Air Pollution Forecasting in the United Kingdom: 1997

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Executive Summary

Daily air pollution forecasts for ozone, nitrogen dioxide, sulphur dioxide, carbon monoxide and particles are issued by AEA Technology Environment, National Environmental Technology Centre. The forecasts are an important part of the UK Department of the Environment, Transport and the Regions air pollution information systems. An air pollution forecast is

important because it allows individuals who may be affected by episodes of high air pollutant concentrations to take preventative measures. Air pollution information is made available to the public by a Data Dissemination Unit through television and radio weather forecasts, teletext, newspapers, a free telephone information service (freephone number 0800 556677) and the World Wide Web.

This is the fifth report on air pollution forecasting in the UK and summarises the achievements and success rates of the air quality forecasting service for the year January to December 1997. On 19 November new bandings were introduced, along with the forecasting of particles and carbon monoxide, and the replacement of the term “air quality” with “air pollution”. The forecasting success rates have therefore been reported in two sections:

- Under the old bandings twenty five of the 28 instances of POOR air quality for ozone during the summer of 1997 were correctly forecast, and forty seven out of a total of 97 instances of POOR air quality for nitrogen dioxide were correctly forecast with the success rate varying from region to region. Nine out of a total of 32 instances of POOR air quality for sulphur dioxide were correctly forecast.
- Under the new bandings there were no instances of HIGH air pollution for ozone, nitrogen dioxide or carbon monoxide. One instance of HIGH air pollution for sulphur dioxide was not forecast and two out of the 6 instances of HIGH air pollution for particles were correctly forecast. This area of forecasting is subject to substantial research and review in order to enable us to capture, better, local impacts on the particle concentrations.

The most significant change to the forecasting service during the year was the requirement to predict concentrations of PM_{10} within the framework of the new bandings. A combination of box modelling techniques to predict the local contribution and a trajectory model to predict the long range transport component of PM_{10} are required to forecast ambient concentrations.

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Introduction

The Department of the Environment, Transport and the Regions (DETR) provides an hourly update on air pollution levels, together with a 24-hour air pollution forecast, which is widely disseminated through the media. An air pollution forecast allows individuals who may be affected by episodes of high air pollutant concentrations to take preventative measures. These can include increasing medication or taking steps to reduce exposure and dose.

Air Pollution Bulletins continue to be made available to the public each day by the DETR's Data Dissemination Unit (DDU), via television teletext, newspapers and a free telephone information service (currently 0800 556677). Teletext pages have been updated hourly since June 1994. Information on current air pollution and forecasts are also made available on the World Wide Web:

- http://www.aeat.co.uk/netcen/airqual
- http://www.environment.detr.gov.uk/airq/aqinfo.htm

This site also includes a comprehensive Air Quality Archive. Air pollution information is always made available for inclusion in television, and radio weather forecasts and is usually broadcast during periods of HIGH air pollution.

Detailed, region by region, forecasts of air pollution for inclusion in these bulletins are provided by AEA Technology, National Environmental Technology Centre (NETCEN). The forecast consists of an air pollution band for each pollutant for the following 24 hours, for each geographical region. During the period covered in this report there were 9 geographical regions (see Figure 1.1) but in February 1998 the new region of East Anglia was introduced (see Figure 1.2).

From January 1st to November 18th 1997 air quality was classified according to four banding levels set out by the DETR, with the forecasters aiming to predict POOR and VERY POOR levels of O_3, NO_2 and SO_2. On 19 November 1997 a new set of bandings were brought in by DETR, including levels for CO and particles (PM_{10}) as well as re-defined bandings for O_3, NO_2 and SO_2. Under the new bandings forecasters are aiming to predict HIGH and VERY HIGH levels of air pollution. At the same time the term 'air pollution' has been substituted for the term 'air quality'.

In addition to the public dissemination of the daily air quality forecast, NETCEN also provides DETR with an 'early warning' forecasting service of major air pollution episodes.

Our first report (Stedman and Willis, 1994) described the techniques that are used to forecast air quality in the UK and presented an analysis of the forecasting success rate for the year from April 1992 to March 1993. Subsequent reports (Stedman and Willis, 1995; Stedman and Willis, 1996, Stedman *et al*, 1997) presented analyses of the forecasting success rate and discussed modifications to the forecasting system. This report, the fifth on air pollution forecasting in the UK, presents an analysis and some discussion of the forecasting success rate for the year period from January to December 1997. We consider the new bandings introduced in November 1997, and the likely changes to episode frequencies. The forecasting success rate is discussed in two sections: one for each set of bandings. The testing and implementation of modelling to aid in the forecasting of PM_{10} is discussed in Section 5 and Section 6 covers a number of other forecasting issues, including other models and data exchange.

