CMAQ Development for UK National Modelling

Demonstration of CMAQ for Defra's Evidence Needs

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Executive summary

The Community Multi-Scale Air Quality model (CMAQ) is an open-source model developed by the USEPA able to produce outputs for a range of air pollutants and processes simultaneously for research and regulatory purposes.

The Department for Environment, Food and Rural Affairs (Defra) commissioned a review involving a collaboration of three of the groups in the UK using CMAQ for national scale policy the overall aim of which was to investigate and demonstrate how CMAQ might meet Defra's needs with respect to the national modelling and assessment of UK air quality policies and to develop a configuration optimised for those needs. The three groups participating in the project are King's College London (KCL), University of Hertfordshire (UH) and AEA, with further input from rdscientific (Professor Dick Derwent).

Defra uses various air quality models in order to help build the evidence about what contributes to poor air quality. Defra's main evidence needs are associated with the following policy drivers:

- Compliance with European Union Air Quality Directives
- Assessment of policy options including revision of the Air Quality Strategy
- Health protection impact assessments
- Ecosystems impact assessment
- Impacts of Climate Change and Climate Change Measures
- Negotiations for the new EU Directive

Several groups of modellers have used CMAQ to model air quality in the UK. This report focuses on the work of Objective 1 in the first phase of the project and considers how CMAQ might be used or, if necessary, developed to help meet Defra's evidence needs.

The report considers each of the evidence needs in turn and identifies the potential role to be played by CMAQ. It has identified that CMAQ has the potential to provide a consistent modelling environment to meet a wide range of Defra's modelling needs alone or in combination with other models. It is a deterministic model and can be used to predict conditions under different meteorology and emission scenarios. The report identifies the main limitations of CMAQ in the context of Defra's evidence needs. These are:

- Modelling uncertainty (a limitation for all models)
- Low spatial resolution for annual modelling at UK scale within acceptable timescales
- High computational requirements which limit the number of scenarios that can be modelled in a specified time

The report outlines the developments required to make the CMAQ model more useful for the purpose of meeting Defra's evidence needs. These should be considered in any implementation plan for CMAQ in Defra's suite of air quality modelling tools for policy purposes.

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Appendix 1 Description of CMAQ Decoupled Direct Method, Adjoint Model and Tagged Species Source Apportionment Method.

1 Introduction

The Department for Environment, Food and Rural Affairs (Defra) works with others at local, national and international levels to reduce air pollution. It uses various air quality models in order to help build the evidence about what contributes to poor air quality. Defra's main evidence needs are associated with the following policy drivers:

- Compliance with European Union Air Quality Directives
- Assessment of policy options including revision of the Air Quality Strategy
- Health protection impact assessments
- Ecosystems impact assessment
- Impacts of Climate Change and Climate Change Measures
- Negotiations for the new EU Directive

The United States Environmental Protection Authority (USEPA) sponsored the development of the Community Multi-scale Air Quality (CMAQ) modelling system. CMAQ was designed to approach air quality as a whole by including state-of-the-science capabilities for modelling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. Several groups of modellers have used CMAQ to model air quality in the UK. This report does not constitute a CMAQ evaluation, but considers how CMAQ might be used or, if necessary, developed to help meet Defra's evidence needs.

Section 2 of the report summarises how CMAQ has been implemented by various UK modelling groups. It describes two developments of the CMAQ model that have potential application in the UK: the Decoupled Direct Method (DDM) and the Adjoint Model. The technical details of these features are provided in an Appendix to this report. They are considered highly relevant to the possible use of CMAQ to meet the evidence needs described later in the report. Finally, Section 2 considers how other models might be nested within CMAQ to provide higher spatial resolution.

Sections 3-8 consider the application of CMAQ for each of the main policy drivers in turn. These sections describe in outline how the evidence needs are currently met and consider how CMAQ could be used as an alternative to or in concert with the current modelling approach. They consider the potential role of DDM, Adjoint Models and nesting in the context of each policy driver.

Section 9 takes account of the discussion in Sections 3-8 and identifies the key developments that have the potential to increase the utility of CMAQ within the context of Defra's evidence needs.

2 CMAQ Models

2.1 Introduction

This section summarises how CMAQ has been implemented by various UK modelling groups. It describes two developments of the CMAQ model that have potential application in the UK: the Decoupled Direct Method (DDM) and the Adjoint Model. Finally, it considers how other models might be nested within CMAQ to provide higher spatial resolution.

2.2 Current CMAQ facilities

The U.S. Environmental Protection Agency's Community Multiscale Air Quality (CMAQ) model is a three-dimensional Eulerian (i.e., gridded) atmospheric chemistry and transport modelling system that simulates ozone, acid deposition, visibility, and fine particulate matter throughout the troposphere.

Weather conditions provide the primary physical driving forces in the atmosphere (such as the changes in temperature, winds, cloud formation, and precipitation rates). The Weather Research and Forecasting (WRF) and the Mesoscale Model (MM5) can provide gridded meteorology for CMAQ air quality model simulations.

The meteorology inputs dictate the following CMAQ configuration parameters:

- Horizontal grid coordinate and projection
- Horizontal grid resolution
- Maximum spatial coverage
- Vertical grid extent (model top)
- Temporal extent (start/end date/time, time step length)

Several groups within the UK have developed the capability to run CMAQ, including the following groups that took part in phase 1 of the intercomparison exercise:

- AEA Technology
- E.ON Engineering Limited
- RWE npower Technology Services
- University of Hertfordshire
- ERG- King's College London

Table 2.1 provides a brief outline summary of the information provided about CMAQ implementation by the user groups for Phase 1 of the Defra Model Intercomparison Exercise (MIE). The implementation by different user groups is broadly similar. More detailed analysis of the model implementation by different groups is reported separately in a project report which aims to identify best practice and a preferred configuration for Defra policy applications[1].

Model run times depend on how the model is set up (number of grid nodes, reaction schemes etc.) and on the computational resources available. The MIE Phase 2 involved running CMAQ with different emission scenarios. Run times for an annual simulation covering the European and UK grids are estimated to be around 10 and 20 days respectively, with an estimated elapsed time of 4 weeks - this accounted for data preparation, archiving, basic model analysis, but not running WRF (the Weather Research

[1] Beevers S, Kitwiroon N, Beddows A, Carslaw, D, Good N, Chemel C, Xavier Francis, Sokhi R, Derwent D, Fraser A, Murrells T, and Venfield H. (2012). CMAQ Development for UK National Modelling - Development of a provisional CMAQ-UK Configuration. Version: 23rd October 2012

Forecasting model). This can be reduced by running the model as a series of months simultaneously. Scenarios can be run simultaneously if the computing resource is available.

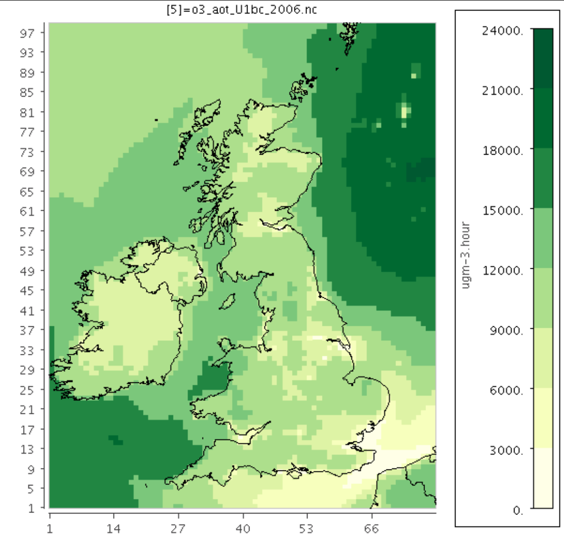
Table 2.1: Summary of information supplied by CMAQ user groups to the Defra Model Intercomparison Exercise Phase 1 (MIE1)

	AEA	E.On/ RWE npower	University of Hertfordshire	ERG-Kings College
CMAQ Version	4.7or 4.6	4.7.1	4.7 or 4.6	4.7 or 4.6
Horizontal grid resolution	Europe 50 km UK 10 km	45 km 78 x 73 15 km 96 x 75 5 km 195x130	45 km 76 x 76 15 km 93 x 108 5 km 177x219 (Deposition) 18 km 260 x 240 (regional)	a) Europe 81 km b) UK & Ireland 27 km c) Great Britain 9 km d) South East England 3 km e) London 1 km
Vertical grid	17-26 layers depending on application	15 layers	15-34 layers depending on application	23 layers
Chemistry scheme	CB05 + extensions for Cl, aqueous and aerosol chemistry	CB05	CB-IV, CB05	Various
Dry deposition	Pleim-Xiu scheme	Pleim-Xiu scheme	Resistance analogue	Resistance analogue
Wet deposition	Derived from RADM	Sub grid and resolved cloud model with scavenging and washout	Derived from RADM	Derived from RADM
Emissions	a)Europe EMEP b) UK NAEI c) Biogenic Potential Inventory	a) Europe EMEP b) UK NAEI c)GEIA Biogenic Inventory d) JEP power stations	a) Europe EMEP b) UK NAEI c) TNO	a) Europe EMEP b) UK NAEI c) LAEI
Meteorology	WRF 3.0 using initial and boundary conditions from ECWMF	WRF 3.0.1	WRF 3.2.1 using analysis nudging and initial and boundary conditions from ECWMF	WRF 3.1 with NCEP initial and boundary conditions

Figures 2.1-2.3 show some examples of the outputs that can be obtained from CMAQ. The outputs were obtained using AEA's implementation for 2006.

Figure 2.1: Examples of ozone AOT40 and annual mean nitrogen dioxide for 2006.

AOT40 for ozone, 2006, µgm^{-3}.hour



Annual mean background nitrogen dioxide concentration, 2006, µgm^{-3}

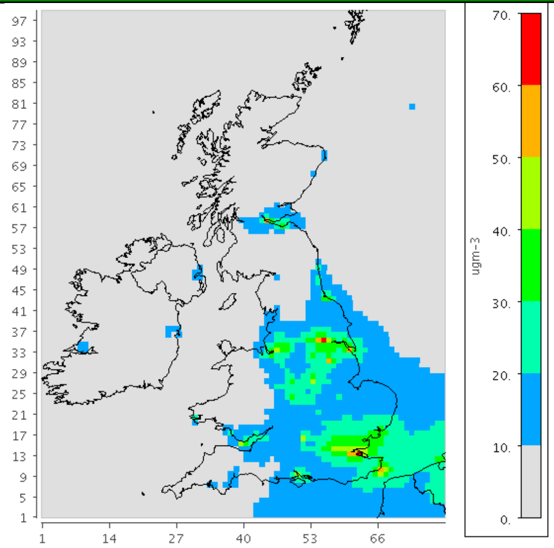
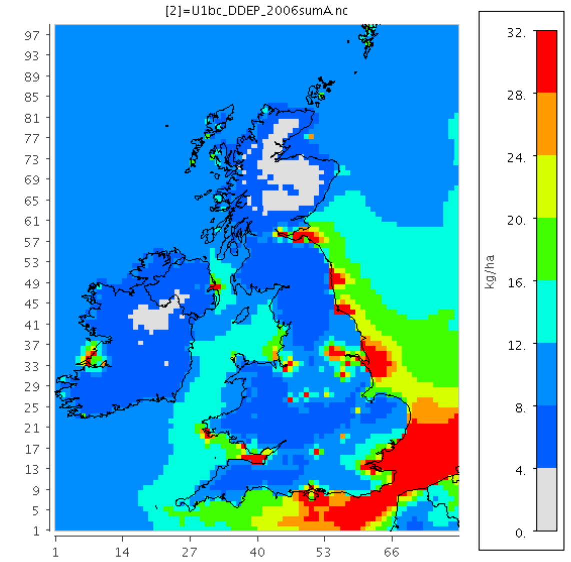


Figure 2.2: Examples of annual wet and dry deposition of SO_2+SO_4 for 2006.

Annual dry (surface) deposition of SO_2+SO_4, 2006



Annual wet deposition of SO_2+SO_4, 2006

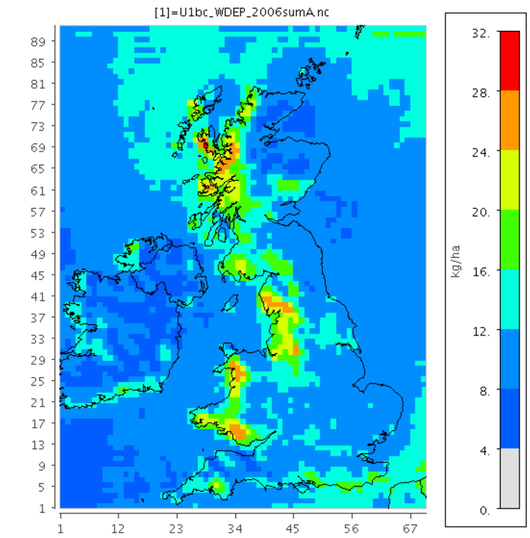
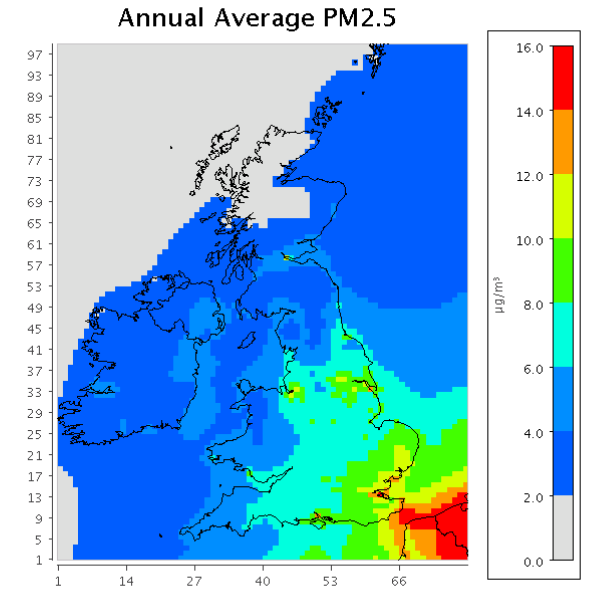
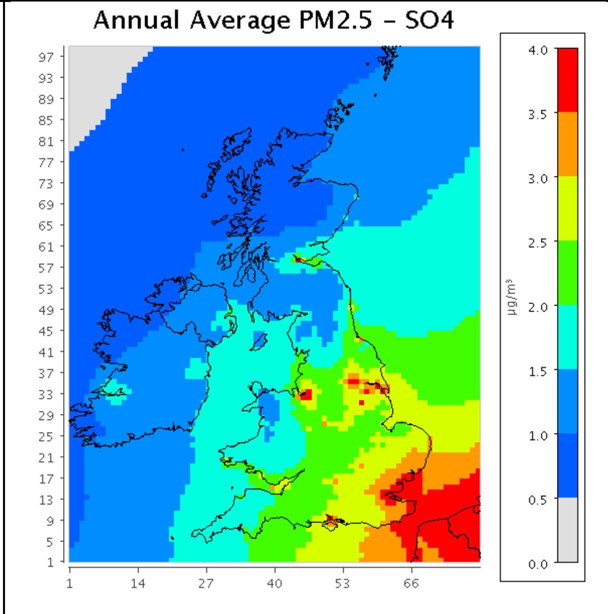


Figure 2.3: Examples of annual mean $PM_{2.5}$ and inorganic components for 2006.

