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Executive Summary

This report summarises the main activities, results and conclusions from the project "***Modelling of Tropospheric Ozone***" under contract AQ0704, funded by the Air Quality and Industrial Pollution Division of The Department for Environment, Food and Rural Affairs (Defra) and the Devolved Administrations (DAs, the Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland) over the period January 2007 to August 2009.

The overall purpose of the project was to maintain, develop, and apply tools for modelling tropospheric ozone formation and distribution over a range of spatial scales (global, regional and national). The modelling has been used to support and guide Defra's policy on emission reductions and objectives for pollutants that influence ozone, and to verify compliance with UK policy and with European directives on ground-level ozone.

To achieve the key objectives of the project, the work undertaken can be broadly categorised as

- **application** of existing models of tropospheric ozone formation for policy purposes,
- **analysis of trends** in ambient measurements of ozone, NO_x and VOCs to support our scientific understanding of the factors controlling them and
- further **research, development and evaluation** of the models and the underpinning science for predicting concentrations of ozone and related air quality policy.

The Objectives involved:

- Policy development and scenario analysis
- Detailed assessment of relationship between ozone, nitrogen oxide and nitrogen dioxide levels, and factors controlling them
- Improvements to photochemical reaction schemes
- Maintenance and Improvements to the Ozone Source Receptor Model and Comparison With Eulerian Models
- Development of a methodology for assessing the costs, benefits and trade-offs of measures for controlling emissions from use of Volatile Organic Solvents
- Development of an air quality model intercomparison protocol

The report summarises details of the project work given in the two annual project reports and recent quarterly reports, but includes the results and conclusions from the most recent work on improvements to the Ozone Source Receptor Model (OSRM) and the final screening and initial evaluation of the Eulerian model, CMAQ carried out in the final stages of the project.

The other project activities, technical reports and research publications emanating from the project are listed and the report concludes with a summary of the enhances made in the development of the Master Chemical Mechanism and associated condensed chemistry codes, including the treatment of biogenic VOCs and formation of secondary organic aerosols, introducing the Secondary Organic Aerosol concept for policy assessments. It also summarises the demonstration of CMAQ as a Eulerian model able to provide a realistic description of the UK's ground-level ozone climate.

A set of recommendations for future work is presented.

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1 Introduction

The concentrations of ground-level ozone, a pollutant that affects human health, ecosystems and materials, widely exceed environmental quality standards across the UK and Europe. Ozone is not emitted directly into the atmosphere, but is a secondary photochemical pollutant formed in the lower atmosphere from the sunlight-initiated oxidation of volatile organic compounds (VOCs) in the presence of nitrogen oxides (NO_x).

The non-linear nature of ground-level ozone production requires the use of sophisticated chemical transport models to understand the factors affecting its production and subsequent control on a wide spatial scale. The Department for Environment, Food and Rural Affairs (Defra) and the Devolved Administrations (DAs, the Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland) have funded the development of ozone modelling tools over the years. This project has sought to build on earlier work, requiring a modelling capability to treat ozone formation (a) on all spatial scales from urban areas at high spatial resolution to the global scale so that ozone production on the regional and global scales is linked and (b) from timescales of hours to reproduce the diurnal behaviour of ozone to decades so that the influence of climate change and changes in emissions can be assessed.

The overall purpose of the project is to maintain, develop, and apply tools for modelling tropospheric ozone formation and distribution over a range of spatial scales (global, regional and national). The modelling has been used to support and guide Defra's policy on emission reductions and objectives for pollutants that influence ozone, and to verify compliance with UK policy and with European directives on ground-level ozone.

To meet these aims and to address the intended applications, the project involved a programme of work comprised of six main objectives some of which were modified or extended since the project started in January 2007:

Objective 1: Policy development and scenario analysis

Objective 2: Detailed assessment of relationship between ozone, nitrogen oxide and nitrogen dioxide levels, and factors controlling them

Objective 3: Improvements to photochemical reaction schemes

Objective 4: Maintenance and Improvements to the Ozone Source Receptor Model and Comparison With Eulerian Models

Objective 7: Costs, Benefits and Trade-offs: Volatile Organic Solvents

Objective 8: Development of air quality model intercomparison protocol

Objectives 5 and 6 were offered as options in the original proposal, but were not taken up by Defra in the final project specification. These were proposed to be on the development of stomatal flux calculations for vegetation and on the investigation of the impact of meteorology on ozone modelling.