Figure 1.1 UK Air Quality Forecasting Regions, 1997, And The Locations Of Automatic Monitoring Sites

Figure 1.2 UK Air Pollution Forecasting Regions, 1998, And The Locations Of Automatic Monitoring Sites

New Bandings for Air Pollution

Before 18 November 1997 the DETR classified air quality using the four banding levels for O_3, NO_2 and SO_2 shown in Table 2.1.

Table 2.1: United Kingdom Department of the Environment, Transport and the Regions Air Quality Guidelines (ppb, hourly average) (until 18 November 1997)

	VERY GOOD	GOOD	POOR	VERY POOR
O_3	< 50	50 - 89	90 - 179	≥ 180
NO_2	< 50	50 - 99	100 - 299	≥ 300
SO_2	< 60	60 - 124	125 - 399	≥ 400

Since 19 November 1997 a new banding scheme has been in use. This scheme includes bandings for PM_{10} and CO as well as the three pollutants previously forecast and these pollutants are now forecast every day (Committee on the Medical Effects of Air Pollutants, 1997). The new banding levels which the DETR now uses to classify air pollution for O_3, NO_2, SO_2, CO and fine particles are shown in Table 2.2. We have assessed the forecasting success rate for the "Information" threshold between MODERATE and HIGH.

Table 2.2: United Kingdom Department of the Environment, Transport and the Regions Air Quality Guidelines (ppb, hourly average) (since 19 November 1997)

	Standard	Information		Alert
	LOW	MODERATE	HIGH	VERY HIGH
Sulphur Dioxide (ppb, 15 minute mean)	less than 100	100 - 199	200 - 399	400 or more
Ozone (ppb)	less than 50 (8 hour running mean)	50 - 90 (hourly mean)	90 - 179 (hourly mean)	180 or more (hourly mean)
Carbon Monoxide (ppb, 8 hour running mean)	less than 10	10 - 14	15 - 19	20 or more
Nitrogen Dioxide (ppb, hourly mean)	less than 150	150 - 299	300 - 399	400 or more
Fine Particles ($\mu g/m^3$, 24 hour running mean)	less than 50	50 -74	75 - 99	100 or more

In the last forecasting report (Stedman *et al*, 1997) the likely number of exceedances for 1995 and 1996 under the new banding scheme was discussed. The findings were that there would be a similar number of ozone episodes as under the old scheme, fewer SO_2 episodes and virtually no NO_2 episodes. During 1996 and 1995 there were very few days with HIGH or even MODERATE levels of CO, under the new scheme, but there were a large number of days with HIGH levels of PM_{10}. Table 2.3 lists the number of days with measured HIGH or VERY HIGH pollution levels for each pollutant for 1997 for the country as a whole, if the new bandings had been used throughout the year. A comparison with the number of POOR and VERY POOR days defined by the old bandings confirms earlier conclusions, and since there are such a large number of episode days for PM_{10} it is important to have good forecasting techniques.

Table 2.3: Total number of episode days in 1997 classified by new and old bandings

	1997 Network Data			
	HIGH	VERY HIGH	POOR	VERY POOR
Ozone	8	0	8	0
Nitrogen Dioxide	0	0	72	0
Sulphur Dioxide	17	1	30	1
Carbon Monoxide	0	0	-	-
Particles	49	14	-	-
Total	74	15	110	1

Current Air Pollution Forecasting Techniques

A forecast of air pollution for the following 24 hours is prepared each afternoon, for inclusion in the 16:00 air pollution bulletin. A revised forecast is also issued at 11:00 if VERY HIGH air pollution is being measured or is expected. It is also possible to issue new or revised forecasts at any hour of the day.

The air pollution forecasts are based on information from a number of sources. The forecast is prepared with reference to all available information and on the basis of a number of years of 'hands on' experience of UK air pollution monitoring (Stedman and Willis, 1994). Sources of information include:

- On-line measured concentrations from the UK monitoring networks, for all pollutants. Data are averaged for comparison with the relevant bandings (ie 15-minute, hourly, 8-hourly or 24-hourly averages).
- Weather forecasts for the following day, provided by the UK Meteorological Office (MO).
- 'Real time' results from the trajectory ozone forecasting model (Stedman and Williams, 1992). The model is run each day during the summer by the MO, taking the output of numerical weather prediction models as its input, with the results automatically transferred to NETCEN via a computer link. This model provides estimates of ozone concentration for one day ahead for 20 sites and for two days ahead for five sites.
- Ozone data from selected monitoring sites in North West Europe is available each day via email. Moves towards the co-ordination of ozone data exchange in North West Europe are discussed in Section 6.5.
- Results from the urban pollutants forecasting box model, also provided by MO. The NO_x emissions estimates used in this model are provided by the National Atmospheric Emissions Inventory. This model provides estimates of NO_x and NO_2 concentration and meteorological parameters for 10 sites for one day ahead for the whole year and meteorological parameters for 10 sites for two days ahead during the winter.
- Carbon monoxide concentrations are forecast using the box model by assuming that the dispersion and emission conditions that are likely to lead to elevated CO are similar to those likely to lead to high concentrations of NO_x and NO_2.
- Elevated SO_2 concentrations can result from poor dispersion of low level emission sources and forecasts of such episodes are based on the box model results and a knowledge of local low level emissions (which are significant in cities such as Belfast). SO_2 episodes due to the impact of plumes from individual major point sources are predicted by reference to meteorological forecasts, and further research is under way to improve the reliability of these forecast (see Section 6.2).
- Results from a trajectory model adapted to forecast particulate sulphate are used in the forecasting of secondary PM_{10}. Primary PM_{10} is forecast using the results from the urban pollutants forecasting box model. Both of these are discussed in more detail in Section 5.

Analysis Of Air Pollution Forecasting Success Rate

introduction

Air quality in the UK is generally within the VERY GOOD/ LOW or GOOD/ MODERATE air quality bands. Episodes of POOR/HIGH or VERY POOR/VERY HIGH air quality are, however, also experienced. Episodes during the winter are generally associated with periods of poor pollutant dispersion caused by low temperatures and light winds (see for example Bower *et al*, 1994). Air pollution episodes during the summer are often photochemical in nature and are associated with light winds, high temperatures and strong sunlight.

The forecasts that are issued tend to err on the side of caution and consequently more occurrences of POOR/ HIGH air quality were predicted during 1997 than were measured. This is because it is considered by DETR to be better for public information and health, to predict POOR/ HIGH and be wrong than predict GOOD/ MODERATE and fail to warn the public of potentially POOR/ HIGH air quality.

The forecasting success rates are discussed in two sections: the old bandings in Section 4.2 and the new bandings, including forecasts of CO and particles, in Section 4.3.

Forecast Analysis For Old Bandings, 1 January 1997 To 18 November 1997

The forecasting success rates for ozone, nitrogen dioxide and sulphur dioxide are presented in Tables 4.1, 2.2 and 2.3 respectively. Each table gives an analysis of forecast versus measured POOR air quality during 1997. The air quality band for each region is the band for the highest concentration measured at any monitoring site within that region.

There was one measurement of VERY POOR air quality for SO_2 during the period covered by this report. There were no measurements of VERY POOR air quality for O_3 or NO_2. For the tables of forecast analysis, VERY POOR air quality has been included in the totals of POOR air quality. The instance of VERY POOR air quality is discussed in the text.

Forecast Analysis for Ozone

Twenty five of the 28 "region-days" with POOR air quality for ozone were correctly forecast (89%, see Table 4.1). All the instances of POOR air quality were correctly forecast for SE England, the Midlands and London, and 5 out of 6 days were correctly predicted in NE England.

A cautious approach by the forecasters resulted in this very high level of achievement, but also led to a number of region-days being forecast which did not occur. A significant number of these were 'near-misses' where the 90 ppb threshold just failed to be breached. There were usually exceedances of EPAQS recommended guideline on these days, with the 8-hour running mean exceeding 50 ppb, the National Air Quality Standard, and this would be considered MODERATE air pollution within the new bandings.

The frequency of days with POOR air quality for ozone during 1997 was lower than in 1996, and much lower than the more photochemically active year of 1995, which had 57 episode days (Stedman and Willis, 1996).

VERY POOR air quality for ozone was neither forecast nor measured during 1997.

Table 4.1 Forecast Analysis for Ozone, 1 January 1997 to 18 November 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland
POOR days measured	1	6	4	1	8	7	0	0
POOR days forecast	5	19	17	15	28	12	3	5
forecast & measured	0	5	4	0	8	7	0	0
forecast & not measured	5	14	13	15	20	5	3	5
not forecast & measured	1	1	0	1	0	0	0	0

Forecast Analysis for Nitrogen Dioxide

Forty seven out of a total of 95 “region days” (50%) with POOR air quality for nitrogen dioxide were correctly forecast during this period (see Table 4.2). Fifty four out of a national total of 95 “region days” with POOR air quality for nitrogen dioxide were measured in London, of which 31 days (57%) were correctly forecast. In the Midlands three out four days were correctly forecast while, while in NE England only 5 out of 16 days were forecast. A large proportion of these episodes were recorded at Lincoln Roadside, a new site on a very busy road with a high-sided street canyon. This site appears to show higher concentrations than ever measured before at a non-London roadside site. Consequently a period of “hands-on” experience was required before the forecasters could accurately predict the NO_2 levels at this site.