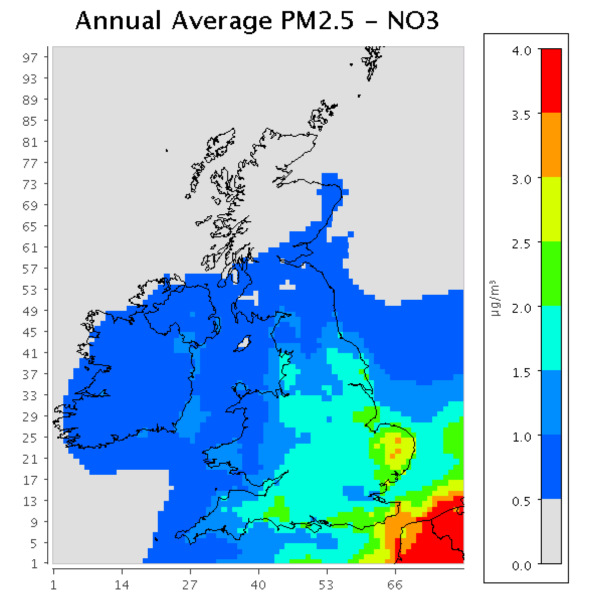
Annual mean $PM_{2.5}$, 2006



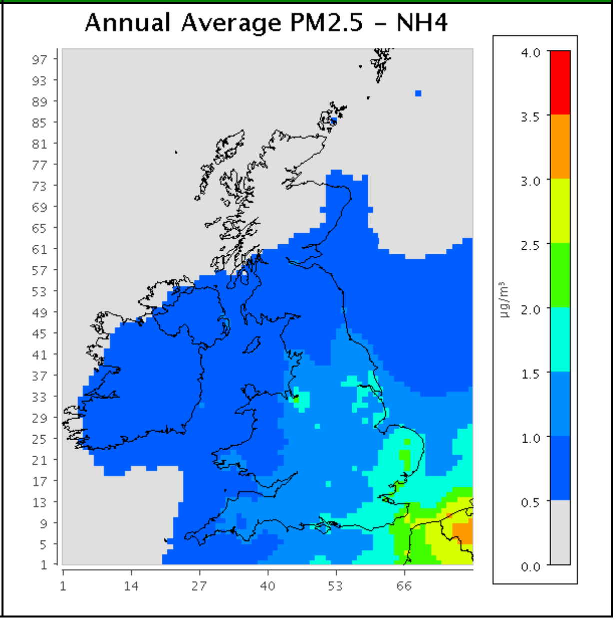
Annual mean Sulphate $PM_{2.5}$, 2006



Annual mean Nitrate $PM_{2.5}$, 2006



Annual mean Ammonium $PM_{2.5}$, 2006



2.3 CMAQ Decoupled Direct Method

CMAQ predicts concentrations at each node of the Eulerian grid at specified time intervals (usually hourly) for a specific set of input parameters-for example, specific emissions or boundary conditions. It is useful for policy development to be able to investigate how concentrations will change if the input parameters, particularly emissions, change. One way to investigate the change is to rerun the model with revised emissions and compare the output concentrations. However, this “brute force” approach requires the model to be rerun for every perturbation of the input parameters and it may not be possible to carry out the required number of model runs in a reasonable time with the available computing resources. The CMAQ Decoupled Direct Method allows the user to determine the sensitivity of the model outputs to the model input parameters. It is thus possible to investigate multiple scenarios within one model run.

The Appendix provides an outline description of the CMAQ Decoupled Direct Method.

The decoupled direct method takes account of perturbations in initial values, boundary conditions and emissions. Hakami et al [2] showed how the approach can be extended to take account of perturbations to reaction rate coefficients. The implementation of DDM in CMAQ 4.7 allows the user to calculate the sensitivity coefficients for emissions, initial conditions, boundary conditions and reaction rates. There are several options available to the user. The user can:

- specify first or second order sensitivity coefficients (second order only for gases)
- investigate the sensitivity of concentrations to an additional emission source from a specified grid cell or from a region. CMAQ 4.7 DDM-3D allows the user to specify a diurnal profile for these emissions
- investigate a fractional change in emissions from a particular category e.g. mobile sources, point sources
- limit the changes in the input parameters to a particular region
- limit the changes in parameters to a period between specified dates
- limit the changes in parameters to part of the day

CMAQ 4.7 DDM-3D calculates the sensitivity coefficients in parallel with the base case model run. The additional calculations require additional computational effort: the additional effort depends on, for example, the number of parameters and on the detailed model set-up. We are uncertain how much the implementation of DDM-3D will slow down the base case model run. Discussion with users at the 2011 CMAQ Conference indicated that operation with 20 parameters increases the base run time by a factor of 2 and that operation with 100 parameters was feasible.

2.4 CMAQ adjoint model

DDM computes the sensitivities of all model outputs throughout the domain to specified model inputs and parameters. Thus, the method is well-suited for characterizing how concentrations everywhere are impacted by a limited number of changes in emissions or other parameters of interest. However, for some applications, the user may want to know how specific model outputs are influenced by numerous model parameters. You might want to know how average pollutant concentrations at a single monitor or group of monitors are influenced by many model parameters, or by numerous emitters (say, to calculate the average exposure index for $PM_{2.5}$). As the number of emitters or input parameters of interest grows, it would quickly become cumbersome to compute forward sensitivities to each parameter. The CMAQ adjoint model provides an efficient method for calculating sensitivity of a few model outputs to numerous model input parameters.

The Appendix provides an outline description of the CMAQ adjoint model.

The CMAQ adjoint model is currently under development and has not been included in the definitive versions of CMAQ. We are not aware of any applications in the UK. A version (CMAQ_ADJ v 4.5.4) is available from the developers' website[3]: more recent versions can be obtained from the developers. CMAQ_ADJ v 4.5.4 is set up to determine the sensitivity of the concentrations at a receptor at the end of the simulation to earlier concentrations at grid nodes ("grid species concentrations") and to emissions. Hakami et al has shown how the adjoint variables can be used to determine the sensitivities for other parameters (e.g. temperature).

Figure 2.4 shows some sample output from CMAQ_ADJ v4.5.4 showing how the sensitivity of the ozone concentrations at a ground level receptor in the middle of the plot at time T is

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[2] Hakami A et.al. 2007. The Adjoint of CMAQ, Environ. Sci. Technol., 41, 7807
[3] http://people.cs.vt.edu/~asandu/Software/CMAQ_ADJ/CMAQ_ADJ.html

affected by the ground level concentrations of nitrogen dioxide at other locations in the area 6, 12 and 18 hours beforehand.

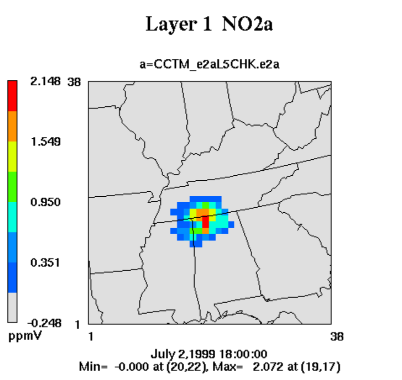
Figure 2.5 shows how the ozone concentration at a ground level receptor in the middle of the plot at time T is affected by the ground level emissions of nitrogen dioxide at other locations throughout the preceding 47 hours.

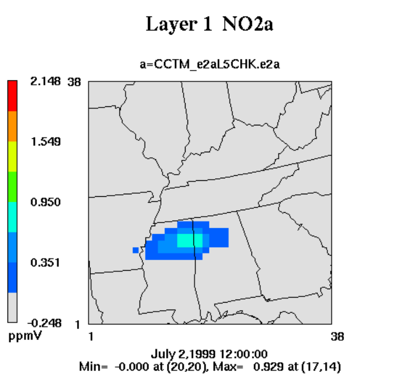
CMAQ_ADJ v 4.5.4 is set up to carry out simulations of 24 hours, although multi-day simulations are possible with some adjustments. In practice, the forward model would be run for each day followed by the adjoint model.

Adjoint models can also be used in conjunction with numerical optimisation programs to adjust model parameters (e.g. initial conditions) to provide the best fit with measured concentrations. Data assimilation allows the optimal combination of three sources of information: an a priori (background) estimate of the state of the atmosphere, knowledge about the physical and chemical processes that govern the evolution of pollutant fields as captured in the chemistry transport model, and observations of some of the state variables. CMAQ_ADJ v 4.5.4 provides data assimilation routines.

Figure 2.4: Sensitivity plots for dO_3/dNO_2 backwards in time every 6hrs.

T- 6 hours	T-12 hours	T -18 hours





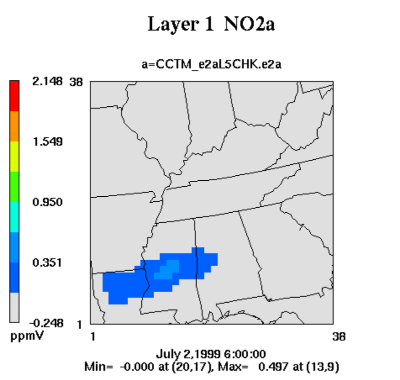
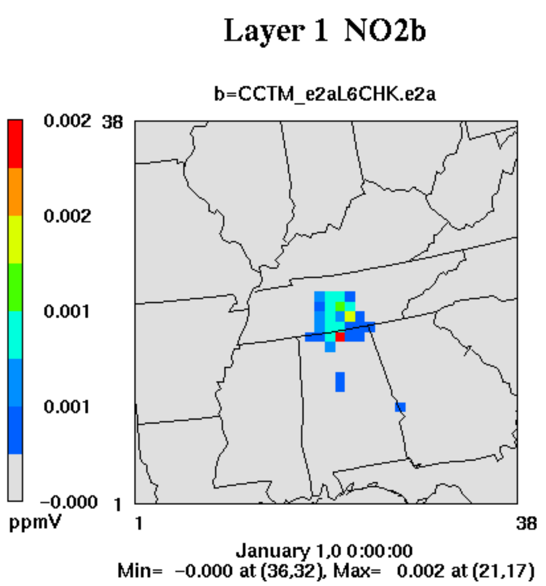


Figure 2.5: Sensitivity plots for dO_3/dNO_2 emissions at constant rate over the previous 47 hours.



2.5 CMAQ –Tagged Species Source Apportionment

The "Tagged Species Source Apportionment (TSSA)" method is a method for tracking transport and nonlinear chemical conversions of both primary and secondary products from the selected emissions sources such as sulphate (SO_4^{-2}), nitrate (NO_3^-), ammonium (NH_4^+), elemental carbon (EC), secondary organic aerosol (SOA), as well as other aerosol species. All of this can be archived from a single model run to provide PM source apportionment at any location in the UK. The TSSA in CMAQ v5 is under development at the USEPA.

TSSA algorithms

The TSSA algorithm last appeared in CMAQ v4.5 and was developed at the University of California[4] . The TSSA employs tracer, or "tagged species" to quantify the transport and transformation of emissions from selected sources and regions. Using TSSA within a CMAQ model run produces a 3-D concentration field showing the primary and secondary concentrations from a selection of single or grouped emissions categories/regions, determined by the user. Examples include road transport/Germany or large power stations/France.

The TSSA algorithm is inserted into each CMAQ processes, including emissions, advection, diffusion, chemistry, deposition, cloud and aerosol physics and chemistry conserving mass throughout the model run [5].

2.6 Nesting of dispersion models within CMAQ

The CMAQ model has relatively low spatial resolution. Grid square sizes are typically 10 km for grids covering the whole of the UK and 1 km for limited urban areas (e.g. London). There are often steep spatial gradients in concentrations of pollutants in urban areas especially near roads. The CMAQ model is not able to predict concentrations at the high spatial resolution required. On the other hand, dispersion models such as ADMS and AERMOD are capable of modelling at high spatial resolution, but are unsuitable for modelling transport and chemical reactions over long distances. Ching[6] in the USA and ERG[7] and CERC[8] in the UK have investigated the use of dispersion models nested within CMAQ.

There are four main hurdles to the implementation of nested dispersion models:

1. Dispersion models such as ADMS and AERMOD use hourly meteorological data and assume that emissions and meteorological conditions remain constant throughout the whole time that the pollutants travel from source to receptor. This is satisfactory if the meteorological conditions change only slowly but leads to errors at distant receptors if the meteorological conditions change. Strictly, this limits the size of the CMAQ grid squares for nesting to a few kilometres. The restriction is less important where the nested dispersion model is only required to predict long-term concentrations (e.g. annual mean) because the errors introduced are expected to average out over the year.

2. The CMAQ model provides a single concentration over each grid square. There will therefore be step changes in the concentrations predicted by the combined model at

[4] Wang, Z. S., Chien, C-J. and Tonnesen, G. S. 2009. Development of a tagged species source apportionment algorithm to characterize three-dimensional transport and transformation of precursors and secondary pollutants. Journal of Geophysical Research, 114, D21206, doi:10.1029/2008JD010846.

[5] Byun, D. W. and Ching, J. K. S. 1999. *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System*. EPA/600/R-99/030. United States Environmental Protection Agency.

[6] http://www.cmascenter.org/conference/2006/ppt/session6/ching.ppt

[7] http://uk-air.defra.gov.uk/reports/cat20/1105091516_UrbanFinal.pdf

[8] http://www.harmo.org/Conferences/Proceedings/_Kos/publishedSections/PPT/H14-263-PR.pdf

the boundaries. The step change may be considered to be trivial in many cases but may produce distinguishable effects when the modelling results are presented as maps. Spatial interpolation of the CMAQ fields may improve the appearance of the maps.

3. There is an issue of double counting of the contribution of sources to pollutant concentrations from CMAQ and the dispersion model. This may not be important where the CMAQ component is small compared to the dispersion model component (e.g. near roads). CERC have addressed this problem and suggest that the total concentration is calculated as the sum of the CMAQ contribution and the dispersion model contribution **less** the dispersion model contribution associated with the emissions distributed uniformly over the square. An alternative approach would be to calculate a flux-weighted average concentration on the upwind face(s) of the grid from the CMAQ outputs.

4. Large point sources can make a small contribution to ground level concentrations over a wide area potentially extending 50 km or more from the source. Nesting a dispersion model of a point source within a CMAQ grid requires care to ensure there is no double counting of emissions and that the step change at the boundary is minimised. Similar step changes were observed in the CREMO project when large point sources were modelled using ADMS model nested within AEA's TRACK model. Particular problems may arise where a point source is close to the edge of a CMAQ grid square. The step change may be considered to be trivial in many cases but may produce distinguishable effects when the modelling results are presented as maps. This problem may be overcome to some extent using the Plume in Grid model within earlier versions of CMAQ rather than ADMS. Plume in Grid was limited to larger grid sizes (larger than approximately 12 km) and was not widely used: it is not supported in the current version of CMAQ (4.7.1) but a new version of Plume in Grid is currently under development and is expected to be incorporated in CMAQ in 2012.

2.6.1 Example of Nested Dispersion Modelling in London

Nesting street scale ADMS dispersion models within CMAQ has already been undertaken in London by King's College and CERC. CMAQ-Urban as described in Beevers et al.[9] has been submitted to DEFRA's model intercomparison exercise[10]. The CMAQ-Urban model is a one-way coupling of CMAQ and ADMS which deterministically predicts hourly grid resolved concentrations at 20m x 20m, for NO_X, NO_2, O_3, PM_{10} and $PM_{2.5}$. Within CMAQ-urban the ADMS roads model (v2.3)[11] has been used to describe the near field dispersion from roadways, using the hourly meteorological inputs: wind speed and direction, temperature, surface sensible heat flux and planetary boundary layer height, predicted from the WRF model. The ADMS model was run for each hour of the year using similar methods to those described in Kelly et al.[12], to produce hourly concentration fields or model kernels. Each kernel represents the concentration of a primary pollutant (with no chemistry applied) across a regular grid as it dilutes away from a road source of unit emissions. The concentrations across each kernel were predicted at 5m intervals and within 225m of each source, using a constant road emissions rate of 1 g km^{-1} s^{-1}. Road geography is highly important and so the emissions from roads in London were represented using the centreline of each carriageway divided into 10m sections. The 10m granularity of the road sources was considered to be

[9] Beevers SD , Kitwiroon N, Williams ML, Carslaw DC. 2012b. One way coupling of CMAQ and a road source dispersion model for fine scale air pollution predictions. Atmopheric Environment (in press).