The work undertaken can be broadly categorised as **application** of existing models of tropospheric ozone formation for policy purposes (Objectives 1 and 7), the **analysis of trends** in ambient measurements of ozone, NO_x and VOCs to support our scientific understanding of the factors controlling them (Objective 2) and further **research, development and evaluation** of the models and the underpinning science for predicting concentrations of ozone and related air quality policy (Objectives 3, 4 and 8).

In fulfilling the requirements of the project, the work was undertaken by a consortium led by AEA (Dr Tim Murrells, Project Manager, with Andrea Fraser, Sally Cooke, Clare Allen, Andrew Kent, Susannah Grice and John Abbott) and involving Professor Dick Derwent (rdscientific), Dr Mike Jenkin (Atmospheric Chemistry Services) and the University of Leeds (Professor Mike Pilling and Dr Andrew Rickard) with contributions from the Met Office and Dr Mike Holland (EMRC).

This final report on the project summarises the work, the main conclusions and policy relevance for the duration of the project from January 2007 to August 2009. The summary is taken from the two annual project reports for work carried out in 2007 (Murrells et al, 2008a) and 2008 (Murrells et al, 2009) and the two most recent quarterly reports covering work undertaken in 2009. Further details are referred to in these reports. This report also summarises the results and conclusions from the most recent work of Objective 4 on improvements to the Ozone Source Receptor Model (OSRM) and the final screening and initial evaluation of the Eulerian model, CMAQ carried out in the final stages of the project since the last quarterly report.

2 Application of Tropospheric Ozone Models for Policy Support

Objective 1 involved the application of models and associated knowledge to directly inform Defra's policy on ozone air quality. This Objective was broken down into three sub-tasks:

Objective 1a: Involved the modelling of ozone for national and international policy development using the OSRM and Photochemical Trajectory Model (PTM) to run scenarios relating to ozone policy for Defra on an *ad-hoc* basis.

Objective 1b: Involved the support for policy implementation using available tools to guide and assist policy implementation and provide expert advice as required by Defra, again on a mainly ad-hoc basis. This activity led to the publication of several reports on specific topics

Objective 1c: Involved the modelling support for the Third Daughter Directive reporting, using the empirical modelling approach of the Pollution Climate Mapping programme and the OSRM to provide the modelling outputs (ozone metrics) to meet the Supplementary Assessment Modelling requirements of the Third Air Quality Daughter Directive reporting each year.

Modelling in Objective 1 to evaluate the potential impacts of solvent control policies on ozone was extended in **Objective 7** by the development of a methodology for assessing the wider costs and benefits of solvent reduction and substitution policies covering a range of economic, health, social and environmental impacts. The methodology would enable full life cycle analysis of alternative approaches to inform and underpin future policy development to meet domestic and international commitments. It also illustrated the role of air pollution models based on detailed chemical mechanisms in providing inputs to wider policy analysis tools.

The following is a summary of the main conclusions from these activities.

2.1 UK Ozone Climate in 2006 and 2007

The UK ground-level ozone climate for 2006 and 2007 was characterised by the Pollution Climate Mapping (PCM) empirical modelling approach and the Ozone Source Receptor Model (OSRM), as required under Objective 1c. Both models indicated 2006 was a relatively high ozone year, with elevated concentrations measured in the summer when peak episodic conditions prevailed, while 2007 was a relatively low ozone year.

Results from the PCM were used to fulfill the Supplementary Assessment Modelling requirements of the Third Air Quality Daughter Directive reporting of ozone for each year. These are based on ozone monitoring data and are summarised for the EU Target Value for ozone concentration metrics for human health and vegetation in 2010 (an average over the past 3 years) and the Long-term Objectives for ozone in the following tables, respectively.

UK summary results of air quality assessment in 2006 relative to the Target Values for ozone for 2010

Target Value	*Number of zones exceeding*
Max Daily 8-hour mean Target Value	none
AOT40 Target Value	none

UK summary results of air quality assessment in 2006 relative to the Long-term Objectives for ozone

Long-term Objective	*Number of zones exceeding*
Max Daily 8-hour mean Long-term Objective	43 zones (41 measured + 2 modelled)
AOT40 Long-term Objective	41 zones (32 measured + 9 modelled)

In 2006, there were particularly high numbers of exceedences of the 120 µg m^{-3} Long-term Objective value in East Anglia and the South-East.

The corresponding tables of results from the PCM for 2007 ozone monitoring data are summarised in the following tables for the EU Target Values.

UK summary results of air quality assessment in 2007 relative to the Target Values for ozone for 2010

Target Value	*Number of zones exceeding*
Max Daily 8-hour mean Target Value	none
AOT40 Target Value	none

UK summary results of air quality assessment in 2007 relative to the Long-term Objectives for ozone

Long-term Objective	*Number of zones exceeding*
Max Daily 8-hour mean Long-term Objective	41 zones (24 measured + 17 modelled)
AOT40 Long-term Objective	3 zones (1 measured + 2 modelled)

In 2007, the areas with the most number of days exceeding the objective concentration threshold for human health tended to be in the east of England.