VERY POOR air quality for NO_2 was not forecast or measured during this period.

Table 4.2 Forecast Analysis for Nitrogen Dioxide, 1 January 1997 to 18 November 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland
POOR days measured	7	16	4	10	1	54	0	3
POOR days forecast	20	17	13	25	4	62	3	5
forecast & measured	4	5	3	4	0	31	0	0
forecast & not measured	16	12	10	21	4	31	3	5
not forecast & measured	3	11	1	6	1	23	0	3

Forecast Analysis for Sulphur Dioxide

Table 4.3 Forecast Analysis for Sulphur Dioxide, 1 January 1997 to 18 November 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland
POOR days measured	1	11	1	0	4	2	13	0
POOR days forecast	1	11	1	0	1	5	37	0
forecast & measured	0	2	0	0	0	1	6	0
forecast & not measured	1	9	1	0	1	4	31	0
not forecast & measured	1	9	1	0	4	1	7	0

VERY POOR air quality for SO_2 was measured on 5/11/97, at Middlesbrough, with a maximum hourly average concentration of 450 ppb. This was due to some local residents celebrating Bonfire Night by burning a pile of old tyres next to the monitoring station. The exact location and duration of the event was not predicted by the forecasters! SO_2 concentrations were low at all other monitoring sites due to the relatively efficient dispersion of the emissions from bonfires not located directly next to monitoring sites.

Nine out of a total of 34 "region-days" (26%) with POOR air quality for sulphur dioxide were correctly forecast (see Table 4.3). This is lower than the number of POOR days recorded during the whole of 1996. More than a third of POOR days measured were recorded in Northern Ireland: 13 days with POOR air quality for SO_2 were measured, of which 6 were forecast. In NE England 11 episode days were recorded of which only 2 was forecast (18%, or 20% if we exclude the VERY POOR), while in SE England none of the 4 episode days measured at Rochester were forecast. This site tends to be affected by a number of nearby point sources, such as refineries and power stations, whose effects are harder to predict. Research work is currently under way to attempt to improve our methods for forecasting point source related SO_2 episodes (see Section 6).

Forecast analysis for NEW bandings 19 november 1997 to 31 december

The forecasting success rates for nitrogen dioxide, sulphur dioxide, fine particles and carbon monoxide are presented in Tables 4.4, 2.4 and 4.7 respectively. Each table gives an analysis of forecast versus measured HIGH air pollution during the last part of 1997. The air pollution band for each region is the band for the highest concentration measured at any monitoring site within that region.

There were no measurements of VERY HIGH air pollution for any of the pollutants during the period covered by the new set of bandings. There were no measurements of HIGH air pollution for ozone during this winter period.

Forecast Analysis for Nitrogen Dioxide

Neither VERY HIGH nor HIGH air pollution for NO_2 was measured or forecast during the last part of 1997.

Table 4.4 Forecast Analysis for Nitrogen Dioxide, 19 November 1997 to 31 December 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland
HIGH days measured	0	0	0	0	0	0	0	0
HIGH days forecast	0	0	0	0	0	0	0	0
forecast & measured	0	0	0	0	0	0	0	0
forecast & not measured	0	0	0	0	0	0	0	0
not forecast & measured	0	0	0	0	0	0	0	0

1.1.1 Forecast Analysis for Sulphur Dioxide

VERY HIGH air pollution for SO_2 was not measured in the last part of 1997 and HIGH was recorded once in Northern Ireland, which was not correctly forecast.

Table 4.5 Forecast Analysis for Sulphur Dioxide, 19 November 1997 to 31 December 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland
HIGH days measured	0	0	0	0	0	0	1	0
HIGH days forecast	0	0	0	0	0	0	0	0
forecast & measured	0	0	0	0	0	0	0	0
forecast & not measured	0	0	0	0	0	0	0	0
not forecast & measured	0	0	0	0	0	0	1	0

1.1.2 Forecast Analysis for Particles (PM_{10})

VERY HIGH air pollution for particles was not measured during the last part of 1997. Of the six episode days measured across the country two were correctly forecast (33% success rate), one each in Scotland and Northern Ireland. The two days of HIGH air pollution in Wales were both recorded at Port Talbot, which is situated close to a steel works and therefore susceptible to local pollution which it is difficult to forecast.