[10] http://uk-air.defra.gov.uk/library/reports?report_id=654

[11] CERC, 2006, *AMDS-Roads An Air Quality Management System User Guide*. Cambridge Environmental Research Consultants Lid., Cambridge

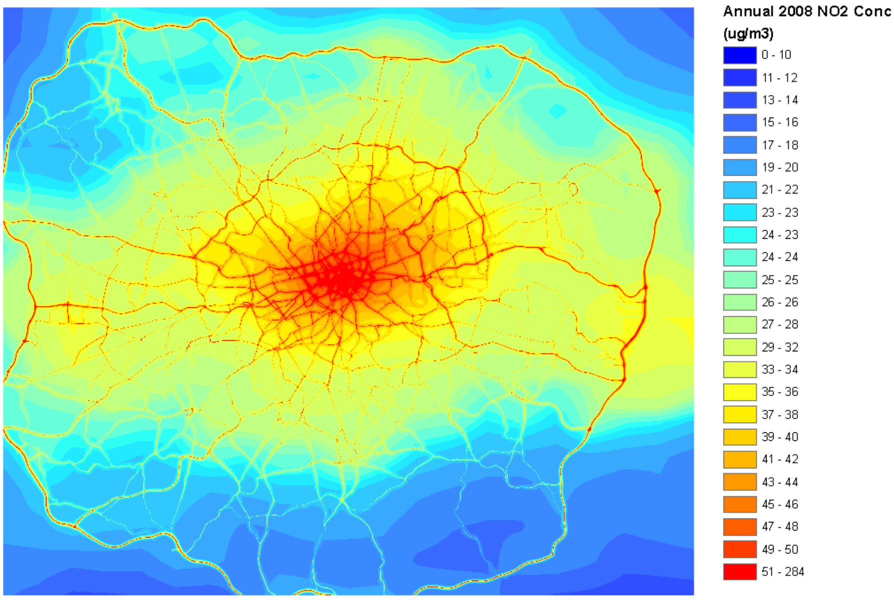
[12] Kelly FJ, Anderson HR, Armstrong B, Atkinson RW, Barratt B, Beevers SD, Mudway IS, Green D, Derwent RG, Tonne C, Wilkinson P. 2011. The impact of the Congestion Charging Scheme on air quality in London. Health Effects Institute http://pubs.healtheffects.org/view.php?id=358

representative of complex road curves but also the distance between carriageways on larger roads such as motorways. Six road categories (and associated kernels) were used in London, including open roads (motorway), typical roads (average urban roads surrounded by low rise buildings) and 4 types of street canyon (classified by their orientation: north-south, east-west, southwest-northeast and southeast-northwest). The "typical roads" had a road width of 20m and a building height of 10m and "street canyons" had a width of 30m and a building height of 25m. The "street canyon" width and height details were manually sampled from the 3D building model in London. Once created, each kernel was applied to the 1746 major road emissions estimates in the LAEI consisting of ~340,000 10m road sources, and the hourly concentration of NO and primary exhaust NO_2 combined onto a fixed grid of 20m x 20m in London.

The near road chemistry was simulated using a simple chemical scheme described in Carslaw and Beevers[13]. The reaction rates and photo-dissociation rates were taken from the photolysis rate pre-processor (JPROC)[14], part of the CMAQ run, and the time of flight from road sources, estimated each hour, as a concentration weighted average at each receptor location, assuming a straight line between source and receptor and using WRF wind speed at 10m height.

A sample plot of annual 2008 NO_2 concentrations simulated from CMAQ-Urban is shown in Figure 2.6. The annual 2006 and 2008 NO_X, NO_2 and O_3 simulations were assessed against the over 100 monitoring sites across London and good agreement was observed at roadside, urban background and suburban locations. Current computer run times suggest that it is feasible to operate CMAQ-Urban over urban areas at UK national scale.

Figure 2.6: Annual 2008 mean NO_2 concentrations for London ($\mu g\ m^{-3}$)



[13] Carslaw, D.C. and S.D.Beevers. 2005: Estimations of road vehicle primary NO_2 exhaust emission fractions using monitoring data in London, Atmospheric Environment, 39, 167-177.
[14] Roselle., S.J., Schere, K.L. and Pleim, J.E. 1999. Chapter 14: Photolysis rates for CMAQ, In: Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA/600/R-99/030

3 Policy Driver 1: Compliance with Directives

3.1 Introduction

The Air Quality Directive (2008/50/EC) requires Member States to assess the ambient air quality with respect to assessment thresholds and limit values (and target values) for sulphur dioxide, nitrogen dioxide and oxides of nitrogen, particulate matter (PM_{10} and $PM_{2,5}$), lead, benzene and carbon monoxide. The Directive also requires Member States to assess the concentration of ozone with respect to target values and long-term objectives set out in the Directive. Similarly, the Fourth Daughter Directive (2004/107/EC) requires the assessment of the concentrations of arsenic, cadmium, mercury, nickel and polycyclic aromatic hydrocarbons with respect to assessment thresholds and target values. The Directives allow Member States to carry out the assessment using a combination of fixed measurements and modelling. The modelling provides information on the spatial distribution of air quality.

Currently, compliance with the Directives is assessed primarily by the Defra funded project AQ0634, *UK Ambient Air Quality Assessments* (UKAAQA). The three main directive reporting tasks within this project and their associated evidence needs are:

- Annual compliance assessment
- Air quality plan development
- Hot spot modelling

The potential application of CMAQ to these tasks is considered below.

The Air Quality Directive also requires Member States to inform members of the public with forecasts of the air quality for the following afternoon/day(s). The forecast should provide information on the geographical area of expected exceedances of information and/or alert thresholds, and expected changes in pollution (improvement, stabilisation or deterioration), together with the reasons for those changes. The UK currently uses a number of methods to obtain this information, including CMAQ modelling. The provision of air quality forecasts is outside the scope of this report.

3.2 Annual compliance assessment

3.2.1 The evidence needs

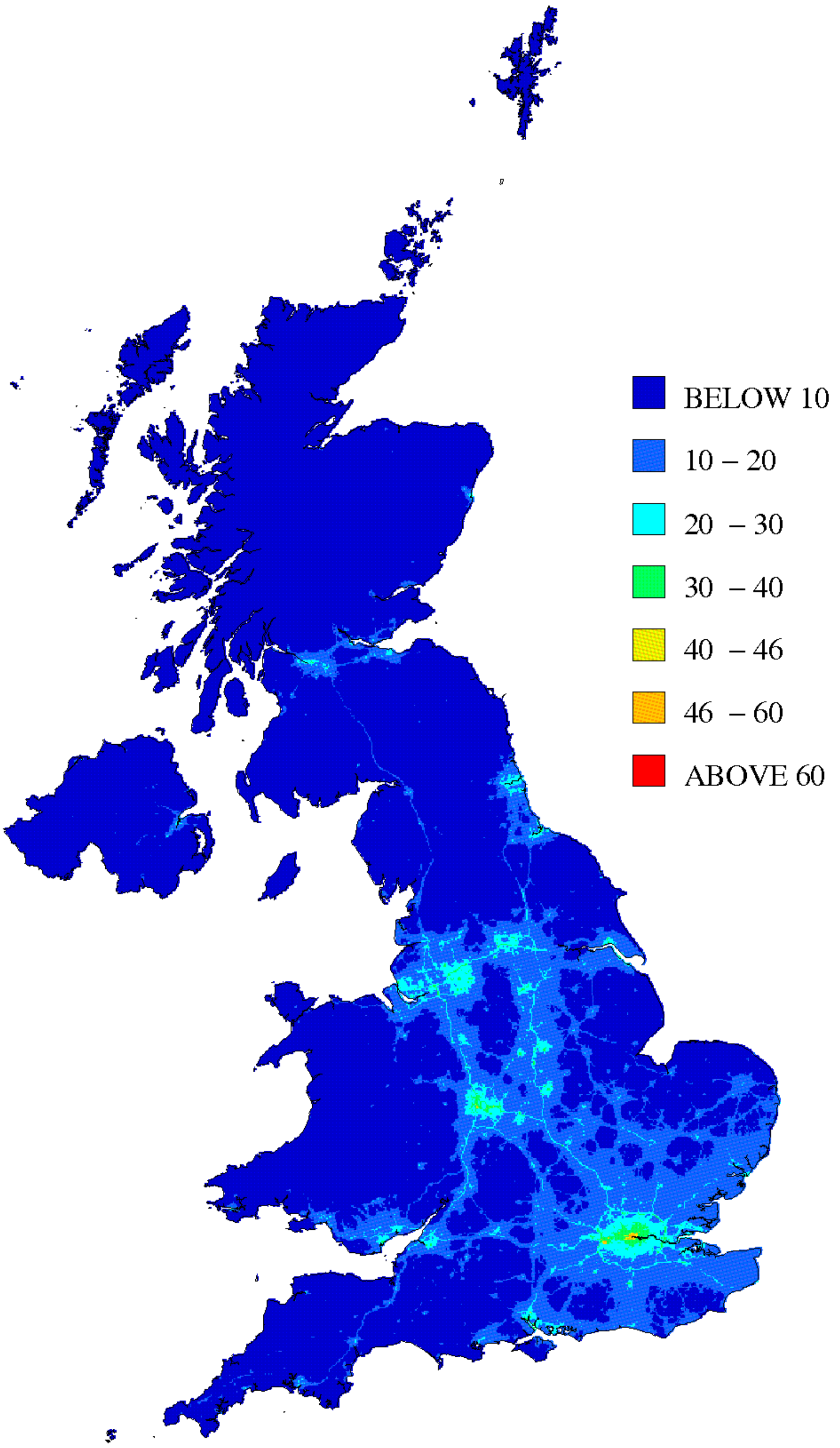
Defra's key evidence need here is to generate supplementary information which can be used in directive reporting. This equates to a need for modelled maps that meet the following requirements:

- Maps for NO_X, NO_2, PM_{10}, $PM_{2.5}$, SO_2, CO, benzene, O_3, Pb, As, Cd, Ni and benzo(a)pyrene (B[a]p) for various annual metrics defined in Directives 2008/50/EC and 2004/107/EC.
- These maps must be able to represent different types of monitoring sites defined in the directives (i.e. rural background, suburban background, urban industrial, urban background and urban traffic) in order to meet the requirements for use as supplementary information.
- Adequate resolution (currently 1x1km background concentrations, with roadside locations also mapped separately)

- These maps must exclude locations for which monitoring is not required by the directives (e.g. junctions)
- Natural sources to be included in the assessment where relevant and calculation of a natural sources layer, which can be subsequently deducted from total levels for reporting
- A deadline of mid-July of the subsequent calendar year in order to provide input in time for the deadline for submission of the completed air quality assessment in September.

Currently, the Pollution Climate Mapping (PCM) model is used to meet this evidence need for Defra. The basis of the model is the calculation of ‘background’ concentrations across the UK on a 1 km x 1 km grid using measured data (or in some instances model results) to derive the regional background, with near sources (those within about 15 km) modelled as area sources using a kernel approach based on ADMS 4, and large point sources modelled explicitly using ADMS 4. Roadside concentrations are based on an empirical approach with concentrations defined for an effective distance of 4 m from the kerb. The model produces annual mean concentrations, relying on empirical relationships to derive shorter-period concentrations for most pollutants except sulphur dioxide. Figure 3.1 shows an example of the maps produced using the PCM model; it shows the annual average background nitrogen dioxide concentration for 2008.

Figure 3.1: Annual mean background nitrogen dioxide concentration, 2008, μgm^{-3}



3.2.2 Outline assessment of CMAQ's suitability for this role

CMAQ is able to calculate the concentrations of each of the pollutants specified in the Directives. Most of the CMAQ implementations in the UK only consider NO_X, NO_2, PM_{10}, $PM_{2.5}$, SO_2, CO, benzene and ozone. However lead, arsenic, cadmium and nickel can be modelled as inert tracers. Benzo(a)pyrene is semi-volatile and is present in both the gaseous and particulate phases: a version of CMAQ has been developed in Germany to take account of the different rates of deposition from the gaseous and particulate phases. Mercury (not currently modelled by PCM) is also present in the atmosphere as elemental mercury, inorganic mercury compounds and organic mercury: CMAQ has been used extensively in the US to model the transport of mercury.

The output from CMAQ provides hourly concentrations at gridded receptors. All the metrics specified in the Air Quality Directives can be calculated from the hourly concentrations at each receptor.

The output from CMAQ provides concentrations on a regular grid. The gridded output is suitable for representation in a Geographical Information System (GIS). It is possible to apply a mask to exclude results using GIS capabilities in order to distinguish between urban, suburban and rural areas.

Current UK implementations of CMAQ typically employ a 9 or 10 km resolution horizontal grid to cover the UK with higher resolution grids (up to 1 km resolution) covering specific areas within the UK (e.g. London). Annual model runs for the UK at 10 km resolution typically take 20 days depending on the computing resources available. It is thus not likely that it will be feasible to carry out complete CMAQ modelling at 1 km resolution over the whole of the UK.

The PCM model currently uses a kernel approach for modelling area sources at 1 km resolution. It uses kernels based on meteorological data from a single weather station (Waddington). It may be feasible to derive similar kernels at 1 km resolution using CMAQ rather than ADMS at a few locations throughout the UK. This would allow modelling of the 1 km resolution area emissions with some loss of resolution in the meteorological field.

The PCM model currently uses a semi-empirical model to estimate the contribution from road traffic at receptors close to roads. CMAQ is currently not set up in the UK to model concentrations close to roads (e.g. at 10m) and it is not likely that it will be in the near future.

Examples of the NO_2 air quality plans submitted in September 2011 illustrate the zone level compliance assessment for the West Midlands Urban Area for background locations (Figure 3.2) and traffic locations (Figure 3.3).

Figure 3.2. Map of modelled background annual mean NO_2 concentrations 2008. Modelled exceedances of the annual limit value are shown in orange and red.