The OSRM is a process model calculating the formation of ozone in the UK based on a chemical transport modelling approach using emissions inventory and meteorological data. It showed broadly similar patterns compared with the empirical maps in terms of these ozone metrics for 2006, identifying significantly higher concentrations in the south and east of the UK, however there were some specific spatial differences and overall the OSRM in 2006 generally under estimated ozone concentration metrics compared with measured data. For 2007, the OSRM showed higher concentrations in the eastern coastal fringes of the UK and generally overestimated Third Daughter Directive ozone metrics compared with measured data. This continues the trend found previously indicating that the OSRM overestimates these ozone metrics in low ozone years (2004, 2005 and 2007) and underestimates them in high ozone years (2003 and 2006) compared with measured data.

Maps that have been generated from the outputs of the OSRM and empirical PCM model for the health-based Long-Term Objective metrics are presented in Figures 1.1 and 1.2 for 2006. Figure 1.1 presents the map of the number of days exceeding 120 µg m^{-3} in 2006 from the OSRM and Figure 1.2 shows the same metric derived from the PCM empirical model.

The PCM empirical model continues to produce results that are closer to the measured concentrations than the OSRM and should continue to be used in its current capacity, contributing modelled data in fulfilment of the UK's Third Daughter Directive reporting obligations to the European Commission.

Further details are given in Murrells et al (2008a, 2009).

Figure 1.1. Number of days exceeding 120 µg m^{-3} (2006) (OSRM map)

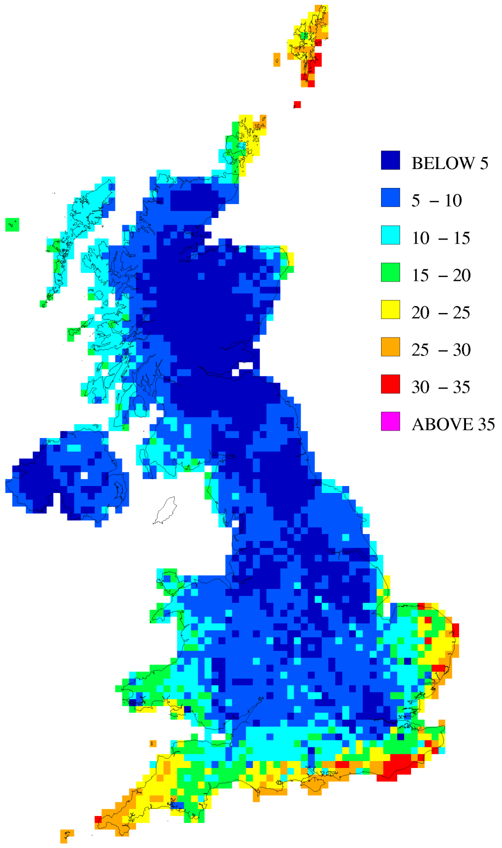
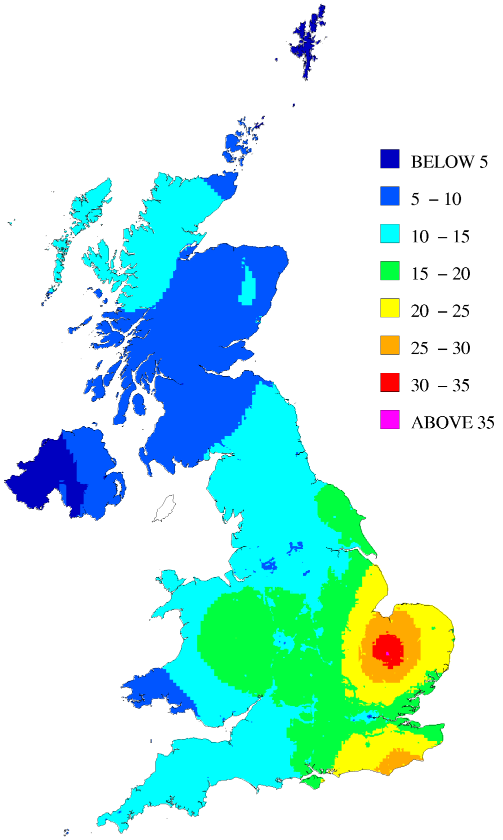


Figure 1.2. Number of days exceeding 120 µg m^{-3} (2006) (PCM empirical map)



2.2 Modelling Impacts of Emission Scenarios on Future UK Ozone Using the OSRM

As required under Objective 1a, the process modelling capability of the OSRM was used to model a number of future emission scenarios relevant to policy.

