boundary layer for a significant portion of the hour (or vice versa) as the boundary layer height changed.
- Dispersion calculated in a straight line to the edge of the grid, even if wind speed would not allow emissions to reach that far. This could lead to predictions of peak concentrations at distant sites earlier than they actually occur.
- Emissions considered for one hour only, then ignored. This goes some way to compensate for the previous point, but only if the wind direction and emissions are constant.
- No consideration of wind trajectories. When the wind direction changes from one hour to the next a receptor at medium distance may not be predicted to receive any contribution from a source, when in reality the centreline of

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the plume may have passed overhead. An example of this is the 2nd September at Bottesford, described by Acres [8].

It should be remembered that dispersion is a turbulent process, which is of a chaotic nature. No dispersion model will be able to achieve a high degree of accuracy over a very short timescale, and even hourly averages should really only be considered as an estimated mean for a distribution of possible concentrations under particular meteorological conditions.

In reality meteorological conditions change gradually, but continuously; and do not have exactly the same values across large regions. The emissions from a power station do not disappear after one hour (as assumed by the model), but remain in the atmosphere. In many cases the emissions will be transported out of the modelled area within one or two hours, but under adverse conditions high concentrations may persist close to the source for longer. Under such conditions (e.g. calm, or light and variable winds) there may be mixing of instantaneous emissions with elevated concentrations remaining from earlier emissions.

Fortunately such events are rare, and do not significantly impair the long term performance of the model; however on an individual hour basis such events may contribute to the under-prediction of the maximal concentration values noted at all the monitoring sites.

3.4 Sensitivity analyses

Figure 5 shows a comparison between the predicted concentrations based upon meteorological data with a random amount of error incorporated either into the input or the processed data. The agreement between ensemble statistics taken across the entire grid is good, but when short-term results at a single point are considered, there is considerably more scatter. This suggests a very high sensitivity to individual meteorological parameters (either input or processed), but in a non-biased way, such that ensemble statistics are affected less.

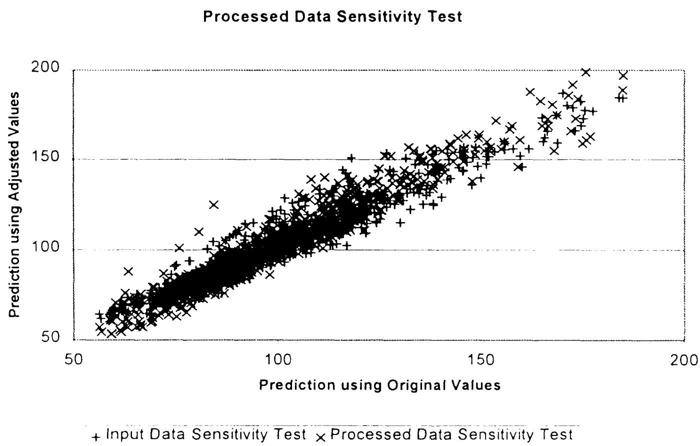

Figure 5: Sensitivity of ADMS3 predictions to random scatter to the input meteorological data

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The sensitivity to changes in individual parameters is shown in Figure 6, which gives relationships between ground level concentration and several of the input and processed meteorological parameters. These are derived from the maximum predicted concentration at any grid point assuming full load operation at all three stations. The meteorological parameters are varied around the worst case condition for all stations combined. The results from the sensitivity analyses of individual parameters demonstrate the highly non-linear nature of the model. Step changes in predicted concentration occur as a result of small changes to any of the input parameters. Reference to the ADMS-3 Meteorological Output file suggests that some of the more dramatic changes occur as a result of the transition from stable to unstable conditions. For input parameters the calculated boundary layer height is also thought to have a significant effect. There is clearly a change in the behaviour of the plume as the boundary layer rises, possibly relating to the point at which the plume becomes entirely trapped within the boundary layer.

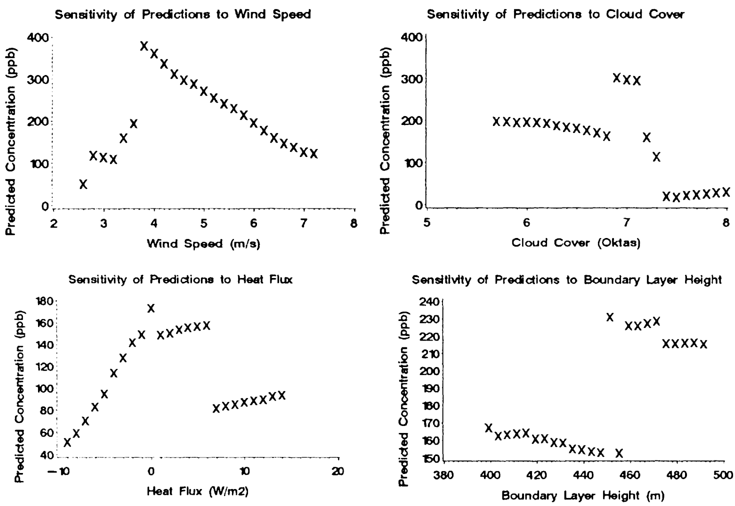

Figure 6: Sensitivity of ADMS predictions to small changes in the input meteorological conditions.