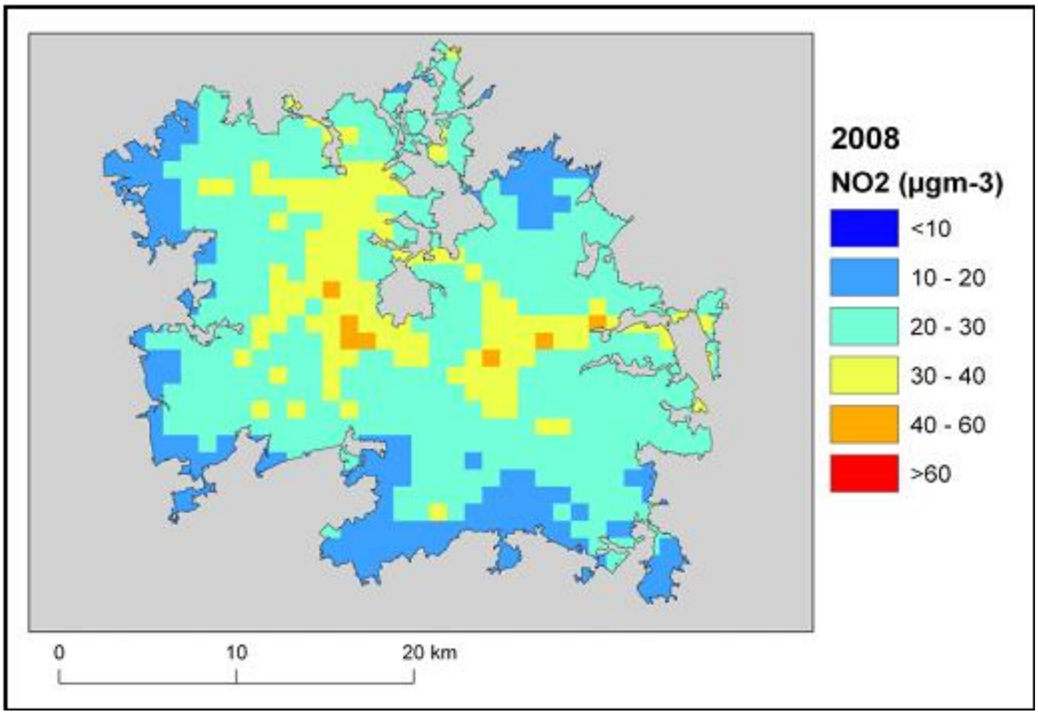
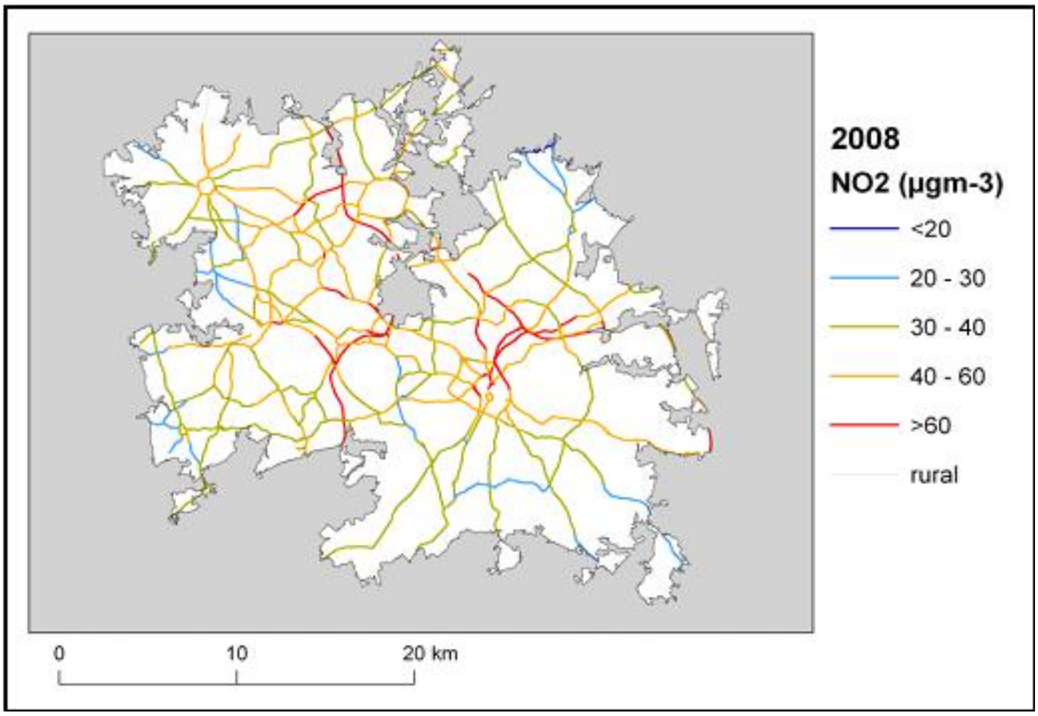


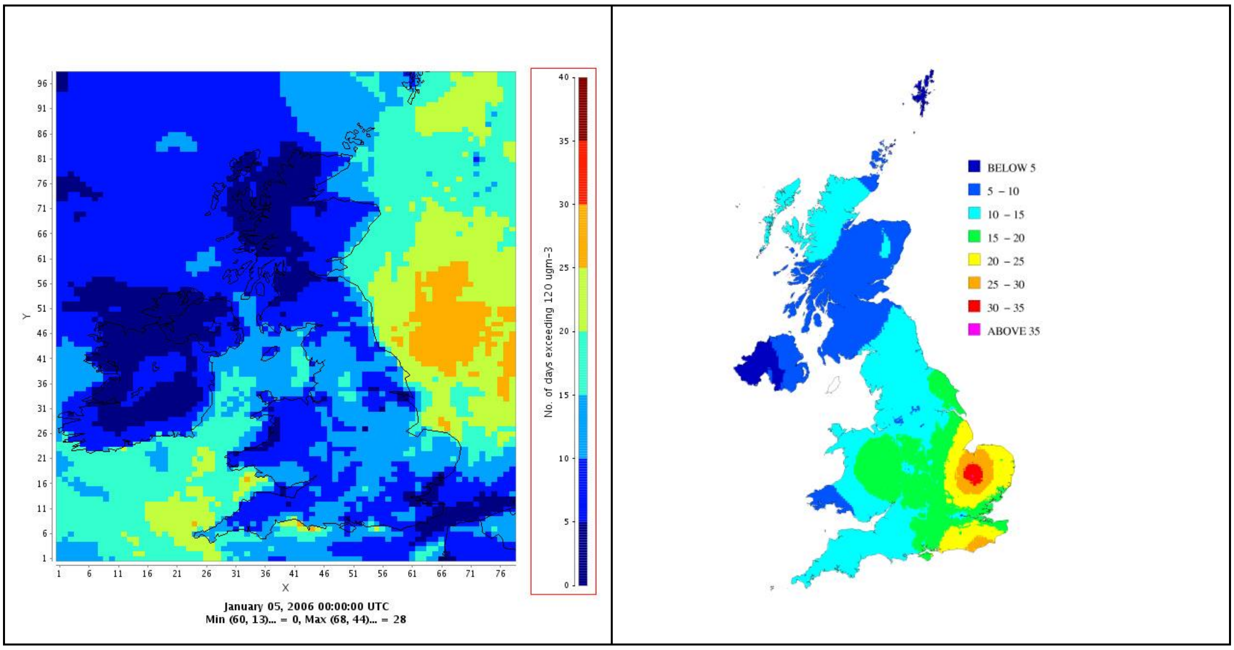
Figure 3.3. Map of modelled roadside annual mean NO_2 concentrations 2008. Modelled exceedances of the annual limit value are shown in orange and red.



CMAQ models implemented in the UK generally include the uptake and transport of seasalt but have not taken into account resuspended dust from natural sources. Jimenez-Guerrero et al have coupled CMAQ with a resuspended dust model in order to model the transport of dusts from the Sahara desert.[15] Further development of the UK CMAQ models would be required in order to allow the contribution from natural sources to be deducted from total levels for reporting of anthropogenic particulate matter concentrations.

The PCM model currently uses measured data to provide regional background concentrations. CMAQ could be used to provide the regional background concentrations for many pollutants. However, it is not obvious that there would be any advantage in replacing measured regional background concentrations with modelled concentrations for annual compliance assessment. Currently, measured concentrations are considered to be a more reliable basis for estimating regional background concentrations for compliance assessment than models. For example, measurements are used to estimate regional ozone concentrations rather than the Ozone Source Receptor Model (OSRM)[16], a model which is used primarily for emission scenario modelling in support of Defra national policies. Defra's recent model intercomparison did not show that CMAQ as implemented by UK modellers performed significantly better overall than other models. There can be substantial differences between modelled and measurement-based approaches: this is demonstrated in Figure 3.4 which shows the number of days exceeding 120 µg m^{-3} for ozone predicted by CMAQ and interpolated from the measurements. In this case the measurements of ozone at a few rural monitoring sites have an influence on the spatial distribution, e.g. the monitoring site at Wicken Fen in East Anglia. The use of models such as CMAQ has the potential benefit of improved spatial resolution over the interpolated background but may introduce modelling errors where there is a discrepancy between the modelled and measured concentrations. Data assimilation techniques, for example 4D Var approaches using the CMAQ adjoint model, may prove useful in the future in minimising the differences between the modelled and measured concentrations at the monitoring sites.

Figure 3.4: Number of days exceeding 120 µgm^{-3} for ozone in 2006 modelled by CMAQ and PCM



[15] Pedro Jimenez-Guerrero, Carlos Perez, Oriol Jorba and Jose M. Baldasano: Contribution of Saharan dust in an integrated air quality system andits on-line assessment. Geophysical Research Letters, Vol. 35, L03814, Doi:10.1029/2007gl031580, 2008

[16] http://uk-air.defra.gov.uk/reports/cat05/1003151144_ED48749_Final_Report_tropospheric_ozone_AQ0704.pdf

3.2.3 Assessment of potential for preparing annual mean maps

Most of the limit values, target values and assessment thresholds in the Directives are specified as annual means. PCM models the annual means for most pollutants and thus enables direct comparison for compliance assessment against annual mean objectives. The main obstacle to using CMAQ for this application is its relatively low spatial resolution. CMAQ could be used to provide improved spatial resolution of annual mean rural background concentrations, which are currently estimated by interpolation from measurement data. However, the rural background concentrations are generally only a small part of the total concentrations so that the potential improvement in model performance is likely to be small. The potential for improvement is offset because use of modelled rather than measured background concentrations would introduce modelling errors. CMAQ may be able to derive area source kernels to replace those currently derived using ADMS: this would allow CMAQ to provide similar spatial resolution for area sources as the PCM. However, a dispersion model such as ADMS or AERMOD would still be required to model concentrations near to large point sources. The need to avoid double counting of the large point source contributions requires further consideration.

3.2.4 Assessment of potential for preparing maps for ozone metrics

The Directives specify various short-term metrics for other pollutants. For ozone, the target values and long term objectives are expressed in terms of the maximum daily 8-hour mean for the protection of human health and the AOT40[17] metric for the protection of vegetation. Compliance assessment is currently based on measurements of ozone concentrations at rural background sites. Ozone concentrations are generally lower in urban areas because of its reaction with nitric oxide emitted from local sources (the NO_x titration effect). The PCM model calculates an empirical urban ozone decrement based on modelled annual mean oxides of nitrogen concentrations. It also takes into account the effects of altitude.

CMAQ was developed in order to predict ozone concentrations and the Directive metrics are readily calculated from the model output. UK scale modelling of ozone is currently carried out at 10 km spatial resolution and significantly higher resolution at the UK scale is not feasible without substantially increased computing resources. The effect of titration in urban areas as the result of area source emissions could be taken into account at higher spatial resolution in several ways:

- the PCM urban ozone decrement approach
- hourly area kernels derived from dispersion models and NO_x titration models (e.g. Abbott [18])
- detailed dispersion models with integral NO_x titration models (e.g. ADMS Roads)- (note that detailed dispersion models have not been applied at the UK scale)

3.2.5 Assessment of potential for preparing maps for short-term sulphur dioxide metrics

The Air Quality Directives specify short-term limit values for sulphur dioxide in terms of the hourly average and daily average concentrations. The PCM model currently uses the dispersion model ADMS4 to predict the combined contribution from large point sources to percentile hourly and daily ground level concentrations that correspond to the limit values. The model predicts these contributions at 5 km resolution. The PCM model calculates the contribution from area sources to annual mean concentrations using a kernel approach at 1 km resolution. It then uses a simple algorithm to estimate the total percentile concentrations. Figure 3.3 shows the predicted 99.18th percentile 24 hour mean concentrations for 2008: this metric corresponds to the third highest 24 hour concentration specified in the Directive.

[17] AOT40 (expressed in (µg m-3).hours) means the sum of the difference between the hourly concentrations greater than 80 µg m-3 (=40 parts per billion) and 80 µg m-3 over a period using only the 1 hour values measured between 8:00 and 20:00 Central European Time each day
[18] Abbott, J.. 2005, Primary nitrogen dioxide emissions from road traffic: analysis of monitoring data. www.airquality.co.uk/reports/cat05/0703151041_primno2v3.pdf

Figure 3.5 shows that the highest short-term sulphur dioxide concentrations occur in the vicinity of a small number of large point sources. The PCM model currently models these at 5 km resolution. UK scale CMAQ models typically predict concentrations at 10 km resolution however it may be feasible to model more limited areas (e.g. excluding the north of Scotland, Northern Ireland, Cornwall) at resolutions approaching 5 km. It is uncertain whether CMAQ or ADMS would provide better performance at this resolution. There would be two main advantages of using CMAQ in this way:

- ADMS is expected to perform better than CMAQ in the near field (30km), however it assumes that the hourly meteorological conditions for each hour apply throughout the whole of the modelling domain. As implemented in PCM this assumption is applied out to distances of up to 100 km: potentially several hours travel time from the source. CMAQ on the other hand would take into account the changing meteorological conditions en route between source and distant receptors.

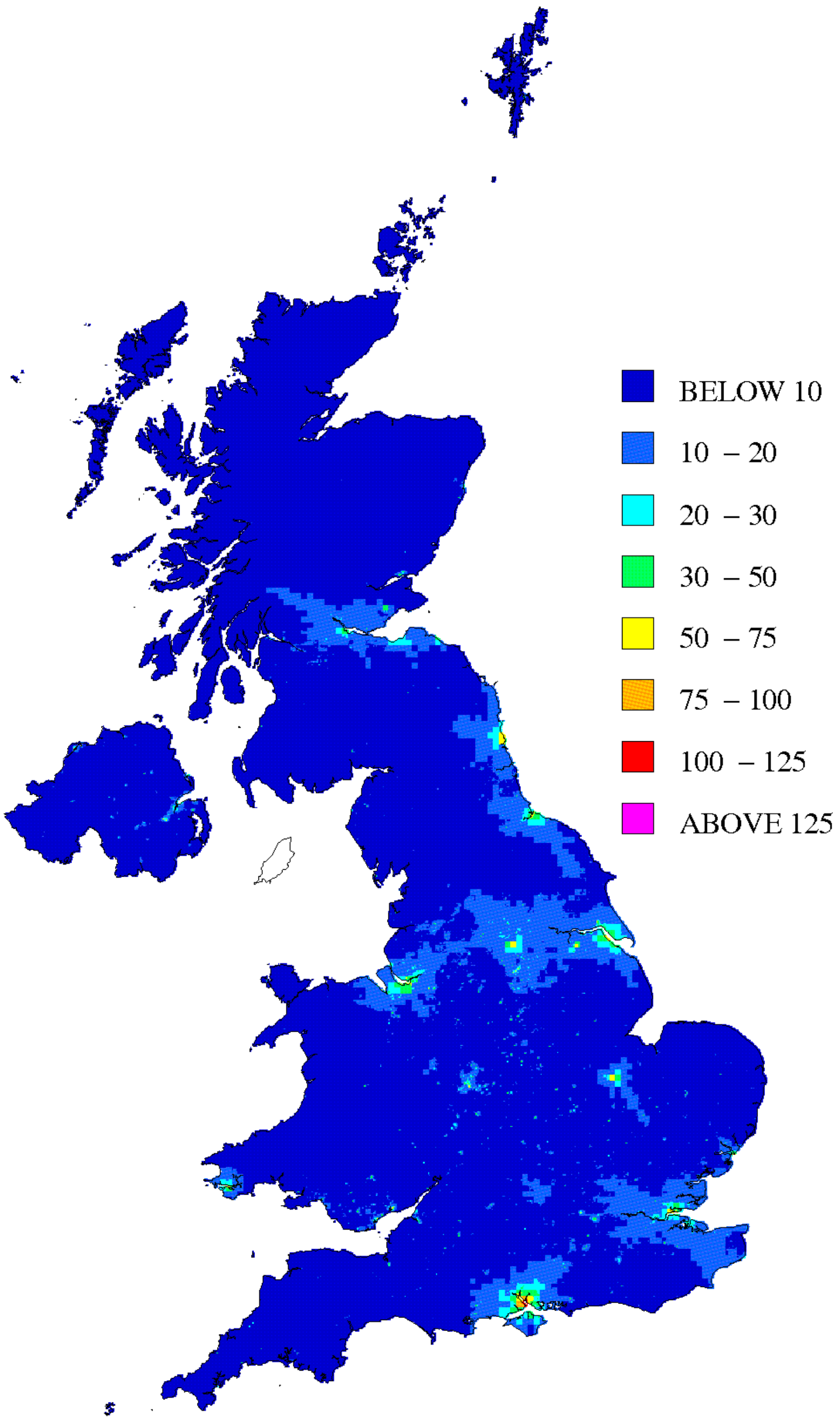
- The contribution from area sources could be taken into account directly (at 5 km resolution) without relying on approximate methods of addition of percentile concentrations.

