MODELLING OF AIR QUALITY AND ACID DEPOSITION IN THE UK AND EUROPE - DEMONSTRATING THE VALUE OF A ‘ONE ATMOSPHERE’ APPROACH

Ian R. Rodgers[1], Alan T. Cocks[1] and Stephen Griffiths[2]
[1] RWE npower [2] Power Technology, Powergen
Ian.Rodgers@rweinnogy.com, Alan.Cocks@rweinnogy.com,
Stephen.Griffiths@powertech.co.uk

ABSTRACT

The effects of pollutant emissions to the atmosphere must be assessed at a range of scales from local through to transboundary. This assessment is complex because multiple pollutants contribute to a given environmental effect, and a single pollutant may contribute to multiple environmental effects. The policy and investment decisions required to reduce environmental effects need a framework which can simulate this complexity, and allow cost effective solutions to be found. Models of long-range atmospheric transport play a key role in this process. Such models have indeed been used for many years in Europe to inform policy makers and to assist in identification of least-cost emission reduction legislation. To date, however, a modelling framework capable of integrating all the spatial scales, time scales and processes of concern – a ‘one atmosphere’ model - has not been used for this purpose in Europe.

A UK and European version of the USEPA Models-3/CMAQ system has been developed over the last few years by the UK electricity generators’ Joint Environmental Programme to meet these diverse air quality and acid deposition modelling needs. The model offers four key advantages through its ability a) to simulate and couple processes from local to transboundary scales, b) to simulate both short-term episodes and annual effects, c) to simulate all the key atmospheric processes of concern within a single modelling framework, including the coupling of acid deposition, particulates and ozone and d) to examine the sensitivity of model results to the underpinning science via a modular software design.

It is concluded that the model is suitable for adoption and further development as a high-resolution long-range transport model for the UK and Europe.

INTRODUCTIONThe effects of pollutant emissions to the atmosphere must be assessed at a range of scales from local through to transboundary. This assessment is complex because multiple pollutants contribute to a given environmental effect, and a single pollutant may contribute to multiple environmental effects. The policy and investment decisions required to reduce environmental effects need a framework which can simulate this complexity, and allow cost effective solutions to be found. Models of long-range atmospheric transport play a key role in this process.

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In practice long-range transport models fulfil a number of roles. They allow examination of, and debate about, the underlying science; they are used by project developers or power station operators for specific projects as part of the environmental impact assessment process; they are used for debate with regulatory bodies and they are used to inform policy development.

The environmental issues which an integrated modelling framework should be capable of addressing includes acidification and eutrophication of ecosystems, contribution of groups of sources to national air quality, health effects of atmospheric particulates, atmospheric concentrations and deposition of toxics, tropospheric ozone effects on human and plant health and transboundary transport of pollution.

The coupling and interdependency between the processes underlying these different issues must be correctly and consistently treated. Consideration needs to be given in particular to the spatial and temporal scales over which the model should operate, and whether or not it needs to interface with other models of atmospheric dispersion which operate at different scales. The table below indicates the range of length scales of relevance:

<table>
<tr><th>Spatial scale (km)</th><th>10^0</th><th>10^1</th><th>10^2</th><th>10^3</th><th>10^4</th></tr>
<tr><td>Designation</td><td colspan="5">|------- local -------|
|---------- regional --------------|
|------------ national ---------------|
|----------------- continental -------------------|</td></tr>
<tr><td>environmental issue</td><td colspan="5">|-------- g.l.c. from primary emissions --------|
|-------- Secondary Particulates --------|
|------------------ Ozone ---------------|
|------------ Acidification/Eutrophication -------------|
|----------------------- Toxics -----------------------------|</td></tr>
</table>

An integrated modelling system is required to provide the capability to model across this range of length scales. It is important for an industry such as the Electricity Supply Industry that large point sources of emissions, such as power stations, are correctly represented within the model. The table below considers in a similar fashion the timescales of relevance to processes of concern to the JEP.