- The impact on UK ozone concentrations of four additional transport emission reduction measures were modelled for the Air Quality Strategy Review (AQSR). For the road transport measures that involved reductions in NO_x emissions due to tighter Euro 5/6(VI) standards on vehicle emissions, the results tended to show a worsening in the health-based ozone metrics. A slight improvement in ozone was observed when measures reducing NO_x emissions from shipping were included.

- A separate study looked at the impact of reducing shipping emissions alone, using assumptions used in the Air Quality Strategy Review. All metrics show that reducing NO_x emissions from shipping by 9% leads to a reduction in ozone concentrations. Reducing SO_2 emissions by 33% also leads to a small beneficial effect on ozone, but the impact is considerably smaller than the effect of reducing NO_x emissions. It was recommended that the effect of shipping emissions on ozone concentrations be given a more detailed analysis.

- The OSRM was used to model the impacts of changing VOC emissions from road transport across Europe arising from the EU Fuel Quality Directive and the uptake of bioethanol-petrol blends. The focus was on the impacts of potential increases in acetaldehyde emissions from engine exhausts and an increase in evaporative emissions from cars as a consequence of the relaxation of volatility limits of summer blends of petrol to enable the market penetration of bioethanol blends across Europe. The overall conclusion from the modelling study was that the effect of introducing up to 10% bioethanol petrol blends in Europe is unlikely to show any effect on UK ozone levels in the UK up to 2020.

Much more detail on modelling for each of these policy areas was given in Murrells (2008a).

2.3 Modelling and Assessments Relating to Ozone Policy Using the UK PTM

As part of Objective 1a, the UK PTM was used to study trends in both episodic peak and annual mean of the daily maximum ozone metrics from 1990-2010. The aim was to determine the contribution to the observed trends in the ozone metrics from:

- NO_x and VOC precursor emission reductions
- intercontinental trans-Atlantic ozone transport
- non-linearities in ozone formation
- the ambition level achieved in international policy negotiations

The conclusion was that the balance between the contributions appear to be significantly different for the episodic peak and annual mean ozone metrics, but all four influences appear to be important to one or other of the ozone metrics.

The UK PTM model was also used to evaluate the contribution to ozone formation from solvents using the detailed emission speciation data from the National Atmospheric Emissions Inventory (NAEI) and the explicit chemical mechanism described in the Master Chemical Mechanism (MCM). The contributions from usage of solvents and other products such as aerosol sprays are only slightly lower than that of VOC emissions from road transport. The contributions to episodic ozone from all 53 emission sub-sectors that make up the solvent and other product usage sector in the NAEI were examined. It was concluded that there is no one solvent sector that dominates overall. The picture is one of detail and complexity, with many different solvent activities and applications and no dominant activity or process upon which to focus policy

Much more detail on modelling for each of these policy areas was given in Murrells et al (2009).

2.4 Other Support for Ozone Policy Implementation

During the project, a number of ad-hoc tasks were undertaken to assist Defra with implementation of policies relating to ozone air quality, as required under Objective 1b. This involved the provision of data, advice, reports and guidance on a variety of topics.

A report entitled "*Climate Change Consequences of VOC Emission Controls*" was prepared for Defra to be used as a guide for industry, providing a simple approach, with worked examples, for quantitatively assessing the climate change consequences of VOC emission control by incineration (Murrells and Derwent, 2007). Defra expect the report to be used as supplementary background technical information for a wider set of guidelines for industry operators and regulators covering the issue of VOC abatement and its environmental consequences.

Advice and data were given on VOC emission trends from the industrial coatings industry and its impacts on ozone. The UK emission time-series expressed as POCP-weighted emissions from the sector were provided. Long time-series trends in ozone concentrations and exceedences back to 1980 were also provided for this query.

Advice was given on the ozone consequences of reductions in natural gas leakage. Following a query by Ofgem, some advice was given to Defra on how to potentially quantify the reductions in UK ozone levels that would arise if greater controls were placed on the leakage of natural gas from gas distribution systems.

Advice and data were given on VOC emissions from paints and their contribution to ozone formation. Time-series data from the NAEI showing trends in emissions from the paints industry were provided, together with POCP values for paint solvent emissions and their contribution to episodic ozone concentrations.