- The long-range contribution from European and shipping sources could be taken into account directly. PCM currently adds a small contribution to modelled concentrations attributed to “long range” sources. The contribution is derived as the intercept of the regression line used to calibrate the model. In practice, this long range contribution does not significantly affect the model predictions. However, the most recent compliance report[19]suggested that using a long-range transport model to predict sulphur dioxide concentrations from non-UK sources might improve the performance of the model.

Use of CMAQ at 5 km resolution would reduce the modelling resolution for area sources (small industry, domestic, roads etc.), which are currently modelled at 1 km resolution. Local high short-term concentrations of sulphur dioxide occur where there is either substantial local domestic coal burning or near some industrial/ commercial sources.

[19] http://uk-air.defra.gov.uk/reports/cat09/1101250943_dd122008mapsrep_v4.pdf

Figure 3.5: Predicted 99.18th percentile 24 hour mean sulphur dioxide concentrations for 2008: PCM model



3.2.6 Assessment of potential for preparing maps for short-term nitrogen dioxide metrics

The Air Quality Directives specify short-term limit values for nitrogen dioxide in terms of the hourly average concentrations. PCM does not model against this limit value. Instead, it uses monitoring data from sites throughout the UK to show that the annual average limit value for nitrogen dioxide is more stringent than the hourly limit value.

The highest nitrogen dioxide concentrations are observed in urban areas, particularly near roads. CMAQ is not capable of modelling at the high resolution required for detailed modelling of oxides of nitrogen in urban areas near roads. However, the model could be used to provide regional background concentrations: a detailed dispersion model such as ADMS Urban could then be nested within the CMAQ grid.

3.2.7 Assessment of potential for preparing maps for short-term PM_{10} metrics

The Air Quality Directives specify short-term limit values for PM_{10} in terms of the daily average concentrations. PCM does not model against this limit value. Instead, it uses monitoring data from sites throughout the UK to develop a statistical relationship between the annual average concentration and the number of exceedences of the short-term limit value.

Many sources contribute to PM_{10} concentrations. Table 3.1 lists the components modelled and the approach taken by PCM. The table also shows whether the components can be modelled by current UK implementations of CMAQ.

Table 3.1: Components of particulate matter modelled using PCM and CMAQ

Component	PCM approach	CMAQ capability
Secondary inorganic	Based on monthly measurements	Yes
Secondary organic	HARM/ELMO model at 10 km resolution	Yes
Large point source primary emissions	ADMS dispersion model at 1 km resolution	Only at 10 km spatial resolution
European primary emissions	TRACK model at 10 km resolution	Yes
Rural calcium rich dusts	ADMS kernels at 1 km resolution with soil resuspension model	No
Urban calcium rich dusts	Measurement based	No
Regional iron rich dusts	Constant estimated value based on analysis of measurements	No
Iron rich dusts suspended by vehicles	ADMS kernels at 1 km resolution with vehicle wake resuspension model	No
Sea salt	Measurement based	Yes
Area source primary emissions	ADMS kernel at 1 km resolution	May be able to develop CMAQ kernels at 1 km resolution
Roadside increment	Empirical model	No

CMAQ as currently implemented in the UK does not take into account the contribution from dust emissions and the roadside increment. The roadside increment is a major component at locations where PM_{10} concentrations approach the daily limit value and so it will not be feasible to use CMAQ alone for the assessment of compliance. Nesting of roadside dispersion models within CMAQ should be feasible, however. These may be simple (the empirical PCM roadside increment approach) or very detailed (e.g. ADMS Urban) although detailed high resolution dispersion models have not yet been applied at the UK scale. It would be feasible, with some work, to nest the PCM soil and vehicle wake resuspension models within the CMAQ grid.

The use of CMAQ may result in improvements in the prediction of the contributions from secondary inorganic particles, secondary organic particles, European primary emissions and sea salt. CMAQ's approach for these components is more sophisticated than that currently used in PCM.

CMAQ models primary emissions from large point sources at lower spatial resolution than PCM. However, for PM_{10} this may not be important because this component makes a relatively small contribution to total concentrations.

3.2.8 Summary of the potential of CMAQ for compliance assessment

CMAQ alone will not be able to provide the evidence needed to support UK compliance assessment against the Air Quality Directive limit and target values. The model has the potential to provide modelled estimates of regional or rural background concentrations that can be used in conjunction with other models with higher spatial resolution. Existing methods of compliance assessment use estimates of regional or rural background primarily based on measured concentrations. CMAQ should be used to supplement the measurements if it can provide greater spatial resolution without introducing modelling errors. The CMAQ Adjoint Model has the potential to assimilate measured concentrations within the model predictions. However, the CMAQ Adjoint model is still under development and has not been used substantially in the UK.

CMAQ can be used in conjunction with nested dispersion models to provide high resolution estimates of pollutant concentrations for compliance assessment. The dispersion models can be simple (e.g. the existing PCM tools) or very detailed. The choice of dispersion model will remain a compromise between sophistication, ease of implementation, computational speed and the availability of reliable input data.

There is a risk of double counting of emissions when nesting dispersion models for large point sources within CMAQ. This matter needs further consideration. One approach might be to exclude UK point sources from the CMAQ model run or from the nested dispersion model.

3.3 Air quality plan development

3.3.1 The evidence needs

The Air Quality Directives require the UK to prepare air quality plans where the levels of pollutants in ambient air exceed any limit value, plus any relevant margin of tolerance. The air quality plans are required to show how the limit value will be achieved in future.

The key evidence needs here are:

- Source apportionment
- Baseline projections for future years
- Ground level maps and summary statistics
- Projections including the impacts of additional measures beyond those included in the baseline

Source apportionment is particularly important as it is needed to demonstrate that Defra has an adequate understanding of the sources that are driving exceedences and hence enable Defra to target measures effectively to tackle exceedences. Projections including the impact of measure are important since these are required in order to demonstrate that the air quality plan is expected to deliver compliance.

The requirements are similar where target values have been exceeded, although in this instance a report on measures is needed rather than an air quality plan.

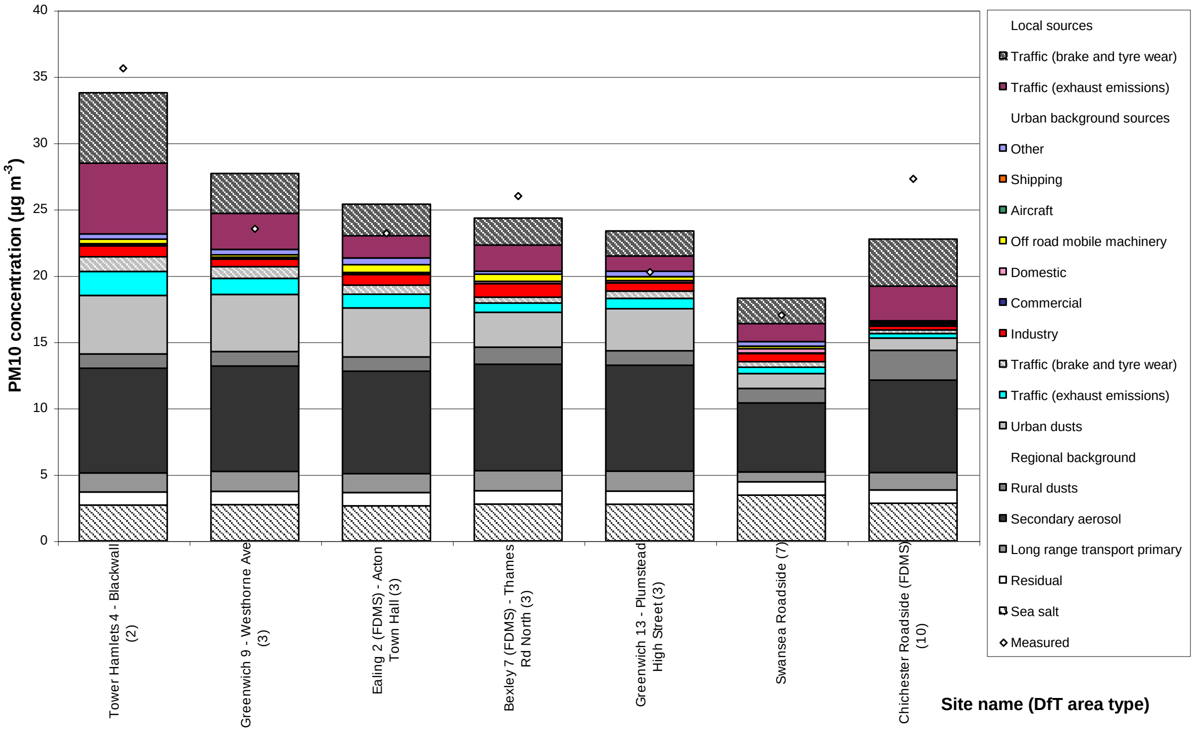
3.3.2 Source apportionment

The main application of CMAQ for compliance assessment is the estimation of regional and rural contributions to total concentrations, using other more spatially detailed models to take account of local sources. CMAQ thus directly provides an estimate of the overall contribution from the long range sources that contribute to the regional concentrations . For some pollutants (e.g. sulphur dioxide), this may be sufficient because the regional background component is relatively small. In other cases, where the regional or rural component are significant, more detail is required of the speciation or sources.

For particulate matter, PCM currently provides a breakdown of the main components of particulate concentrations. For example, Figure 3.6 shows the breakdown at roadside sites. The local and urban background components are broken down according to source type (traffic, industry etc.), while the regional background components are broken down by species (e.g. rural dusts, secondary aerosol, sea salt). A single CMAQ model run will be able to provide details of the breakdown of particulate matter in the regional background concentration (long range primary, secondary aerosols, sea salt and, with some development, long range dusts).

Examination of Figure 3.6 shows that secondary aerosol in the regional background is one of the largest contributors to PM_{10} (and also $PM_{2.5}$) concentrations. Reducing this component could provide an effective means of reducing particulate matter concentrations. Policy makers need to understand the potential reduction that can be achieved by reducing oxides of nitrogen, sulphur dioxide, ammonia and VOC emissions from UK and European sources.

Figure 3.6: Breakdown of particulate matter components at roadside sites



Similarly, high ozone concentrations usually occur as the result of photochemical reactions of oxides of nitrogen and volatile organic compounds released into the atmosphere many hours before. The regional background ozone concentrations are often higher than in urban areas because of the rapid reaction of ozone with nitric oxide released from local sources in urban areas. Policy makers need to understand the potential reduction in regional ozone concentrations that can be achieved by reducing oxides of nitrogen and VOC emissions from UK and European sources.

CMAQ potentially has a useful part to play here although Defra has access to other models that can fulfil many of these requirements. For example, the OSRM model can be used to assess the contribution from specific emissions source categories in the UK and Europe to ozone concentrations. The FRAME model can be used to assess the contribution from specific UK and European emission source categories to secondary inorganic aerosol concentrations. A key aspect here is the chemical mechanisms in these models defining the formation and removal of ozone and its precursors in the atmosphere.

The simplest way of using a model to assess the contribution from specific sources to regional background particulate matter or ozone concentrations for source apportionment is to run the model excluding the specific sources of interest. This “brute force” approach is feasible for simpler models such as OSRM for ozone and FRAME for secondary inorganic aerosol because the models have been developed to allow relatively short run times. The individual contributions from many sources can be modelled over reasonable timescales by excluding each source type in term. Run times for CMAQ are considerably longer with UK scale model runs at 10 km resolution taking many days and so it is feasible to carry out few “brute force” model runs within acceptable timescales.

The CMAQ Decoupled Direct Method enables the user to investigate the sensitivity of model outputs to many input parameters within the same model run. Thus it is possible to investigate the sensitivity of ozone or secondary particulate concentrations to reductions in oxides of nitrogen and VOC emissions from road vehicles, industrial sources, etc. within the same model run. The sensitivities calculated relate to incrementally small perturbations in the emissions. If the modelled concentrations were linearly related to the emissions, it would be possible to calculate the contribution from each source category to modelled concentrations directly from the sensitivities. However, ozone and secondary inorganic aerosol concentrations are not generally linearly related to emissions and so only an approximate source apportionment can be carried out using CMAQ DDM. Hakami et al have shown that the errors in source apportionment for ozone can be reduced to acceptable levels when using second order sensitivities. However, the current version of CMAQ –DDM only allows the calculation of first order sensitivities for particulate matter.

The UK complies with air quality directive limit values for particulate matter and target values for ozone throughout nearly the whole country. Exceedence of the limit values occurs in relatively few areas. The CMAQ Adjoint model would allow the user to investigate the (first order) sensitivities of regional background concentrations in a specific area to emissions of all pollutants at all locations in the model domain in one model run to shed light on the sources causing the exceedences.

3.3.3 Baseline projections for future years

The main potential application of CMAQ for compliance assessment is the estimation of regional and rural contributions to total concentrations, using other more spatially detailed models to take account of local sources. The PCM model estimates the regional or rural contributions on the basis of measured concentrations. However, the measurements alone provide no information about future concentrations. PCM scales the contributions from specific source categories to take account of changes in emissions on the basis of the output from various long range models:

- Primary particulate concentrations are calculated by scaling the TRACK model output for changes to emissions
- Secondary particulate components are scaled using sensitivity coefficients derived from the EMEP unified model on a 50 km grid
- Oxides of nitrogen concentrations are calculated using a source apportionment derived from the EMEP unified model on a 50 km grid
- Ozone regional background concentrations are not scaled.

The CMAQ model could be used to develop future projections of the regional background concentrations for future scenarios for all of these pollutants. The main advantage would be that the same model could be used consistently for all the pollutants. Use of the CMAQ

DDM to provide sensitivity coefficients would allow forecasts to be made efficiently for several future scenarios in one model run.

3.3.4 Ground level maps and summary statistics

CMAQ provides model outputs on a regular spatial grid. A range of mapping tools have been developed specifically to extract data and calculate summary statistics from CMAQ output and present the output as maps of ground level concentrations.

3.4 Hot spot modelling

The annual compliance assessment and/or other sources of information occasionally identify potential local pollution hot spots. Recent examples of this include SO_2 from a brick works in Stewartby and a nickel exceedance of the target value in Pontadawe. Defra's evidence needs here might include:

- Detailed modelling to confirm the spatial extent and magnitude of exceedance
- Source apportionment to help target measures to eliminate the exceedance

CMAQ does not provide the necessary spatial resolution for this application. Established dispersion models such as ADMS or AERMOD are well-suited to this task.

4 Policy Driver 2: Assessment of Policy Options Including Revision of the Air Quality Strategy

4.1 Introduction

Modelling of policy options is currently available under a number of Defra funded projects (e.g. UKAAQA and "*Modelling of Tropospheric Ozone, AQ0704*). There are three types of assessment of policy options that we have identified as particularly important to Defra.