<table>
<tr><th>Time scale</th><th>seconds</th><th>minutes</th><th>hours</th><th>Days</th><th>months</th><th>years</th></tr>
<tr><td>Designation</td><td colspan="6">|------- rapid -------|
|----- short-term ---------|
|---- diurnal ----|
|---- episodic ---|
|- seasonal -|
|-- annual --|</td></tr>
<tr><td>issue</td><td colspan="6">|--------------- GLC from primary emissions -------------------- |
|----- Secondary Particulates -----|
|---------------------------------- Ozone ----------------------------------|
|------ Acid’n/Eutroph’n ------|
|----- Metals -----|</td></tr>
</table>

The shaded region indicates the range of timescales considered appropriate to be simulated in a single modelling framework. To play an effective part in current assessments, a model is potentially required, therefore, to simulate processes over length scales of 10km to 1000km, and time scales of days to years.

THE ADVANTAGES OF A 'ONE ATMOSPHERE' MODEL

In the past, the response of model developers to the challenge set by the wide range of spatial and time scales, and wide range of issues for which the models were to be used, was to segment the problem and to build models which aimed to simulate just one part of the whole problem. As a result of this simplification process, models developed separately for transboundary and National-scale modelling, for simulation of annual and short-term processes, and for the modelling of acid deposition and atmospheric photochemical processes, to take three examples.

The inevitable consequence of the development of these issues-specific models is, at best, the parameterisation of processes outside the scope of the models (and at worst the complete neglect of these processes), or attempts to couple together different models. Examples of this include the development of within-grid treatments of plume rise and deposition from large point sources, and linking of city-scale and transboundary models.

Many of these difficulties would be avoided by the use of a single, consistent, modelling framework capable of modelling a wide range of timescales, spatial scales and processes in a single model simulation – a 'one atmosphere' model. This would obviate the need to run different models to simulate different processes with all the attendant risks of inconsistencies in treatment.

Models of long-range transport have been used for many years in Europe to inform policy makers and to assist in identification of least-cost emission reduction legislation, but to date a 'one atmosphere' approach has not been used for this purpose in Europe.

SELECTION OF MODELS-3

The decision was made, following a detailed review of available models, that the US-EPA modelling framework Models-3 most closely met these requirements. The EPA refers to the integrated nature of the Models-3 system as a third generation "one atmosphere" model. The phrase is intended to imply that all relevant processes are calculated simultaneously in a single model run. Models-3 provides a nested grid capability, and it has a modular approach to the model science that enables alternative science treatments to be selected for a given process.

The Models-3 modular framework has been designed to allow software developments, or advances in the science modules, to be incorporated in as simple a manner as possible. There are three main "science" modelling components (the Emissions Modelling System, the Meteorological Modelling System, and the Community Multi-scale Air Quality System) and a number of management tools.

CMAQ is comprehensive in scope and allows the transport, chemical transformation and deposition of a wide range of chemical species to be studied over spatial scales ranging from local to regional or trans-national. Additionally, its temporal resolution is sufficient to allow episodic air quality events to be studied. For a comprehensive technical description of the model see US EPA [1].

BUILDING A VERSION OF MODELS-3 FOR THE U.K. AND EUROPE

A model has been built using a sequence of nested grids, from an outer 108km grid covering Western Europe, through a 36km grid covering the UK and part of Europe to a 12km grid covering England and Wales and a 4km grid covering an area of central U.K. A 21-layer vertical grid has been used for all four model horizontal grid resolutions. The model results described here were generated using meteorology and emissions for 1999.

Meteorological data for 1999 supplied by the UK Met. Office were used to generate the input data sets required by the meteorology preprocessor. Two distinct Met. Office datasets were used for this purpose, both of which cover limited geographical areas: Mesoscale High Resolution data covering the immediate vicinity of the UK and Northern Europe, and Regional High Resolution data for the outer 108km grid. Surface properties were derived by using a land use pre-processor which produces a gridded data set relating the surface properties to one of 11 categories.

Gridded hourly emission files for the pollutants were constructed using the SMOKE emissions modelling system [2]. For area sources, emissions are confined to the lowest vertical layer, whereas point sources may emit into higher layers. SMOKE converts annual emissions inventory data into a temporally resolved and speciated format suitable for input to Models-3. The gridded emissions for the higher resolution grids were obtained from the UK National Atmospheric Emissions Inventory [3]. For UK power stations, the actual stack height and exit parameters were used where possible. For other source types, data from power stations, CHP plant, and other industrial installations were used to derive representative stacks.