Table 4.6 Forecast Analysis for Fine Particles, 19 November 1997 to 31 December 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland	\
HIGH days measured	0	0	0	0	0	0	2	2	
HIGH days forecast	0	0	0	0	0	0	1	1	
forecast & measured	0	0	0	0	0	0	1	1	
forecast & not measured	0	0	0	0	0	0	0	0	
not forecast & measured	0	0	0	0	0	0	1	1	

1.1.3 Forecast Analysis for Carbon Monoxide

Table 4.7 Forecast Analysis for Carbon Monoxide, 19 November 1997 to 31 December 1997

	NW England	NE England	Midlands	SW England	SE England	London	N Ireland	Scotland	\
HIGH days measured	0	0	0	0	0	0	0	0	
HIGH days forecast	0	0	0	0	0	0	0	0	
forecast & measured	0	0	0	0	0	0	0	0	
forecast & not measured	0	0	0	0	0	0	0	0	
not forecast & measured	0	0	0	0	0	0	0	0	

Neither VERY HIGH nor HIGH air pollution for carbon monoxide was measured or forecast during the last part of 1997.

1.2 Comparison With Previous Years

Table 4.8 shows the forecasting success rate for the whole UK over the last four years. This is the percentage of episode days which were correctly forecast The number of days with POOR air quality for ozone that were correctly forecast was 89%, a small improvement on 1995 (82%), though not as good as 1996 (100%). The success rate for forecasting of POOR NO_2 was lower than in 1996, though about the same in London (57%). This may be due, in part, to an increase in the number of monitoring sites. The success rate for SO_2 in 1997 was lower than in 1996, both in Northern Ireland and across the country as a whole.

Table 4.8 Forecasting Success Rates for the Whole of the UK

	93/94	95	96	97 (old)	97 (new)
Ozone	69%	82%	100%	89%	*
Nitrogen Dioxide	32%	70%	52%	49%	*

Sulphur Dioxide	27%	42%	38%	28%	0%
Carbon Monoxide	-	-	-	-	*
Particles	-	-	-	-	33%

* No HIGH or VERY HIGH days recorded.

The number of HIGH days recorded in the last part of 1997 indicates the drop in episode days following the move to the new banding structure. In particular nitrogen dioxide episodes were very rare (none in period included) and sulphur dioxide episodes were also less frequent (only one in this period).

2 Forecasting PM_{10}

2.1 Introduction

An important new task following the introduction of the new air pollution bandings in November 1997 is the forecasting of episodes of elevated concentrations of airborne particles, specifically PM_{10}. The forecasting of PM_{10} episodes is a challenge because of the range of sources that contribute to ambient particle concentrations. The relative contributions from these sources must be understood before a reliable forecasting strategy can be implemented. The sources of PM_{10} in the UK have been reviewed by the Quality of Urban Air Review Group (QUARG, 1996) and source attribution methods involving the combination of data from several DETR monitoring networks has recently been developed at NETCEN (Stedman, 1998). Ambient PM_{10} can be considered to be made up from three distinct types of particles:

- Primary combustion particles - these are particles derived from vehicle exhaust or stationary combustion sources. These particles are generally black due to the presence of carbon.
- Secondary particles - consisting of sulphates and nitrates from the atmospheric oxidation of sulphur dioxide and oxides of nitrogen. These particles and their precursors can be transported over distances of 100s of km.
- Coarse particles - in contrast to the primary combustion or secondary particles, these resuspended dust, soil, mechanically derived and sea salt particles are generally larger than 2.5 μm in diameter.

We have used an empirical regression method to disentangle the different origins of measured daily PM_{10} particle concentrations. An equation of the following form can be obtained:

[measured PM_{10}] = A.[measured black smoke] + B.[measured sulphate] + C

with these three terms representing, primary combustion, secondary and coarse particle concentrations, all in μgm^{-2}. This method was originally applied (Stedman, 1998) on a network mean basis (mean of all sites on a daily basis) and regression coefficients have subsequently been derived for the cities listed in Table 5.1.

Table 5.1. Regression coefficients for PM_{10} data

	Smoke coefficient, *A*	SO_4 coefficient, *B*	Intercept, *C*	r^2
London Bloomsbury	0.64	2.26	10.96	0.78
Birmingham Centre	0.59	2.41	8.30	0.71
Bristol Centre	1.03	2.35	10.83	0.70
Manchester Piccadilly	0.60	2.46	9.77	0.74
Newcastle Centre	0.66	3.13	7.73	0.84
Belfast Centre	0.71	2.30	9.21	0.79
Cardiff Centre	0.86	1.71	13.07	0.73
Leeds Centre	1.00	2.58	4.56	0.84
Network Mean	1.00	3.00	5.00	0.84

The forecasting of episodes of elevated PM_{10} concentrations therefore requires the use of appropriate models to forecast these different contributions on a daily basis. The regression method described by Stedman (1998) significantly simplifies the derivation and testing of the required models because the individual models can be compared with measured black smoke and sulphate data. The models that have been developed for forecasting primary combustion and secondary PM_{10} are discussed below. This is followed by an investigation of the reliability of the combination of these two models during a 10 week period during the winter of 1997/98.