These are:

- Bespoke modelling of measures/scenarios
- Marginal-Abatement Cost Curve (MACC) tool modelling
- Local Air Quality Management (LAQM) inputs

4.2 Bespoke modelling of measures/scenarios

Recent examples include biomass modelling and modelling of the potential impacts of a national framework for Low Emission Zone (LEZ) scheme. Many of the evidence needs for this bespoke modelling are likely to be similar to the compliance modelling and air quality plan development described above. It follows that CMAQ will have similar utility for this type of task. Thus CMAQ would be most useful for assessing the effects of policy options on regional or rural background concentrations typically at around10 km resolution at the UK national scale and at up to 1 km resolution for more localised urban studies.

4.3 MACC tool modelling

MACC tool modelling provides a relatively quick and inexpensive method for Defra to evaluate costs of certain measures or groups of measures versus potential benefits of measures in terms of concentration levels and exceedance extents. The MACC tool allows the user to estimate the effects on concentrations at specified receptor locations of changes in the emissions from particular categories of emissions. The existing MACC tools for nitrogen dioxide and PM_{10} are based on sensitivity coefficients taken from the PCM model. The sensitivity coefficients in the PCM model were derived from various models as follows:

- Regional background primary particulate concentrations: the TRACK model
- Regional secondary particulate components: EMEP unified model on a 50 km grid
- Regional background oxides of nitrogen concentrations: EMEP unified model on a 50 km grid
- Urban background concentrations: ADMS kernels
- Local roadside concentrations; PCM empirical model

CMAQ could be used to derive the sensitivity coefficients for the regional concentrations but does not have sufficient spatial resolution for the local roadside contributions. Derivation of the sensitivity coefficients using CMAQ by "brute force" methods would require many model runs, which may not be feasible if time is constrained. The CMAQ DDM would provide the means to calculate the sensitivity coefficients efficiently in one model run.

4.4 Local air quality management inputs

Part IV of the Environment Act 1995 requires local authorities to review and assess the air quality in their areas regularly. Technical Guidance LAQM.TG(09) describes recommended methods for carrying out the assessment of air quality. The guidance recommends that local authorities assess the contribution to pollutant concentrations in their areas from local and background sources. The LAQM support pages on Defra's website[20] provides annual mean background maps at 1 km spatial resolution of the contributions from various emission sources. The background maps are derived from the PCM model output. The contribution estimates can be downloaded for each local authority area from the website. Projections for background concentrations are available for each year to 2020.

The background maps for $PM_{2.5}$, PM_{10} and NOx have the most detail. For each 1 km square, they provide separate contributions from sources within the square and outside the square for the following source categories:

- Motorways
- Trunk roads
- Primary A roads
- Minor roads
- Brake and Tyre wear (PM only)
- Industry
- Domestic
- Aircraft (NOx only)
- Rail
- Other

In addition, the maps provide the contributions from large point sources, sea salt and residual (PM only), secondary particulates (PM only) and the rural background (NO_x only).

The maps only provide estimates of total background concentrations in the case of benzene, 1,3-butadiene, carbon monoxide and sulphur dioxide.

The Technical Guidance recommends that local authorities use a NO_x to NO_2 conversion tool provided on the website to convert modelled roadside NO_x concentrations to NO_2. The conversion tool requires regional background ozone, oxides of nitrogen and nitrogen dioxide concentrations as input. The tool includes suitable values derived from the PCM for each local authority area.

Defra provides the maps for all local authorities and so the modelling is carried out at the UK national scale. Practical UK-scale CMAQ models typically predict concentrations at 10 km resolution: they do not provide the spatial detail currently provided in the background maps. It is possible, however, for individual local authorities or groups of local authorities to model limited areas (e.g. London) at 1 km resolution. The existing background maps provide estimates of the contributions from specific source categories, which provide the basis for source apportionment. "Brute force" sensitivity analysis by individual local authorities using CMAQ at 1 km resolution would use considerable computing resources. The CMAQ Decoupled Direct Method would enable the user to investigate the sensitivity of model outputs to each emission class within the same model run. The calculation of first order sensitivity coefficients would be sufficient in most cases where local concentrations are linearly dependent on emissions.

[20] http://laqm.defra.gov.uk/review-and-assessment/tools/tools.html

Nesting of dispersion models within the CMAQ grid is possible. In this case, the CMAQ model would provide estimates of the contributions from regional or rural background sources. However, it is not clear that there is any advantage over the measurement-based approach currently used in the background maps for local authority review and assessment.

5 Policy Driver 3: Health Protection Impact Assessments

5.1 Introduction

Defra needs to quantify the overall impact of air pollution on human health and the effects of reducing air pollution. The Committee on the Medical Effects of Air Pollutants (COMEAP) developed methods to quantify the impacts on human health for particulate matter, nitrogen dioxide, sulphur dioxide and ozone. Methods developed by the Interdepartmental Group on Costs and Benefits (IGCB) have then be used to assess the monetary benefits of specific measures to reduce air pollution, for example in the development of the Air Quality Strategy.

The COMEAP methods to assess the health impacts for particulate matter, sulphur dioxide and nitrogen dioxide are based on annual mean concentrations and population data at 1 km resolution. The PCM provided the estimates of annual mean pollutant concentrations at 1 km resolution for the COMEAP studies.

The COMEAP methods to assess the health impacts for ozone are based on daily maximum 8-hour mean concentrations. Previous studies have mapped the appropriate ozone metric by interpolation from rural ozone measurements. Ozone concentrations are generally lower in urban areas because of the nitric oxide titration effect. Previous studies using the PCM calculated an empirical urban ozone decrement based on modelled annual mean oxides of nitrogen concentrations.

The largest effects on human health are associated with particulate matter. The COMEAP methods are based on total particulate concentrations and do not distinguish between the various components of particulate matter (e.g. primary emissions, secondary inorganic, secondary organic). In future, methods of health impact assessment may seek to distinguish between different components and so more detailed information on speciated concentrations will be required.

Current methods of assessment are mostly related to annual average concentrations. Some health effects are related to short time exposures above threshold values. Models used for health impact in the future may need to calculate more complex concentration metrics.

5.2 Application of CMAQ

Current UK implementations of CMAQ typically use a 10 km resolution horizontal grid to cover the UK with higher resolution grids (up to 1 km resolution) covering specific areas within the UK (e.g. London). It is not currently feasible to carry out complete CMAQ modelling at 1 km resolution over the whole of the UK. It would however be feasible to use the kernel approach used by PCM to provide the required 1 km spatial resolution with CMAQ providing regional or rural background concentrations.

Previous health impact studies have estimated rural or regional background concentrations on the basis of interpolated measurement data. Use of modelled concentrations from CMAQ rather than interpolated measurements may introduce some errors when assessing current health impacts. However, use of CMAQ could provide an improved basis for assessing projections for future years. Potential improvements resulting from the use of CMAQ are:

- It can explicitly model the changes in regional ozone concentrations resulting from changes in UK and European emissions of oxides of nitrogen, VOCs, etc.

- CMAQ can explicitly model the impact of changing UK and European emissions on regional primary and secondary particulate concentrations.

- It models a wide range of particulate species within the same model run so that it has the potential for the investigation of the health impacts of separate components. Table 5.1 lists the particulate species modelled in CMAQ 4.7.1.

- It produces hourly concentrations and so it is possible to derive a variety of health impact assessment metrics.

Table 5.1: Particulate components modelled by CMAQ

Species	Particle size range		
	Aitkin	Accumulation	Coarse
Inorganic aerosols			
Sulphate	✓	✓	✓
Nitrate	✓	✓	✓
Ammonium	✓	✓	✓
Chloride	✓	✓	✓
Sodium		✓	✓
Water	✓	✓	✓
Elemental carbon	✓	✓	
other fine PM		✓	
Organic aerosols			
Alkene based		✓	
Benzene based		✓	
Anthropogenic oligomerization products		✓	
Toluene based		✓	
Xylene based		✓	
General Anthropogenic	✓	✓	
Biogenic Aerosol			
Isoprene based		✓	
Biogenic oligomerization products		✓	
Sesquiterpene based		✓	
Terpene based		✓	
Other coarse			
Other coarse			✓
Soil			✓

5.2.1 Application of CMAQ in epidemiology research

As part of the UK Medical Research Council (MRC) funded Traffic Pollution and Health in London project a 'hybrid' human exposure model is being developed, which will combine

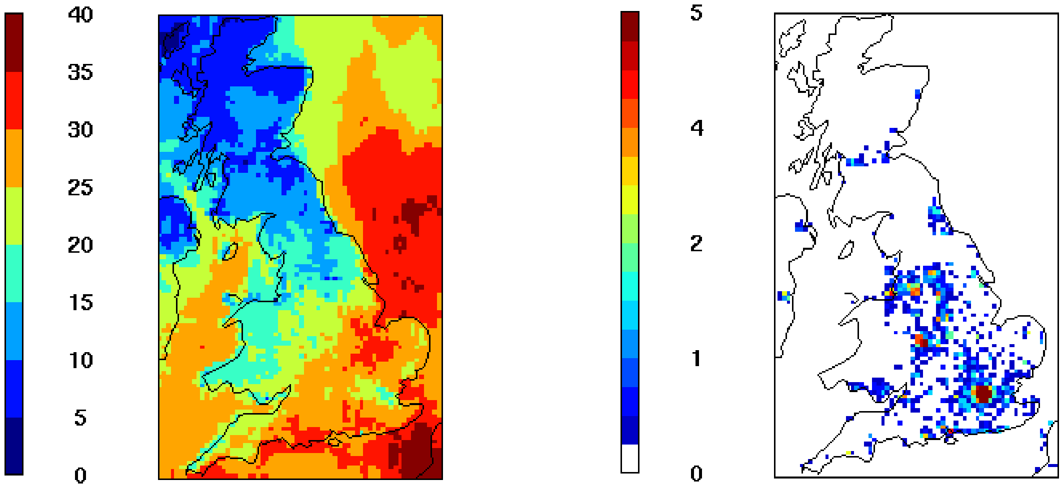
CMAQ-urban with detailed space-time-activity data to create a ‘hybrid’ model of exposure estimates and will be used to study issues relating to exposure misclassification in epidemiology, PM toxicity and exposure to different PM sources. The hybrid model will aid policy makers interested in reducing air quality by providing additional insight into actions that will be most beneficial in reducing human exposure to outdoor air quality. This is important, given the resource implications of meeting EU limit values.

5.2.2 Application of CMAQ in Health Impact Assessment

CMAQ model outputs spatially distributed at post code, borough, city and national levels have been combined using the life table methods of Millar and Hurley (2003)[21]. Furthermore, CMAQ has been used nationally to assess the human health impacts of high 8-hour mean O_3 concentrations. Figure 5.1(i) shows the CMAQ based estimates of number of days when daily maximum 8-hour average O_3 concentrations are greater than 100 µg m^{-3}, which occurred during O_3 episodes in June-July 2006, and which contributed to 80% of the entire year’s exceedences. **Error! Reference source not found.** (ii) shows a 9km grid resolved estimate of the deaths brought forward due to acute O_3 exposure during the June-July 2006 period.

The deaths brought forward were estimated using the concentration-response function from WHO (2004)[22], the CMAQ predicted O_3 concentrations, baseline mortality rate from the UK Office for National statistics (ONS) and high resolution population from European Environment Agency[23] . The premature deaths are higher in and around urban areas with large populations, with nearly 50% of the premature deaths due to O_3, attributable to the June-July period.

Figure 5.1: (i) Number of days when daily maximum 8-hour average O_3 concentration > 100 ug m^{-3} during the June to July period in 2006, (ii) number of deaths brought forward due to short-term exposure to O_3 with a threshold values of 35 ppb for the June – July 2006 period



(i) (ii)

[21] Miller BG, Hurley JF. 2003. Life table methods for quantitative impact assessments in chronic mortality. .Journal of Epidemiology Community Health. 57(3):200-6

[22] WHO. 2004, *Meta-analysis of time-series stidues of Particulate Matter (PM) and Ozone (O_3)*. World Health Organization Europe, Copenhagen.

[23] http://dataservice.eea.europa.eu/

6 Policy Driver 4: Ecosystems Impact Assessment

6.1 Introduction

The UK, through its National Focal Centre, prepares national maps of pollutant concentrations and deposition rates under the UNECE Convention on Long-range Transboundary Air Pollution (LRTAP). The ICP Modelling and mapping manual provides detailed guidance on modelling and mapping requirements and methods.

The following items are mapped:

For critical level exceedance maps:

-ozone concentration (AOT40 values) and ozone flux to vegetation,

- sulphur dioxide concentration,

- nitrogen dioxide concentration,

-ammonia concentration.

For critical load exceedance maps:

- oxidized sulphur (SO_x) deposition (total and non-sea-salt),

- oxidized nitrogen (NO_y) deposition,

- reduced nitrogen (NH_x) deposition,

-base cation and chloride deposition (total and non-sea-salt),

- total nitrogen deposition,

- total potential acid deposition.

Heavy Metal deposition:

- aerosol and wet deposition of lead (Pb), cadmium (Cd), zinc (Zn), and copper (Cu)

- total deposition of mercury (Hg).

The National Focal Centre maps for acidifying and eutrophying species are produced by CEH's CBED model, primarily by interpolating measurement data from the UK monitoring networks. CEH's FRAME model is used to assess the contribution from specific sources and for forecasting concentrations and rates of deposition for future years. The FRAME model in various forms is used for all the pollutants listed above except ozone. The FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange) model is a Lagrangian atmospheric transport model originally developed to assess the long-term annual mean deposition of reduced and oxidised nitrogen and sulphur over the United Kingdom[24]. The latest versions of FRAME can provide model outputs of annual average concentration and deposition at 1 km x 1 km spatial resolution. Increasing the resolution from 5 km x 5 km to 1 km x 1 km resulted in improved estimates of nitrogen deposition near roads and agricultural areas. The FRAME model also provides modelled estimates of concentrations and deposition for the UK Air Pollution Information System (APIS). The APIS database provides estimates of the

[24] http://uk-air.defra.gov.uk/reports/cat05/1003151141_FRAME_Final_report_2009_10_09b.pdf

contributions from specific large industrial sources to deposition estimates for sensitive ecosystems throughout the UK.

Two approaches are used to assess the impacts of ozone on vegetation. The concentration-based approach relates the damage caused by ozone to concentration metrics such as the AOT40 (sum of hourly mean values over a threshold of 40 ppb accumulated over the growing season). The flux-based approach relates the damage caused by ozone to the estimated flux of ozone through the plant stomata.

Maps of AOT40 ozone concentrations are produced using the PCM approach at 1 km resolution by interpolation from rural background concentrations, applying an empirical urban decrement related to modelled oxides of nitrogen concentrations.

Estimates of ozone flux to vegetation are made based on measured or modelled ozone concentrations using Stockholm Environment Institute's (SEI) DO3SE model, which implements the methods set out in the mapping manual. Maps of ozone flux to vegetation at 50 km x 50 km spatial resolution have been prepared during the preparation of the Review of Transboundary Air Pollution (RoTAP) report based on the modelled concentration outputs from the EMEP Unified model. AEA has recently used the OSRM model and the Surface Ozone Flux Model (SOFM) to predict ozone fluxes to vegetation[25] at 10 km x 10 km spatial resolution across the UK. The SOFM model uses similar algorithms to the DO3SE model based on the methods set out in the ICP Modelling and Mapping Manual, the basic guideline for modelling and mapping critical levels for ozone. The International Cooperative Programme (ICP) on Modelling and Mapping of Critical Loads & Levels and Air Pollution Effects, Risks and Trends works under the Convention on Long-range Transboundary Air Pollution.