Small changes in the meteorology can give very significant changes in the predicted concentrations for any given hour. Sensitivity analyses are far from straightforward to interpret because many of the parameters are inter-related in the meteorological processing, and then the concentrations are calculated according to three different formulae, depending upon the value of the ratio h/L_{MO} (Boundary Layer Height/Monin-Obukhov length.)

Air Pollution VIII, C.A. Brebbia, H. Power & J.W.S Longhurst (Editors)

3.5 Comparison with AERMOD

Figure 7 presents contour plots of predicted ground level concentrations of SO_2 produced from both AERMOD and ADMS-3. Although the structure of the two models is quite different, options have been used to provide predictions on as similar a basis as possible from the two models. Information about the predicted statistics at individual receptor points defined at the monitoring sites in the lower Trent Valley was presented in Table 1.

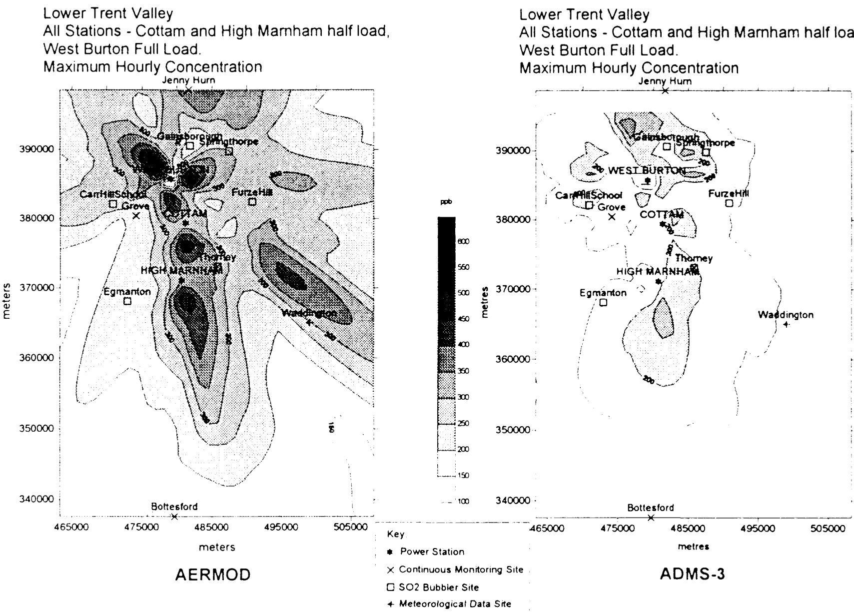

Figure 7: Predictions of AERMOD and ADMS 3 for the Trent Valley, 1998

The predictions of high percentiles produced by AERMOD are significantly different to those generated by ADMS-3. AERMOD gives systematically higher values over much of the grid. Up to the 99^{th} percentile the differences are generally small, but above that the values diverge rapidly. ADMS-3 under-predicts at the highest percentiles, however the over-prediction of AERMOD appears larger than the error in prediction of ADMS-3, particularly close to the point where ADMS-3 changes from over- to under-prediction – near the 99.9^{th} percentile level. By coincidence, none of the monitoring sites lie in areas close to the most extreme maximum concentrations, and even show lower predictions from AERMOD than from ADMS-3 for some statistics. The results from the individual monitoring sites suggest a closer match between the two models than area-wide analyses (as shown in the figure) do.

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4 Conclusions

The various tests carried out here have shown that ADMS-3 produces consistent predictions of ground level concentrations at a variety of fixed monitoring sites around the lower Trent Valley Power Stations. It has been found that there is a pattern of over-prediction of ground level concentrations up to about the 99.9th percentile, above which under-prediction occurs. The stability of these predictions to small perturbations to the input data set is also good, suggesting a generally robust model formulation. By contrast, when individual hours are considered the prediction accuracy is significantly poorer, and a large variation can be induced from small perturbations to the input meteorology.

Certain simplifications in the model can be identified as leading to possible discrepancies. In particular the way each hour is treated entirely separately could lead to under-estimates of ground level concentrations on a few isolated occasions per year, hence explaining the under-prediction of maximal values. Similarly the formulation for plume meander is the same for all hours, whereas in reality the wind direction will show more variability in some hours than in others.

A sensitivity analysis shows that the way the model classifies atmospheric conditions can lead to significant step changes in predicted concentrations as a result of small changes to input meteorological data. Given the inherent uncertainty of meteorological measurements, especially cloud cover, this goes a long way to explaining the behaviour of the model when compared to individual hours.

In comparison with AERMOD, ADMS-3 showed similar predictions up to about the 99th percentile, above which the behaviour of the two models diverged rapidly. This would lead to a large over-prediction of 99.9th percentile by AERMOD. At the maximum level the over-prediction by AERMOD would be at least as great as the under-prediction by ADMS-3.

5 References

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