A ONE YEAR SIMULATION OF ATMOSPHERIC CONCENTRATIONS AND DEPOSITION OVER UK AND EUROPE

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1. INTRODUCTION

There has been an increasing use of integrated mesoscale pollution transport models in Europe. Such models have played a major role in the formulation of European Union (EU) Directives and UNECE protocols and will play a similar role in the EU CAFE (Clean Air For Europe) process and UNECE protocol revisions. They are also being used for the assessment of National abatement policies.

The UK Electricity Industry had developed statistical models of long-range transport over many years but realised their limitations in addressing future environmental questions. The major generators in England and Wales, who own coal and oil fired stations, have sponsored, via their Joint Environmental Programme (JEP), the development of an implementation of Models-3 for UK and European situations.

The England and Wales Environment Agency wished to update and improve its understanding of the current state of the art in the modelling of national scale transport of major pollutants (in particular, acid deposition precursors, and particulates) and the potential application of the "new generation" models to the UK situation. It was decided that this would be achieved, in part, by co-funding a broad review of the capability of Models-3 for atmospheric long-range transport and deposition modelling in the UK.

A key requirement for the regulatory use of such models is the derivation of annual deposition statistics. Therefore, this assessment focused on a comparison of the output of Models-3 simulations over the entire year for 1999 with measured values for the same period. 1999 was chosen as the emissions are representative of current levels and detailed measurement data are available.

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2. BACKGROUND

It was recognised three years ago that the current industry models of long-range transport and deposition could not be extended indefinitely into the future, and that the more complex multi-pollutant and multi-effect analyses that are required would need a new approach to modelling processes.

The requirement was for a model capable of simulating these multi-issue problems across a range of spatial scales (from local to trans-boundary) and a range of temporal scales from short-period events to annual deposition. A further requirement was that the model should be 'future proofed' as far as possible in terms of the representation of key science processes. Following a review of available models, Models-3 emerged as the most promising model with the best fit to our requirements. The key feature of the model was its 'one atmosphere' approach in which the relevant processes for air quality, including particulate formation and photochemical oxidants, and wet and dry deposition of acidifying and eutrophying pollutants to be simulated consistently in a single model run.

Until recently, there had been relatively little work on the development of advanced long-range transport models in the UK, but over the last two years a version of Models-3 suitable for UK and European use has been built with the capability to link the European scale to local scale models.

This work has required the development of new procedures for the key inputs: emissions, meteorology and land use.

A programme of model testing has been carried out to examine the performance of this UK model for air quality and wet deposition, leading to the annual simulation discussed here.

3. STUDY OUTLINE

The model was run with three nested grids ranging from 108km grid resolution for the outer areas of Europe and the Atlantic Ocean, 36km for the United Kingdom and 12km grid resolution over much of England and Wales. In the vertical, a 21 layer hydrostatic grid was used.

For this study a Lambert Conformal projection was used with the following parameters.

Projection Centre	50˚N, 3˚E
Lower Standard Parallel	35˚N
Upper Standard Parallel	70˚N
Central longtitiude	3˚E

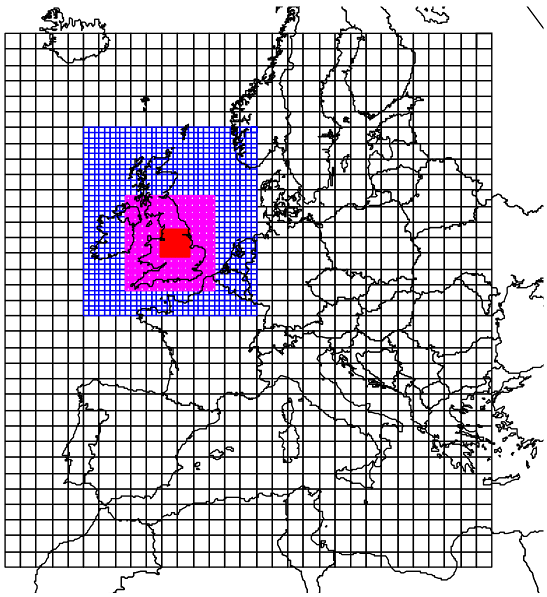

Fig 1: Modelling grids

Predicted daily rainfall and wet deposition of S, oxidised N, and reduced N at 12km resolution were compared with measurements at 10 acid deposition monitoring sites. Predicted hourly ground-level concentrations of SO_2, NO_2, NH_3, and PM_{10}.were compared with measurements at 10 air quality monitoring sites. The species and metrics chosen represent the major parameters determining acid deposition and air quality in the UK. The performance of Models-3 was also compared with that of the major European LRT model, the EMEP Lagrangian model.