6.2 Application of CMAQ

CMAQ is a multi-pollutant model: it can prepare maps of deposition and concentrations for all the pollutants specified in the mapping manual. CMAQ provides hourly predictions of concentrations and deposition rates. All of the metrics used for ecosystem assessment can be derived from the hourly predictions.

Current UK implementations of CMAQ typically employ a 9 or 10 km resolution horizontal grid to cover the UK with higher resolution grids (up to 1 km resolution) covering specific areas within the UK (e.g. London). It is not considered feasible at the moment to model routinely the whole of the UK at substantially higher resolution.

The Mapping Manual considers the spatial resolution required for mapping in some detail. For mapping of acid and nutrient deposition, the mapping manual indicates that substantial underestimates of the exceedence of critical loads can occur if the grid size for the modelled deposition estimates is greater than that for the critical load estimates. Critical load data for the UK is available at 1 km x 1 km spatial resolution and so this is the preferred spatial resolution for modelling of the deposition of acid species. It is not currently feasible to use CMAQ to model the whole of the UK at this resolution. It would however be feasible to nest a dispersion model (e.g. AERMOD, ADMS) within CMAQ to provide the local-scale detailed resolution. Here, CMAQ would provide the regional background concentrations. The CBED maps prepared by the National Focal Centre interpolate the regional background concentrations from measurement data and it is not clear how use of CMAQ would provide improvements in these estimates for current base years. On the other hand, CMAQ would provide an improved basis for the assessment of future scenarios, which cannot be evaluated by interpolation.

The Mapping Manual states that it is helpful to produce the ozone concentration field at a grid of at least 1 x 1 km^2 cell-size to provide a spatial resolution of the ozone exposure on a

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[25] http://icpvegetation.ceh.ac.uk/publications/documents/OzoneandcropsintheUK-published-November2011.pdf

horizontal scale which reflects the variations in the orography. The low spatial resolution of long-range transport models such as CMAQ does not match with the resolution required for the evaluation of ozone exposure of forest ecosystems, and estimates of ozone exposure can be improved by local scale modelling. The necessary concentration values at receptor level can be obtained at high resolution from the CMAQ average values by correcting them for local emission of nitrogen oxides, orography and deposition. The effect of titration in urban areas as the result of area source emissions could be taken into account at higher spatial resolution in several ways:

- the PCM urban ozone decrement approach
- hourly area kernels derived from dispersion models and NO_x titration models (e.g. Abbott[26])
- detailed dispersion models with integral NO_x titration models (e.g. ADMS Urban)- (note that detailed dispersion models have not been applied at the UK scale)

The output from CMAQ does not provide estimates of ozone flux to vegetation. However, it would be possible to apply (with some modification) DO3SE or SOFM to the hourly concentration outputs from CMAQ and thus calculate the ozone fluxes. DO3SE and SOFM also require details of hourly meteorological conditions (wind speed, temperature, humidity, solar radiation/cloud cover, rainfall): this information could also be obtained from the CMAQ output.

6.2.1 Application of DO3SE with CMAQ

The O_3 dry deposition model, DO3SE[27] [28], has been implemented in CMAQ (CMAQ-DO3SE) under research collaboration with the University of York. This provides a UK specific tool for predicting O_3 deposition with the additional benefit that dry deposition is one of the most influential parameters in predicting high O_3 concentrations. In other words, to predict high O_3 concentrations correctly one must make correct dry deposition estimates as this is an important O_3 sink.

DO3SE description

One of the unique features of DO3SE is its use of phenology as a primary driver for predicting seasonal O_3 fluxes. The stomatal O_3 dry deposition is parameterised into 10 EU broad land cover types, including 7 tree species, 5 crop species and 2 grassland species[29] [30].

The O_3 effects on ecosystems can be assessed using the PODy (Phyto toxic Ozone Dose over a threshold y) flux-based method that is accepted by the UNECE LRTAP. The CMAQ-DO3SE provides an integrated system for the assessment of O_3 risk on ecosystems. For PODy calculations, estimates of the plant species specific stomatal O_3 flux (F_{st}) are estimated, following the method provided in the UNECE Mapping Manual. Then the PODy is estimated by accumulating the F_{st} above an O_3 stom-atal flux threshold of y. The **Error! Reference source not found.** shows an example of PODy estimated for beech and

[26] Abbott, J.. 2005, Primary nitrogen dioxide emissions from road traffic: analysis of monitoring data. www.airquality.co.uk/reports/cat05/0703151041_primno2v3.pdf

[27] Emberson, L.D., Simpson, D., Tuovenen, J.-P., Ashmore, M.R. and Cambridge, H.M. 2000. Towards a model of ozone deposition and stomatal uptake over Europe. EMEP/MSC-W 2/2000. ISSN 0332-9879.

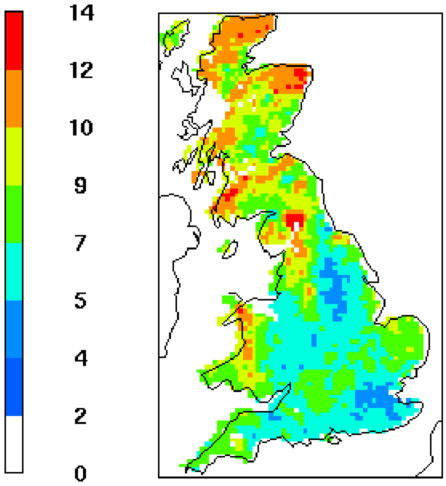
[28] Emberson LD, Buker P, Ashmore MR (2007) Assessing the risk caused by ground level ozone to European forest trees: A case study in pine, beech and oak across different climate regions. *Environmental Pollution,* 147, 3, 454-466.

[29] Simpson, D., Tuovinen, J.-P., Emberson, L. and Ashmore, M.R., 2003. Characteristics of an ozone deposition module II: Sensitivity analysis. *Water, Air and Soil Pollution*. 143, (1-4), 123-137

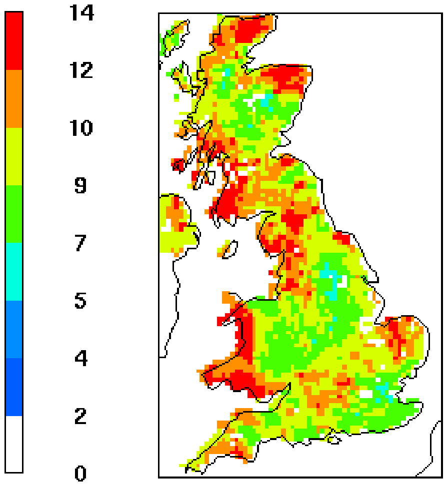
[30] UNECE. 2004. *Modelling and assessment of the health impact of particulate matter and ozone*. EB.AIR/WG.1/2004/11

grassland with threshold of 1.6 nmol m^{-2} s^{-1} for 2006. The PODy critical levels (Clef) for beech and grassland are 4 and 1 mmol m^{-2}, respectively. The Figure indicates that beech and grassland are at risk from O_3 as PODy values exceed the critical level across most of the country.

Figure 6.1: The POD1.6 in mmol m^{-2} for (i) beech and (ii) grassland for 2006



(i)



(ii)

7 Policy Driver 5: Impacts of Climate Change and Climate Change Measures

7.1 Evidence needs

There are two areas in which Defra may need to consider climate change within their modelling capability. The key evidence needs will be similar to those for policy options. These are:

1) Modelling to account for the impact of climate change measures on air quality
2) Modelling to account for the impact of climate change on air quality

Both require assessment of the effect of future emission scenarios on air quality. Evidence need 1) is concerned primarily with the changes to pollutant emissions resulting from measures to reduce greenhouse gas emissions. For example, evidence will be required to assess the impact of changes in particulate matter and oxides of nitrogen emissions from UK or European sources associated with large-scale burning of biomass. Evidence need 2), on the other hand , is concerned with more wide-ranging effects including changes to the weather and to land use/land cover.

7.2 Application of WRF-CMAQ

Figure 7.1 shows a schematic diagram of the main data input streams to the WRF-CMAQ model system that will be affected by climate change. The WRF regional climate model will be affected by changing greenhouse gas emissions, changing land use/land cover and changes to the boundary and initial conditions. The CMAQ regional air quality model will be affected by changing land use/land cover, changing pollutant emissions and changing boundary and initial conditions. Boundary and initial conditions for WRF and CMAQ used by the UK modelling community are provided by various global or hemispherical models. For example, AEA used datasets from ECWMF meteorological data for modelling for 2006 and use the NCEP-GFS forecast for the air quality forecast. Another key objective of this project reported elsewhere seeks to identify the best source of meteorological and chemical boundary /initial condition data for UK modelling applications as well as identifying the best source of land use/land cover data (Beevers et al, 2012).

It will be necessary to specify future boundary/initial conditions and land use/land cover in order to evaluate future climate change scenarios. These will be affected by global greenhouse gas emissions. Global scale modelling of future climate scenarios is carried out by various organisations (e.g. NASA Goddard Institute for Space Studies, University of Carolina, Hadley Centre). Objective 2 of this project seeks to identify the best source of boundary condition data for future scenario modelling applications.

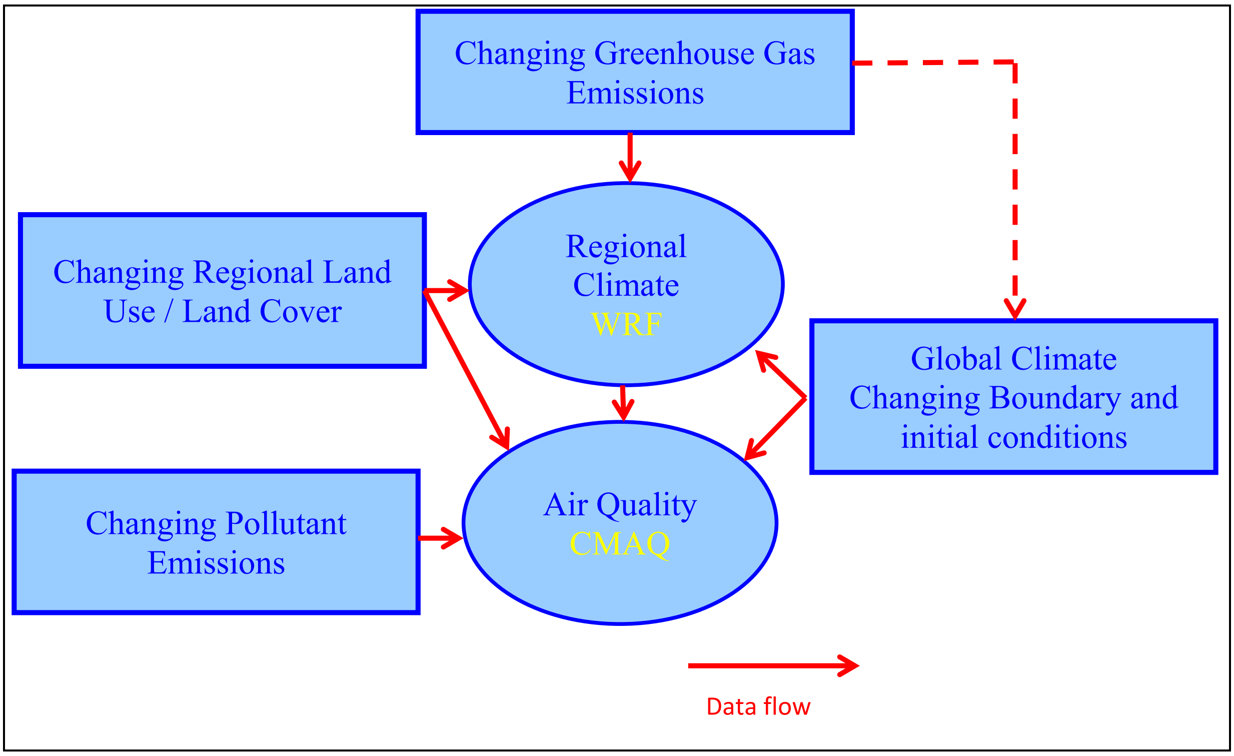
7.3 Nesting of dispersion models

Defra will need evidence on the effect of climate change at various spatial scales from regional to roadside. The CMAQ model will provide evidence of climate change effects at the regional scale. Nested dispersion models can be used to provide concentration predictions at higher spatial resolution. The dispersion models require meteorological data as input. The CMAQ MCIP module output can provide meteorological data based on each climate change scenario suitable for use in most dispersion models. The local dispersion model will then take account of the effects of climate change on dispersion conditions.

7.4 Use of the CMAQ Decoupled Direct Method

WRF-CMAQ requires considerable computing time to carry out national scale annual model runs. It is not therefore usually feasible to investigate many scenarios within a specified timeframe. The use of the CMAQ Decoupled Direct Method would increase the number of emission scenarios that can be investigated. The DDM would also allow the sensitivity of concentration outputs to changes in the concentration boundary conditions. However, there is no equivalent DDM for the WRF model and so it will not be possible to evaluate many global climate scenarios when time is limited.

Figure 7.1: Schematic diagram of the main data input streams to the WRF-CMAQ model system affected by climate change



8 Policy Driver 6: Negotiations for the New Directive

8.1 Introduction

The Air Quality Directive (2008/50/EC) sets legally binding limits for concentrations in outdoor air of major air pollutants that impact public health such as particulate matter (PM_{10} and $PM_{2.5}$, sulphur dioxide, ozone and nitrogen dioxide. The 2008 directive replaced nearly all the previous EU air quality legislation. The 4th Air Quality Daughter Directive (2004/107/EC) sets targets for levels in outdoor air of certain toxic heavy metals and polycyclic aromatic hydrocarbons: these pollutants are not currently covered by the Air Quality Directive.

The European Commission is required to review the air quality directive in 2013 and it is currently initiating work with stakeholders and Member States. The review is expected to look at strengthening provisions for fine particulate matter ($PM_{2.5}$) and to consolidate the 4th Air Quality Daughter Directive. The review will take into account:

— latest scientific information from WHO and other relevant organisations

— air quality situations and reduction potentials in the Member States

— the revision of the National Emissions Ceiling Directive (2001/81/EC)

— progress made in implementing Community reduction measures for air pollutants

The National Emissions Ceiling Directive sets upper limits for each Member State for the total emissions in 2010 of the four pollutants responsible for acidification, eutrophication and ground-level ozone pollution (sulphur dioxide, nitrogen oxides, volatile organic compounds and ammonia). The proposal to amend the National Emissions Ceiling Directive is still under preparation. It should set emission ceilings to be respected by 2020 (or later) for the same four pollutants and also for the primary emissions of $PM_{2.5}$.

The review of the Air Quality Directive will consider whether the existing limit values, target values and exposure reduction targets remain appropriate. It will consider whether new compliance metrics are required, for example for the protection of crops that are affected by exposure to ozone. It will consider whether some of the existing limit values are redundant because other limit values provide more effective control of exposure of the public or sensitive ecosystems.

Defra needs to provide evidence in support of the negotiations for the revision of the Directives. The evidence required will include assessments of:

- the existing and future baseline air quality throughout the UK
- the effect of achievable reductions in pollutant emissions on air quality in the UK and in Europe
- the effect on air quality of reductions in the emissions of pollutants regulated under the National Emissions Ceiling Directive

8.2 Application of CMAQ

The evidence needed to support negotiations for the new Air Quality Directive are similar to those for assessing compliance with the existing Directive (Section 3); for assessing policy options; and for assessing the impacts on human health and ecosystems. The application of CMAQ has been discussed in the previous sections. The advantages of using CMAQ in the preparation of evidence for the negotiations for the new Air Quality Directive include:

- It is a multi-pollutant model so that the effects of policy options on many pollutants can be investigated in the same model run.