2.5 Modelling and Assessments Relating to Secondary PM Policy Using the UK PTM and NAME Models

A common theme that has developed throughout the project has been the application and development of ozone modelling tools to other transboundary air pollution problems, principally secondary organic and inorganic aerosols. Process models for forecasting the response of secondary PM formation to changes in precursor emissions (NO_x, SO_2, NH_3, NMVOCs) require similar chemical transport models to the types used for predicting ozone concentrations and there is overlap in terms of evaluating policies affecting the formation of both pollutants. As part of Objective 1, work was undertaken in this project using the Photochemical Trajectory Model (PTM) and the Met Office NAME model to examine the sensitivity of secondary PM component concentrations to changes in the emissions of PM precursors. The aim was to develop scaling factors that could be used in the empirical Pollution Climate Mapping (PCM) model to gauge the importance of non-linearities for policy-making in relation to changes in precursor emissions.

The PTM was used to develop sensitivity coefficients for each secondary PM component, showing the likely importance of non-linearities in the atmospheric chemistry of secondary PM formation, that could be used in the PCM for policy-making in relation to changes in precursor emissions. The NAME model was used to see whether the model could capture the observed changes in sulphate and nitrate aerosol resulting from the changing emissions over the period 2000 to 2006 and to establish whether the NAME results were robust enough to be of use to provide the PCM model with suitable scaling factors to assist in providing baseline projections of inorganic aerosols. This work was described in Murrells et al (2008a) and in specific reports by Redington (2007) and Derwent (2007).

Further work was undertaken with the UK-PTM to develop a particulate matter (PM) Closure Model. The PTM was used to estimate mass concentrations of $PM_{2.5}$ components at the Harwell site in each day in 2006 and to test the linearity of mechanisms forming secondary PM to reductions in precursor emissions. Emission sensitivity coefficients were developed for the different PM components for 30% across-the-board reductions in precursor emissions of SO_2, NO_x, NH_3, VOCs and CO. These revealed that the chemical environment is ammonia-limited such that policy strategies for secondary PM precursors should focus on the abatement of NH_3.

This work was described in the project report by Murrells et al (2009) and was published in the peer-reviewed journal '*Atmospheric Environment'* (Derwent et al, 2008).

2.6 Methodology for Assessing the Costs, Benefits and Trade-Offs of Solvent Reduction and Substitution Policies

Policy analysis of VOC control is complicated by the wide range of impacts that VOCs have besides formation of ground-level ozone, including:

- Direct chemical effects on human health (including cancers), potentially affecting both workers and the general public depending on exposure routes
- Other occupational risks from use of VOCs (e.g. fire hazard)
- Direct chemical effects on ecosystems
- Global warming effects
- Stratospheric ozone layer depletion
- Formation of secondary organic aerosols with associated health impacts
- Life cycle burdens generated by VOC production, use and disposal (e.g. energy use and release of pollutants to air, land and water)

The work on evaluating the potential impacts of solvent control policies on ozone was extended in Objective 7 by the development of a methodology for assessing the wider costs and benefits of solvent reduction and substitution policies covering a range of economic, health, social and environmental impacts. The methodology would enable full life cycle analysis of alternative approaches to inform and underpin future policy development to meet domestic and international commitments.

An additional purpose of the study was to illustrate the role of air pollution models based on detailed chemical mechanisms like the MCM in providing inputs to wider policy analysis tools. This was illustrated by a case study based on the substitution of trichloroethylene, a toxic solvent used mainly for surface cleaning and metal degreasing, by other VOC solvents including a natural product, limonene. The OSRM, PTM and PCM modelling approaches using reactivity information on these species based on the MCM were used to provide quantitative data on the impacts of replacing trichloroethylene with limonene on ground-level ozone, secondary organic aerosols (SOAs, contributing to PM) and ambient concentrations of toxic trichloroethylene in the UK.

The study concluded with a report by Holland et al (2009) describing a methodology that takes analysis from the point of recommending which VOCs should be considered for further control through identification of alternatives and assessment of costs and health, social and environmental impacts. It brings together a number of techniques into a unified methodological framework including:

- Preliminary screening of options
- Cost-effectiveness analysis (CEA)
- Life cycle analysis (LCA)
- Risk assessment
- Impact pathway analysis (IPA)
- Cost-benefit analysis (CBA)
- Multi-criteria decision analysis (MCA/MCDA)
- Uncertainty assessment

The study has implications for analysis in several areas where policy is being developed, including the socio-economic assessment of chemicals under the EU's REACH Regulation.