4. DATA

The meteorological data was taken from the UK Meteorological Office Unified Model results. These data are available every three hours on a latitude/longitude grid. The resolution is 12km for the mesoscale and 50km for the global data. It was an important element of the study that we should use extant meteorological data. A pre-processor was written to interpolate and re-grid the data; derive surface and boundary layer parameter; and set missing parameters (e.g. cloud water mixing ratio).

The land cover data was obtained from the US Geological Survey and aggregated into the study domain cell size using Arc-Map.

The anthropogenic emissions data (NO_x, SO_2, CO, NH_3, NMVOC, PM_{10} and $PM_{2.5}$) was taken from two main databases: EMEP for European (50km * 50km by sector) and NAEI (National Atmospheric Emissions Inventory) for the UK (1km * 1km by source type). For major point sources in the UK typical stack parameters were used. However for all power stations actual values were entered along with real hourly data for emissions.

5. MODEL RUNS

The emission data was processed using SMOKE v1.4b, and the meteorological data were converted into MM5 format using an in-house preprocessor before being passed through MCIP v2.

The chemical scheme used was RADM2 with extensions for aerosols and aqueous chemistry. (RADM2_AE_AQ). Basic model options were used: ppm method for advection, qssa for the

Fig 2: Monitoring Sites

chemistry, and no plume-in-grid.

The runs were then carried out using CMAQ (v1.4) on two Sun SPARC2 Dual Processor machines with a 400 MHz chip speed. The runs were carried out in 12 monthly sub-runs restarting each month from the previous one. The entire project took around three months to complete.

6. RESULTS

A comparison of the modelled and measured values of NO_2 for this annual simulation is shown in Figure 3. Full analysis of the results from the model simulations at 12km resolution show that:

- The correlation coefficients, taken over all sites, for weekly modelled/measured wet deposition of S, oxidised N and reduced N are 0.59 (range 0.44 to 0.78), 0.46 (range 0.14 to 0.82), and 0.27 (range -0.01 to 0.78) respectively.
- Mean annual modelled/measured ratios for annual wet deposition of S, oxidised N and reduced N, taken over all sites, are 0.7, 1.0, and 1.2 respectively.
- The correlation coefficients, taken over all sites, for daily modelled/measured concentrations of SO_2, NO_2, and PM_{10} are 0.42 (range -0.15 to 0.75), 0.72 (range 0.28 to 0.85), and 0.41 (range 0.34 to 0.56) respectively.
- Mean annual modelled/measured ratios for annual concentrations of SO_2, NO_2 and PM_{10}, taken over all sites, are 1.3, 1.4, and 0.8 respectively.
- There is generally a slight overprediction of annual rainfall at most sites, but this should not be a major factor in determining model accuracy for annual wet deposition.
- Ammonia concentrations are not well simulated and there are significant negative correlations at 3 out of 4 sites. The mean annual model/measured ratio is 2.4. This apparently poor performance arises in part from uncertainties in the temporal and spatial behaviour of ammonia emissions.
- Models-3 performance for wet deposition and atmospheric concentrations compares favourably with the EMEP Lagrangian model.

7. CONCLUSIONS

Models-3 predictions are in reasonable agreement with measurements over the UK for most major environmental metrics and the model is suitable for adoption and further development as a high resolution long-range transport model for the UK and Europe.

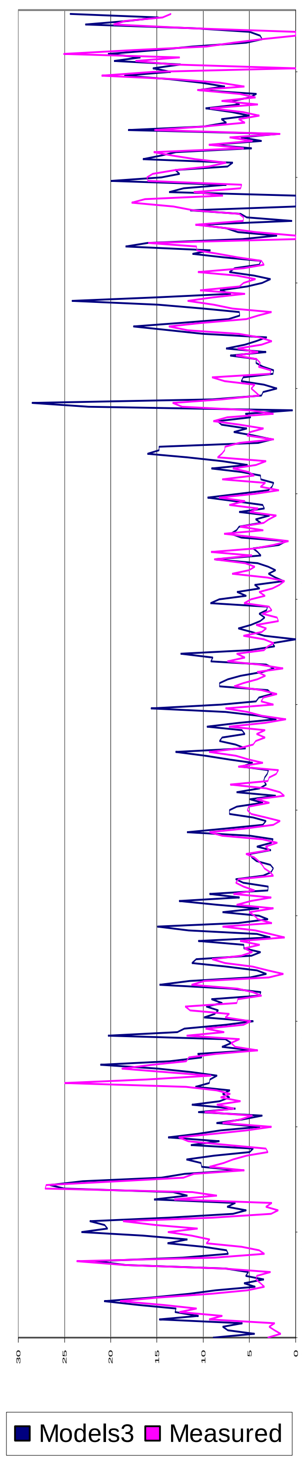

Fig 3: Bottesford: daily modelled and measured ground level concentrations of NO_2

8. ACKNOWLEDGEMENTS

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