Fixed daily mean concentrations have been considered here in order to simplify the analysis because black smoke and sulphate concentrations have been measured on a daily basis. It is recognised that the daily maximum of running 24-hour averages can be higher than fixed daily means. The methods described here represent the initial work that has been undertaken to provide a method for forecasting PM_{10}. There is a continuing research programme to refine these techniques.

2.2 Primary Combustion Pm_{10}

Primary combustion derived PM_{10} originates, in most UK cities, from the same emission sources as oxides of nitrogen (NO_x), including vehicle exhausts. High concentrations of both of these species tend to be associated with poor dispersion of low level emissions caused by light winds and low mixing heights. The box model that is used to forecast hourly NO_x concentrations can therefore be adapted to provide forecasts of primary combustion PM_{10}. The following multi-stage analysis was carried out using daily monitored and forecast pollutant concentrations for the one year period from April 1995 to March 1996. This period was chosen because it includes the major secondary particle episodes in early 1996 and several primary particle episodes in late 1995.

- The regressions listed in Table 5.1 provide a coefficient for the relationship between measured daily mean black smoke concentrations and primary combustion PM_{10} for individual cities.
- An empirical relationship between measured daily mean NO_x concentrations and black smoke was also derived for each city.
- An empirical relationship between the daily mean NO_x concentration predicted by the urban box model and measured black smoke was then derived and checked for consistency with the relationship with measured NO_x. Daily mean NO_x was calculated as the average of the 24 individual hourly forecast concentrations.
- The end result of this analysis is a composite coefficient which can be used to calculate estimates of daily mean primary combustion PM_{10} from predicted NO_x.

The coefficient for the relationship between black smoke concentrations and primary PM_{10} is typically between 0.6 and 1.0 depending on the blackness of the particles in each city, which will depend on the fuel usage. The values of the empirical coefficient between measured NO_x and primary PM_{10} is however reasonably consistent for GB cities, with values ranging from 0.08 to 0.13. The coefficients for the relationship between forecast NO_x and primary PM_{10} is, however, more variable, depending on the absolute values derived from the box model.

Figure 5.1 shows examples of the range of coefficients obtained relationships between measured primary PM_{10} concentrations and both measured and forecast NO_x. The coefficients are reasonably consistent in London for measured and forecast NO_x but in Cardiff the modelled NO_x concentrations systematically underestimate the measured NO_x concentrations, giving the two graphs very different slopes. The Cardiff error is taken into account when the model is used in forecasting.

2.3 Secondary PM_{10}

A trajectory model has be developed to provide estimates of secondary PM_{10} concentrations. This model makes use of the same 96-hour back trajectories and temperature forecasts as the ozone forecasting model (Stedman and Williams, 1992). The simplified chemical scheme has been adapted from Derwent *et al* (1988), and includes a fixed oxidation rate of 1% per hour for the conversion of SO_2 to particulate sulphate.

The model was run using trajectories from 1995 and 1996 and the results compared with measurement network data in order to provide an indication of the reliability of the modelled estimates. Daily measurements of particulate sulphate concentration are available from rural monitoring sites within the acid deposition monitoring networks (RGAR 1997).

To validate the model we investigated the accuracy of the modelled sulphate. The modelled sulphate values were compared with measured particulate sulphate values at seven rural sites: Eskdalemuir, High Muffles, Lough Navar, Strathvaich Dam, Yarner Wood, Sibton and Lullington Heath. Particulate sulphate is not measured at Sibton or Lullington Heath so we have compared the modelled results at these sites with measured concentrations from the nearby sites of Stoke Ferry and Barcombe Mills respectively. At these seven sites we compared data for summer 1995 and 1996, and also looked at distinct episodes for both years. Correlation values (see Tables 5.2 and 5.3) are reasonable and the pattern is generally similar. The model tends to overestimate the peak episode concentrations, despite modelled background being zero at all sites, and generally the modelled values are often within a few $\mu g/m^3$ of the measured data. The modelled means for the summer periods (Table 5.4) are below the measured means due to the zero background. Generally on an episode day the spatial pattern of the modelled results is very similar to that of the measurements. At Lullington Heath/Barcombe Mills the model does not perform so well: the modelled values are much too low and the correlation negligible, except in two of the episodes. It is not clear why this should happen here, but since sulphate concentrations are considered to be due to long range transport it is likely that there are unknown local factors. It is also possible that there are inaccuracies in the emission inventory used (Lubkert and de Tilly, 1989) and this will be addressed in future work. The good agreement between measured and modelled data found at the Sibton/Stoke Ferry shows that lack of co-location is unlikely to be the cause of the difference.