- It can model concentrations throughout Europe so that it will be possible to identify the effects of UK emission reductions at home and abroad.

- The model output includes detailed information about the components of particulate matter concentrations: this will be particularly important for the negotiations with respect to $PM_{2.5}$

- The model provides hourly concentration outputs. A wide range of pollutant metrics can be calculated from these outputs. It will thus be able to evaluate proposed new metrics.

The main disadvantages of using CMAQ stem from its long computational times. The long computational times limit the feasible spatial resolution and the number of model runs that can be carried out. Nesting of dispersion models within the CMAQ grid would provide modelled concentrations at higher spatial resolution than CMAQ alone. The CMAQ Decoupled Direct Method should allow the user to investigate the sensitivity of the model outputs to changes in the emissions.

9 Developments Required

Sections 3-8 identify the main limitations of CMAQ in the context of Defra's evidence needs. These are:

- Modelling uncertainty
- Low spatial resolution for annual modelling at UK scale within acceptable timescales
- Long model run time limits the number of scenarios that can be modelled in a specified time

The limitations are briefly summarised below. The developments required to make the CMAQ model more useful for the purpose of meeting Defra's evidence needs are outlined.

9.1 Modelling uncertainty

Existing models are generally considered too uncertain for modelling regional and rural background concentrations for compliance assessment against the Air Quality Directives. Estimates of these rural and regional background concentrations are made by interpolation of measurement data. Recent model intercomparison studies have not shown that CMAQ performs significantly better than other models when compared with measurement data. The performance of CMAQ will be optimised during the course of this project and we expect that this will improve the performance of the model. Nevertheless, it remains to be seen whether CMAQ alone can provide adequate estimates of regional and rural background concentrations for compliance assessment.

CMAQ can provide important information about the spatial variation in concentrations and the effects of changes in emissions, land use and climate. This information cannot be provided by interpolation alone.

The best estimates of rural and regional background concentrations would take account of both the measurements and the model predictions. 4D Var techniques are currently under development using the CMAQ Adjoint model, but this is not currently available with the definitive CMAQ versions. A simpler approach that could be used would be based on optimal interpolation or kriging of the residuals (modelled minus measured concentrations). This approach is simple to implement but the results may not be entirely consistent with mass balance constraints. We therefore suggest that a simple test of the optimal interpolation approach be undertaken based on the CMAQ output and measured regional or rural concentrations. For each monitoring site, the concentration would be calculated by interpolation of the concentration measurements at other sites and also by interpolation of the residuals from other sites. There will be an advantage in using CMAQ if the errors at the sites are reduced compared to the measured values.

9.2 Low spatial resolution

The spatial resolution of CMAQ can be improved by nesting of a dispersion model within the CMAQ grid. However, using the CMAQ modelled concentrations directly to provide estimates of background concentrations for a particular grid square would lead to some double counting of the effect of the emissions in that square. There are two approaches that can be taken:

- Use the dispersion model to predict the contribution from emissions spread across the grid square and then subtract this from the CMAQ concentration

- Calculate an upwind flux- weighted average concentration from the CMAQ output

It is recommended that the two approaches to preventing double counting are investigated further.

The PCM model uses a kernel approach to modelling area sources in which the contribution to concentrations in each 1 km square is calculated as the sum of the product of the emission from each surrounding square and a kernel dispersion factor. The calculation is carried out for the whole country within a Geographical Information System. Some alterations would be required to the GIS algorithms in order to ensure that the kernel of dispersion factors matched the boundaries imposed by the CMAQ grid. The PCM uses a dispersion model to determine the contribution from point sources: some changes will be required to ensure that the dispersion model domain corresponds to the boundaries imposed by the CMAQ grid.

The PCM model 1 km x 1 km area kernels are currently generated using the ADMS dispersion model. It would be possible to use CMAQ to generate similar kernels for selected locations throughout the country. The advantage would be greater consistency in the modelling approach and the meteorological data. It is recommended that kernels generated by ADMS and CMAQ should be compared.

9.3 Multiple scenarios

Long modelling time limits the number of scenarios that can be modelled using CMAQ in a specified time. The CMAQ Decoupled Direct Method was developed to allow multiple scenarios to be investigated in the same model run. The DDM method results in some errors compared with “brute force” methods of sensitivity analysis. It is recommended that the use of the DDM model is investigated in order to demonstrate whether it will allow multiple scenarios to be investigated efficiently without excessive errors.

9.4 Developments required to meet Defra’s evidence needs

Table 9.1 lists the main elements of work required to develop UK CMAQ applications to meet Defra’s main evidence needs. The table lists the main tasks and subtasks and suggests the earliest start and end dates that these could be achieved given sufficient resources.

Table 9.1: List of tasks to develop CMAQ to meet Defra's evidence needs

Task	Subtask	Comments/suggested recommendations
Model validation	Model validation	Comparison of measured with modelled concentrations for optimum set-up for 3 years e.g. 2006 (to compare with earlier runs), 2010, 2011, 2012 Annual means, short-term SO_2 , PM and ozone metrics
	Kriging interpolation	Evaluate kriging of residuals compared to kriging of measurements
	Advanced assimilation techniques	A long-term development. A possible CASE studentship could be considered for this.
Nesting techniques	Comparison of adjustment methods to avoid double counting	E.g. Upwind flux averaging; subtraction of area source model; no adjustment *vs* higher CMAQ resolution modelling
	Alignment of nested model with CMAQ grid	Area source kernels, point sources, roads modelling
	Development of CMAQ 1 km area dispersion kernels	To investigate potential applications to PCM approach
	Use of CMAQ meteorological data in dispersion models	To obtain consistency between models. Also to allow climate change modelling for future years
	Evaluation of CMAQ nested approach to produce annual maps	
Decoupled Direct Model	Demonstration	
	Development of "standard" scenarios	E.g. % Reduction in UK total NOx, % Reduction in UK total VOC, % Reduction in UK total NOx and VOC
Other	Dust suspension emissions model	

Appendices

Appendix 1 Description of CMAQ Decoupled Direct Method, Adjoint Model and Tagged Species Source Apportionment Method.

Appendix 1 - Description of CMAQ Decoupled Direct Method, Adjoint Model and Tagged Species Source Apportionment Method

Decoupled Direct Method

The following outline description of the CMAQ Decoupled Direct Method (DDM) is based on the descriptions given by Cohan and Napelenok[31] and Carmichael et al[32].

CMAQ provides a numerical solution to the atmospheric diffusion equation representing the transport and reactions of chemical compounds. The atmospheric diffusion equation can be written in simplified form as:

$$\frac{\partial C}{\partial t} = -\nabla(uC) + \nabla(K\nabla C) + R + E$$

where C_i is the vector of species concentrations,

$u(x,t)$ is the wind field, depending on the location x and time t,

$K(x,t)$ is the turbulent diffusivity tensor,

$R_j(x,t)$ are the net rates of chemical production for each of the chemical species, j,

$E_j(x,t)$ are the emission rates.

The atmospheric diffusion equation is subject to initial conditions and boundary conditions at the edges of the model domain.

The numerical solution to the atmospheric diffusion equation ("the forward model") can be represented by:

$$C^k = M\left(y^{k-1}, p\right) \qquad C^0 = C(t^0)$$

The solution C_k is the discrete state vector containing the concentrations of chemical species at time t_k, p is the vector of model parameters (e.g. the emission rates, deposition velocities, boundary fluxes), and M is the discrete model solution operator.

Sensitivity analysis is a formal methodology to assess the rate of change of the solution of the forward model when small perturbations are made to model parameters (including initial values, boundary conditions and emissions). The rate of change of the solution with respect to the ith model parameter (i.e. the sensitivity of the solution with respect to the ith parameter) is denoted by:

$$S_i^k = \frac{\partial C^k}{\partial p_i}$$

The sensitivities of the model solution evolve in time according to the linearized model dynamics, derived by differentiating the equation for forward model with respect to p_i:

$$S_i^k = \frac{\partial M\left(C^{k-1}, p\right)}{\partial C} S_i^{k-1} + \frac{\partial M\left(C^{k-1}, p\right)}{\partial p_i} \qquad S_i^0 = \frac{\partial C^0}{\partial p_i}$$

[31] Daniel S. Cohan and Sergey L. Napelenok: Air Quality Response Modeling for Decision Support. Atmosphere 2011, 2, 407-425; doi:10.3390/atmos2030407

[32] Gregory R. Carmichael, Adrian Sandu, Tianfeng Chai, Dacian N. Daescu, Emil M. Constantinescu, Youhua Tang. Predicting air quality: Improvements through advanced methods to integrate models and measurements. Journal of Computational Physics 227 (2008) 3540–3571

This equation forms the basis for the **direct method** of sensitivity analysis. The sensitivity equations are solved in parallel with the forward model. There is one equation for each of the parameters.

The **decoupled direct method** makes computational savings by reusing the same linear algebra factorizations in the forward model and in all the sensitivity equations. It thus assumes that the model operator M is the same in the forward model and for all sensitivity equations (M is then independent of p), so that:

$$S_i^k = \frac{\partial M\left(C^{k-1}\right)}{\partial C} S_i^{k-1}$$

The decoupled direct method (DDM) is a source-oriented sensitivity analysis approach. An initial perturbation at a particular source location is propagated throughout the modelling domain at future times. The sensitivity to many perturbations (for example, resulting from increased emissions at many locations) is the sum of the sensitivities to individual perturbations because the model is linear.

The DDM predicts local sensitivity coefficients representing responsiveness to infinitesimal changes in a parameter. Linear scaling of local first-order DDM sensitivities may poorly represent the nonlinear impacts of large perturbations. Thus, for highly nonlinear relationships, first-order DDM results can be applied reliably only to characterize local responsiveness or the impacts of small perturbations. Hakami et al[33] extended the analysis to include second order self-sensitivity coefficients $S_{jj}^{(2)} = \frac{\partial^2 C}{\partial {p_j}^2}$ and cross-sensitivity coefficients $S_{jk}^{(2)} = \frac{\partial^2 C}{\partial p_j p_k}$, which characterize how the sensitivity of concentrations to one parameter changes as a second parameter is varied. The concentration corresponding to finite perturbations in parameters j and k , Δp_j and Δp_k is then given by the Taylor Series expansion:

$$C_{p_j p_k} = C_0 + \Delta p_j S_j^{(1)} + \Delta p_k S_k^{(1)} + \frac{\Delta p_j^2}{2} S_{jj}^{(2)} + \frac{\Delta p_k^2}{2} S_{kk}^{(2)} + \Delta p_j \Delta p_k S_{jk}^2$$

showed that the ozone response to large (~50%) changes in emissions can be predicted reliably using this approach.

The equations given above describe the discrete form of the DDM in which the atmospheric diffusion equation is first discretised and then linearised to allow numerical solution. An alternative approach is to linearise the atmospheric diffusion equation first and then discretise the terms of the atmospheric diffusion equation. The continuous and discrete forms provide different results. CMAQ DDM-3D applies a hybrid approach in order to obtain optimum results in which discrete adjoints are used for chemistry, diffusion, and vertical advection, and continuous adjoints are used for horizontal advection.

Adjoint Model

The application of an adjoint model requires the definition of a scalar function, J, based on the model concentration outputs where:

$$J = \sum_t \sum_x g(C(t,x),t,x)$$

where g is a function of the concentrations, C, which are dependent on time, t and location x. A simple example of J would be the average concentration over a period of time at selected receptors. In this case, g would be a numerical scaling factor to take account of the number of receptors and the averaging period for the pollutant of interest and zero for all other chemical species.

In a simple case, for explanation here, we are only interested in the final concentrations at a single "receptor" at the end of a period:

$$J = C(t^F)$$

The adjoint variables are then defined by:

$$\gamma^k = \left(\frac{\partial J}{\partial C^k}\right)^T$$

where γ^k are the adjoint variables at time, k (where 0<k<F)

C^k are the concentrations at time k

T indicates the transpose of the matrix(vector)

The adjoint variables are defined over the model domain ($\gamma = \gamma(x,t)$). They represent the sensitivity of the scalar function J to the concentrations of each chemical species at other locations at earlier times. The final set of adjoint variables:

$$\gamma^F = \left(\frac{\partial J}{\partial C^F}\right)^T$$

can be determined from the definition of J. For the simple case where J is defined as the concentration of a single species at a single receptor at the end of the period, all except one of the adjoint variables is zero.

The adjoint variables at earlier times may then be determined from:

$$\gamma^{k-1} = \left(\frac{\partial M(C^{k-1})}{\partial C}\right)^T \gamma^k$$

where M is the discrete model solution operator (see previous section). The forward model is run first to provide the concentrations at specified timesteps ("checkpoints"). The matrix of $\partial M/\partial C$ is then calculated. The values of the adjoint variables are then calculated backwards in time. Note that the same adjoint variables are used to obtain the sensitivities with respect to all parameters; thus a single backward integration of the adjoint model is sufficient. The sensitivity of the scalar function to many parameters can be assessed without recalculation of the adjoint variables.

TSSA Model

Following equations (Wang, et al., 2009)[34] describes how CMAQ model species and tagged species concentrations are estimated:

$$BulkC_{i(t+\Delta t)} = BulkC_{i(t)} + BulkF_i(emission, advection, diffusion, deposition, chemistry, cloud, aerosol)$$

$$TracerC_{i(t+\Delta t)} = \sum_{j=1}^{\substack{source\\regions}} \sum_{k=1}^{\substack{Source\\groups}} [TracerC_{i,k(t)} + TracerF_{i,k}(emissions, advection, diffusion, deposition, chemicatry, cloud, aerosol)]$$

where ‘$BulkC_{i(t+\Delta t)}$ refers to CMAQ simulated species concentration for species i in each grid cell at time step ‘t+Δt’. The $BulkC_i$ concentration at time step ‘t’plus the change of concentration ($BulkF_i$) during a time step (Δt) through emissions, advection, diffusion, deposition, chemistry, cloud, and aerosol processes.

The contribution of the tagged sources to the bulk concentration within the model grid cell is estimated simultaneously as shown in the bottom equation and the sum ($TracerC_{i(t+\Delta t)}$) of TSSA tracer concentration ($TracerC_{j,k}$) from ‘j’ source regions and ‘k’ source groups plus the change in TSSA tracer concentration ($TracerF_{j,k}$) through associated processes is equivalent to $BulkC_{i(t+\Delta t)}$ for species ‘i’.

The tagged species are initialised with concentration from the model initial condition and updated with the boundary conditions when there is influx to the model domain. The transport of tagged species is solved using the advection and dispersion solvers in CMAQ. For chemical reaction of tagged species, it is updated using integrated reaction rates calculated using the process analysis code in the chemical solver. The deposition is coupled with vertical diffusion in CMAQ and the tagged species are deposited the same way as the CMAQ species (the loss of each tagged species is proportional to the deposition rate of the bulk species and the sum of deposition for all tagged-species equates the deposition of the bulk species). Within cloud process, the TSSA updates the tagged species proportional to the change in the CMAQ bulk species. The tagged species are increased according to increments of emissions. For aerosols, the tagged species are updated with the change being proportional to the change in the bulk species concentration at each time step in the aerosol solver. For the mass transfer between gas and aerosol phase, the tagged species gas and aerosol species are in thermodynamic equilibrium.

[34] Wang, Z. S., Chien, C-J. and Tonnesen, G. S. 2009. Development of a tagged species source apportionment algorithm to characterize three-dimensional transport and transformation of precursors and secondary pollutants. Journal of Geophysical Research, 114, D21206, doi:10.1029/2008JD010846

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