3 Analysis of Trends in Ambient Measurements of Ozone and NO_x

Objective 2 involved a detailed assessment of the relationship between ozone, nitrogen oxide and nitrogen dioxide levels, and the factors controlling them through analysis of the spatial and temporal trends in the measured concentrations of O_3, NO_x and NMVOCs. The analysis has helped to verify our understanding of the complex relationships involved in the coupling between O_3, NO and NO_2 on different spatial scales and the contribution of hemispheric, regional and local photochemical events encapsulated in models. It has also helped to provide more detailed empirical factors to support more accurate modelling of ozone and NO_2 in the PCM based on our theoretical understanding of these observed relationships.

The work looked at the long-term temporal trend in background oxidant (O_3 + NO_2) and the spatial trend in regional oxidant sources enabling a regional modification to the hemispheric baseline contribution to oxidant to be estimated at different geographical locations. Additional analysis of ambient data led to the development of improved oxidant partitioning expressions describing the relationship between the ratio of [NO_2]/[oxidant] and [NO_x]. The expressions were developed to describe the spatial variation in hemispheric and regional oxidant components with year-specific parameters for use in empirical modelling of annual mean background oxidant concentrations in the UK. Analysis of data using the Netcen Primary NO_2 Model was used to examine the trends in primary NO_2 levels evident at different roadside monitoring sites.

Further analysis and interpretation of ambient measurements were undertaken in Objective 2 to find evidence of urban-scale photochemistry. Hourly-mean O_3 and NO_X data from a series of historical photochemical episodes in the UK were analysed to evaluate urban-scale oxidant production in the London conurbation. Photochemical events occurring in London in the summers of 1999, 2003 and 2006 were considered. The analysis provided evidence for urban-scale oxidant production along a transect of sites across London at rates up to 15 ppb h^{-1}. One case was further analysed using monitoring data for hydrocarbons and NO_x in central London together with estimates of the source strengths of free radicals which demonstrated that our current understanding of oxidant formation mechanisms under urban conditions could be reconciled with oxidant production rates inferred from measurements. The diurnal variation in oxidant partitioning was investigated using hourly-mean monitoring data for specific London sites during a summer period in 1999 where a wide range of photochemical conditions were experienced.

All the expressions and research findings of Objective 2 are currently being used to improve the mapping of NO_2 and the partitioning of oxidant in the PCM project. Further details of the analysis can be found in the project annual reports (Murrells *et al*, 2008a, 2009) and recent quarterly reports.

4 Research, Development and Evaluation of Models for Ozone and Other Secondary Air Pollutants

Three of the core project objectives were concerned with the further development and evaluation of models for tropospheric ozone and, in particular, the chemical mechanisms describing the formation of ozone and secondary organic aerosols from natural and anthropogenic emission sources in the regional-scale chemical transport models used for Defra policy.

Objective 3 involved the review of the current status of photochemical reaction schemes and subsequently the further development of the Master Chemical Mechanisms and related schemes in light of new laboratory-based research and other evidence that has improved knowledge of the detailed chemistry involved in ozone and organic aerosol formation from emitted VOC species.

Objective 4 covered the maintenance and improvements to the Ozone Source Receptor Model and a further evaluation of the OSRM and PTM models against selected monitoring data. Following Defra's independent review of ozone models, the project supported a screening and initial evaluation of alternative, Eulerian-based chemical transport models for Defra ozone policy applications. This section describes in some detail the results and conclusions from the most recent work of Objective 4 carried out in the final stages of the project since the last quarterly report.

In preparation of a possible major performance evaluation and comparison involving all Defra's current air quality models used for policy, this project was extended through **Objective 8** to support the development of a model intercomparison protocol that would be used if such an exercise was to be carried out.

4.1 Improvements to Photochemical Reaction Schemes

The work for Objective 3 initially involved a substantial and in-depth review of the Master Chemical Mechanism (MCM)[1] carried out by members of the project consortium. The aim of the review was to enable Defra to assess future funding for further development. The review was undertaken in the first year of this project by the members of the project consortium who have been responsible for the development of the MCM over the past 15 years, namely Dr Mike Jenkin, Professor Dick Derwent, Professor Mike Pilling and Dr Andrew Rickard. The review covered:

- The aims of the MCM
- An introduction to the MCM and its policy background
- MCM protocols
- Current status of the MCM and on-going developments
- The MCM website
- Comparison of the MCM with other chemical mechanisms
- Policy and other applications of the MCM
- Recommended future activities of the MCM including those requied to improve and maintain the status of the MCM.

The direct policy relevance of the MCM as a crucial tool and source of chemical reactivity information in models for assessing the affect of VOC control options on ozone and other transboundary air pollutant formation in Europe was demonstrated in the review.