The secondary particle contribution to PM_{10} measured at the DETR automatic monitoring network sites is likely to be dominated by ammonium sulphate and sodium nitrate. We have investigated using two alternative methods of deriving an estimate of secondary PM_{10} from the trajectory model results. The method for estimating secondary PM_{10} from sulphate measurements presented in QUARG (1996) based on an analysis of sulphate and nitrate measurements for the UK is equivalent to multiplying sulphate by a factor of 2.5 to take into account the presence of both nitrate and counterions. Similar factors were also found by Stedman (1998) when comparing measured sulphate and PM_{10} concentrations at DETR monitoring sites. We have also derived a second estimate of secondary PM_{10} by adding up the modelled estimates of the concentrations of the following species: sulphate, nitrate and ammonium nitrate.

In order to compare these modelled estimates of secondary PM_{10} with PM_{10} measurements we have followed the approach suggested by Stedman (1998) and derived an estimate of secondary PM_{10} by subtracting a primary concentration derived from black smoke measurements and a constant coarse particle concentration from the measured PM_{10}, using the equation and coefficients listed in Section 5.1.

Table 5.2: Correlation coefficient (r^2) of measured and modelled sulphate values for timeseries

Site	Summer 1995	Summer 1996
Eskdalemuir (ES)	0.34	0.50
High Muffles (HM)	0.58	0.46
Lullington Heath/Barcombe Mills (LH/BM)	0.13	0.13
Lough Navar (LN)	0.54	0.50
Sibton/Stoke Ferry (SB/SF)	0.48	0.58
Strath Vaich Dam (SV)	0.43	0.44
Yarner Wood (YW)	0.50	0.41

Table 5.3: Correlation coefficient (r^2) of measured and modelled sulphate values for episodes

Site	April/May 95	March 96	April 96	July 96	August 96
ES	0.69	0.22	0.12	0.45	0.30
HM	0.71	0.62	0.24	0.69	0.40
LH/BM	0.43	0.65	0.12	0.38	-0.49
LN	0.36	0.66	0.26	0.59	0.50
SB/SF	0.40	0.72	0.70	0.29	0.70
SV	0.81	0.47	0.52	0.85	0.37
YW	0.42	0.26	0.57	0.44	0.79

Table 5.4: mean values of measured and modelled sulphate for timeseries (μgSO_4 m^{-3})

	Summer 1995		Summer 1996	
Site	Measured	Modelled	Measured	Modelled
ES	2.5	2.0	2.2	2.7
HM	3.4	2.8	3.2	3.6
LH/BM	4.5	0.8	4.4	1.4
LN	2.5	1.3	1.8	1.3
SB/SF	3.6	5.0	3.9	4.0
SV	1.8	0.8	1.6	1.5
YW	4.9	3.2	3.0	2.3

We compared the model results derived using both B.[modelled sulphate] and [total modelled aerosol] with secondary PM_{10} at 3 sites: London Bloomsbury, Birmingham Centre and Newcastle Centre. Model results are available for London and Birmingham but for Newcastle we used the model results from High Muffles, as the closest trajectory arrival point. At all 3 sites the two sets of model results were very nearly equivalent most of the time, although in many cases the total aerosol model gives slightly lower peak concentrations and in all cases the correlation with measured data was higher for the total aerosol model than for the B.sulphate model. In London the modelled values matched the “measured” secondary PM_{10} well a lot of the time and correlation is reasonable for both (see Table 5.5). Newcastle also shows a good relationship between “measured” and modelled values, with a higher correlation than for London in 1996. Birmingham shows the lowest correlation between modelled and measured values of secondary PM_{10}, although the values are still indicative of the good predictive ability of the model. As with Newcastle and London the correlation is higher in 1996 than in 1995. At all sites most episodes are predicted, some to within a few $\mu g/m^3$ eg on the 2/5/95, 1/8/95 and 20/8/96 in London (see Figure 5.2).

The early part of 1996 was exceptional in terms of the magnitude and duration of the secondary particle contribution to PM_{10} episode concentrations in the UK. In particular, March 1996 saw the largest secondary PM_{10} episode since monitoring began in 1992 (Stedman, 1997) and this episode is excellently modelled at all three urban sites, as well as at the rural particulate sulphate sites, as discussed above. This clearly demonstrates the success of the model.