Models-3 provides a choice of chemical scheme. The model described here was constructed by selecting the RADM2 chemical scheme with coupling to aerosol modelling and cloud processes together with ‘vanilla’ science modules and parameterisations within Models-3; no attempt was made to improve the comparison with measurements by modifying the model.

Atmospheric particulates are represented in the model by three lognormal modes; two ‘fine’ modes (Aitken mode and accumulation mode) for PM2.5, and a coarse mode. The two fine modes are coupled dynamically.

Dry deposition processes in CMAQ are modelled using a dry deposition velocity. A spatially- and temporally-varying dry deposition velocity is calculated in the met pre-processor by employing a resistance analogy method to derive dry deposition velocities for 16 species in the RADM dry deposition module. Wet removal processes are modelled by representing the linkages between atmospheric aerosols and gases, cloud water, and rain.

MODEL VALIDATION

A number of validation studies have been performed using the Models-3 framework, at a range of spatial scales. Summaries are given here of the results of two studies: use of Models-3 to simulate short-term air quality episodes, and 12 month simulation using Models-3 to validate the Model performance for long-term air quality and acid deposition.

Short-term air quality episodes

A study was performed to assess the effectiveness of Models-3 in predicting Ozone levels within the British Isles. Ozone predictions from Models3 were compared to measurements taken from four monitoring sites for the year 1999. The results are

O_3 ppb	Mace Head	Bottesford	Wicken Fen	Yarner Wood
Mean (modelled)	37.5	28.7	29.0	35.4
Mean (measured)	38.2	25.3	22.9	30.9
NME	20%	41%	49%	36%
NMB (mod-obs)	-2%	15%	28%	12%
ME	7	10	6	10
R (Pearson)	0.29	0.67	0.67	0.41

It can be seen that there is a slight tendency (as given by the Normalised Mean Bias) for the model to over-predict when averaged over the entire year. This feature is less pronounced for Mace Head - a site that is less affected by anthropogenic emissions for much of the time. The over-prediction of the mean leads to errors for sensitive parameters such as AOT40. However the number of severe episodes (8 hour running mean > 60ppb) is well modelled and is suitable for EU assessment under EU regulation. It is thought that the over-prediction arises from a specific sub-process omission in the dry deposition module, rather that a more general model formulation issue.

Annual air quality and deposition

This assessment has been undertaken by 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.

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 results of the comparison of the model simulations at 12km resolution with measurements at 10 wet deposition monitoring sites in the U.K. are summarised in the table below:

	Correlation Coefficents	**Mean Annual Modelled/Measured**

	Rainfall	SO_4^{2-}	NO_3^-	NH_4^+	Rainfall	SO_4^{2-}	NO_3^-	NH_4^+
Barcombe Mills	0.62	0.62	0.39	0.47	0.69	0.69	1.03	1.64
Bannisdale	0.71	0.44	0.14	-0.01	0.83	0.58	0.65	0.75
Bottesford	0.82	0.74	0.70	0.72	1.41	0.92	1.05	1.11
Compton	0.85	0.78	0.82	0.78	1.07	0.65	0.81	0.83
Eskdalemuir	0.83	0.58	0.50	0.51	0.98	1.06	1.55	2.11
Flatford Mill	0.68	0.59	0.59	0.19	1.25	0.75	0.92	1.04
High Muffles	0.87	0.68	0.70	0.71	0.95	0.57	0.68	0.78
Preston	0.80	0.73	0.73	0.74	1.15	0.80	0.93	0.91
Tycanol Wood	0.57	0.61	0.61	0.31	1.15	0.63	1.12	1.76
Yarner Wood	0.78	0.61	0.72	0.62	1.10	0.85	1.13	1.84
ALL SITES	**0.77**	**0.59**	**0.46**	**0.27**	**1.01**	**0.72**	**0.99**	**1.17**

The agreement for wet S deposition is reasonable, but there is a tendency for the model to under predict. The annual deposition of oxidised N shows good agreement between modelled and measured values. The comparison for reduced N shows the greatest scatter in annual ratios; nevertheless for 9 of the 10 sites used the ratio lies within a factor of 2. The agreement for rainfall is very good. The methodology used, and full details of the results, are given in [4]

CONCLUSIONS

'One atmosphere' models such as Models-3 provide a suitable framework for integrating important processes over a range of spatial and temporal scales. The model 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.

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