The review report was independently peer-reviewed by three external reviewers selected by Defra and in response to this, the review's authors prepared a set of revised recommendations for future development of the MCM. A work programme was then agreed with the Department as a variation to

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[1] The MCM is a near-explicit chemical scheme which treats the atmospheric degradation of around 135 individual VOC species emitted from man-made and natural sources, initiated by sunlight and in the presence of NO_x leading to the formation of tropospheric ozone and other secondary air pollutants

the contract in 2008 aimed at improving and maintaining the status of the MCM and related mechanisms and assessing and guiding the improvement of the representation of organic chemistry in atmospheric models used in policy applications. The four main tasks involved:

- Development of a hierarchy of traceable reduced mechanisms from the MCM
- Development of new MCM schemes
- A major revision of the MCM protocol
- Development and application of a secondary organic aerosol (SOA) code

Considerable progress was made in all these areas.

A reduced chemical mechanism describing the formation of ozone traceable to the MCM (Common Representative Intermediates mechanism, CRIv2) previously developed was thoroughly tested and shown to perform well in comparison with the MCM over a range of conditions. The CRIv2 was further reduced by progressive and systematic redistribution of emission species and lumping into groups. This led to a hierarchy of traceable reduced mechanisms from the MCM being developed, the most reduced version (CRIv2-R5) now comprising just 22 VOCs, 196 species and 555 reactions and still shows very good performance in comparison with the MCM.

The MCM has been expanded with the development of new chemical degradation schemes for new biogenic VOCs covering a wider reactivity range. Four representative monoterpenes were identified, mechanisms for two of which had already been developed (α- and β̃-pinene). A detailed gas phase mechanism for limonene was developed and implemented into a development version of the MCM. With guidance from the international MCM review panel, a mechanism for dimethyl sulphide (DMS, CH_3SCH_3) has been constructed. DMS is an important biogenic organosulphur compound, which has been routinely detected at coastal locations in the UK and has a potential impact on oxidant chemistry and on particulate formation. Its degradation chemistry is highly complex.

The MCM protocol defines a set of rules for the development of the gas-phase degradation mechanisms in the MCM. The protocol has been updated as new research information has emerged to ensure that different people write consistent and compatible chemistry schemes.

Codes for secondary organic aerosols (SOA) in the MCM were developed, validated and applied. A code for SOA was developed, optimized and validated in the UK-PTM against measurements of organic aerosols from the TORCH campaign and shows good performance. A reduced SOA code for the CRIv2 and CRIv2-R5 was also developed and tested. This represents a major advance in the treatment of secondary organic aerosol formation and hence modelling of PM in chemical transport models. As an application of this, the concept of the secondary organic aerosol potential, SOAP, was developed to reflect the propensity of each organic compound to form SOA on an equal mass emitted basis relative to toluene. SOAPs for 79 different aromatic compounds, including α- and β-pinene, were calculated by running the UK PTM model with the MCM for a range of conditions thus opening the door for efficient policy applications similar to the concept for POCPs.

A total of 5 VOC species exhibit SOAPs that are higher than the reference compound, toluene. The two highest SOAP-ranked VOC species are benzaldehyde and styrene. Another 25 VOCs have a SOAP-ranking between 1 and 100; there are a large number of VOC species that exhibit an insignificant ability to form SOA (SOAP < 1). This is because their degradation reactions do not form reaction products of a sufficiently low vapour pressure to form SOA.

It was also found that the propensity to form SOA for some VOCs depends on the availability of NO_x. For some VOCs (benzene, styrene and benzaldehyde), the SOAPs decrease steadily with NO_x reduction from the base case. Some other VOCs show a dramatic enhancement to their SOAPs with increasing NO_x reduction and these include: o-xylene, m-ethyltoluene and the trimethylbenzenes. There is also a class of VOCs whose SOAPs are largely independent of the availability of NO_x and these include: p-xylene, o-ethyltoluene and p-ethyltoluene.

In combination with the speciated VOC emissions inventory, SOAP-weighted mass emissions of each VOC were calculated. Overall, 15 VOCs account for 97% of SOAP-weighted mass emissions in the UK, toluene being the most prolific. The SOAP ranking was also combined with VOC emissions on a source-sector basis. On the basis of emissions in 2000, road transport sources were the dominant source of SOA because of the high proportion of aromatic compounds in the VOCs emitted from this sector. However, the contribution of road transport to SOA formation will be diminishing as VOC emissions from this source is deceasing with the phasing-out of older, higher emitting petrol cars.

The review of the MCM is given in the report by Derwent et al (2007a). Further details of the MCM development and application work in Objective 3 are given in the project annual reports and have led to a number of publications in the peer-reviewed literature, as listed in Section 6.