These preliminary investigations lead us to believe that the model can be extremely useful in predicting urban secondary PM_{10} episodes. The model has been automated and has been used in the forecasting of PM_{10} since December 1997.

Table 5.5: Correlation coefficient (r^2) of measured and modelled secondary PM_{10} values for timeseries

	Summer 1995		Summer 1996	
Site	B x sulphate	Total aerosol	B x sulphate	Total aerosol
London	0.44	0.48	0.49	0.56
Birmingham	0.43	0.46	0.44	0.52
Newcastle	0.44	0.51	0.54	0.56

2.4 Combining Secondary And Primary Pm_{10}

The previous sections have described the two modelling methods that have been developed to forecast the primary and secondary components of daily PM_{10} concentrations. Both of these types of models have been used since December 1997 to aid the NETCEN air quality experts in the preparation of the daily forecast for PM_{10}. Some example results for selected cities for the 10 week period from December 1997 to mid February 1998 are shown in Table 5.6.

Table 5.6: Measured and predicted mean PM_{10} concentrations (μgm^{-3}) and correlation coefficients for daily means, 1 December 1997 to 13 February 1998 (provisional data)

monitoring site	measured mean	predicted mean	r^2
London Bloomsbury	23	28	0.17
London Camden Roadside	27		0.19
London Marylebone Road	33		0.17

Birmingham Centre	21	21	0.36
Birmingham East	17		0.34
Wolverhampton Centre	20		0.41
Bristol Centre	23	24	0.12
Manchester Piccadilly	23	24	0.27
Salford Eccles	23		0.45
Bury Roadside	28		0.36
Newcastle Centre	18	17	0.25
Belfast Centre	24	22	0.37
Derry	28		0.47
Cardiff Centre	24	22	0.14
Leeds Centre	-	29	
Bradford Centre	26		0.45

The agreement between the measured and predicted mean concentrations is generally reasonably good, with the concentrations at roadside and kerbside sites tending to be under predicted as would be expected. The correlation between the measured and predicted daily means varies from reasonable to poor. Timeseries plots for selected sites are shown in Figure 5.3. Some periods of high concentrations due to a combination of primary and secondary particles, such as the end of January, were correctly predicted at many sites. High concentrations due to primary particles were also reasonably well predicted on several occasions, for example in Birmingham and Bristol in early December and in Belfast and Derry on several days. The absolute magnitude of the data for the largest episode in Derry are in question, but the general shape of the data is still correctly modelled.

Overall the modelling methods that have been developed to assist the air quality experts in forecasting PM_{10} concentrations are proving valuable and further work will be undertaken to refine these methods, including evaluation of a new inventory and new chemical scheme for the secondary PM_{10} model.

3 Development Of The Air Quality Forecasting Service

3.1 East Anglia Region

The forecasting service has been revised in consultation with DETR to include the new region of East Anglia.

3.2 Point Source Emission Episodes

We are investigating the possibility of using an empirical model to improve the reliability of the forecasting of episodes due to emissions from individual major point sources. The meteorological conditions that lead to this type of episode are well understood within commonly used dispersion models, so we are studying a range of point source episodes using dispersion models run with both measured and forecast meteorological data. A report describing this work and making recommendations for the forecasting service is being prepared.

3.3 Neural Network

We are reviewing the performance of the neural network model for forecasting SO_2 in Belfast and NO_2 in London. The model has been running since 16 October 1997.

3.4 Name Model

The 'Name Sulphur Model' is currently under development at the Meteorological Office with a view to testing its applicability for air pollution forecasting. The usefulness of this model within the UK air quality forecasting system will be assessed over a six month period once an operational version of the model running in forecast mode is made available by the Meteorological Office. It is hoped that this model will enable forecasters to predict more accurately HIGH air pollution episodes which are the result of point source emissions.

3.5 Ozone Data Exchange

The European Environment Agency (EEA) have set up a Technical Working Group on Data exchange and Forecasting for Ozone episodes in Northwest Europe. This group is following up on the work of the Ministerial Conference on Tropospheric Ozone in Northwest Europe which was held in London in May 1996. This group has produced a report on ozone forecasting and data exchange in Northwest Europe (Topic Centre on Air Quality, 1997). Air quality scientists from NETCEN have represented the UK within this group and have been closely involved with the drafting of the report. We have also been active in drawing up a specification for a system of co-ordinated data exchange for ozone forecasting within Northwest Europe. A pilot data exchange system has been operational at NETCEN since the summer of 1997 and since April 1998 includes data from Austria, Belgium, Denmark, Finland, United Kingdom, Luxembourg and the Netherlands. A Java based web page to display the ozone data on a map of Europe has also been developed and tested.

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