4.2 Maintenance and Improvements to the Ozone Source Receptor Model

At the start of the project, Objective 4 was provisionally planned to develop the multi-trajectory modelling capacity of the OSRM using forward track trajectories. However, this task was to be dependent on the outcome of the independent review of tools for modelling ozone in the UK commissioned by Defra in 2007. The review undertaken by Professor Paul Monks and colleagues at the University of Leicester made a strong case for moving Defra's ozone modelling activity away from a Lagrangian to an Eulerian basis (Monks et al, 2007). Hence, rather than invest heavily in further developing the treatment of meteorology and transport in the Lagrangian-based OSRM, as originally planned, it was agreed with Defra to revise the scope of Objective 4 to (a) make more limited improvements to the OSRM and evaluate and maintain it for Defra ozone policy applications and (b) to do a screening assessment and evaluation of the Eulerian models, CMAQ and Chimere (see Section 4.3).

4.2.1 Performance Evaluation of the OSRM and PTM

The performance of the OSRM is assessed in Objective 1 each year through its ability to quantitatively reproduce the UK ozone climate as expressed in terms of the two Third Daughter Directive metrics at each AURN monitoring site and to recreate the spatial variability of these metrics indicated by the measurements. However, a more in-depth assessment of the OSRM and the PTM was carried out under Objective 4 considering specific recommendations of the Monks' review.

The assessment considered:

- The use of emission estimates in the OSRM;
- The evaluation of the performance of the OSRM and the PTM by comparison with ambient measurements of ozone concentrations;
- Quality control and outputs and how the OSRM follows the modelling guidelines of the Royal Meteorological Society

In the area of emissions information, it was concluded that the OSRM does treat emissions from UK and other European sources using the best available emissions inventory information, but there is room for improvement.

On model evaluation and comparison with monitoring data, further assessments were made for this study comparing the performance of the OSRM against 2005 and 2006 monitoring data at two rural and one urban AURN site and comparisons also made with the performance of the UK PTM. These showed reasonable model performance, but it was concluded that a much more rigorous assessment is required against other models and this needs to be backed up by strong external peer-review.

On the modelling guidelines of the Royal Meteorological Society, these refer explicitly to atmospheric dispersion modelling and are not always directly appropriate for the applications of the OSRM to Defra policy support. Nevertheless, the general principles they invoke are applicable to the OSRM. All ten aspects of the modelling guidelines were considered and on balance the view was that the OSRM is fit-for-purpose and a better than satisfactory tool, but it is difficult to defend this position based on the current absence of peer-reviewed publications and widely accessible and transparent documentation and there are a number of areas where the OSRM falls short.

Details of the assessment of the OSRM and PTM are given in Murrells et al (2008b) and are summarised in the project annual report by Murrells et al (2009).

4.2.2 Improvements to the OSRM

The limited improvements to the OSRM made under Objective 4 were aimed at maintaining the position of the OSRM as a key Defra ozone modelling tool by ensuring it remained up-to-date with the latest emissions data and chemical scheme linked to the MCM. Attention was also given to updating the initialisation conditions.

4.2.2.1 Emissions Data

With regard to emissions data, the OSRM uses the VOC emission speciation profile from the NAEI. Although the VOC emissions for the main source sectors used in the OSRM are updated with each year according to the inventory, the distribution of the emissions among the many hundreds of VOCs that make up the speciation profile for each source sector are not. To update the VOC profile is a major task and as such is only updated periodically by the NAEI and was last done in around 2002. It was decided, however, to consider whether the VOC profile for key sources could be updated to benefit the OSRM. Attention was directed towards two of the main anthropogenic sources of NMVOCs in Europe, solvent use and road transport. Together, these were responsible for 55% of all UK emissions of NMVOCs in 2006 (Dore et al, 2008) and Derwent et al (2007b) also indicated these sources emitted the most reactive types of VOCs as expressed in terms of the POCP indices of these sources

Examining the VOC profiles for solvent use, it is clear that there is a wide range of organic solvents in use for a myriad of applications such that updating the VOC speciation profile for the solvent use sector would be a major undertaking involving contacting solvent manufacturers, suppliers and trade associations, a task that should be left to the NAEI. It was concluded that there is no reason to believe there should be a major change in the products used as solvents, though this should be reviewed.

For the road transport sector, the VOC profiles are dependent on types of vehicles and fuels used and as such are derived from research studies that measure the composition of VOCs emitted from exhausts and fuel evaporation. A new version of the COPERT emissions model (COPERT 4) has recently been developed for the European Environment Agency and includes a revised VOC speciation profile for vehicle exhaust and evaporative emissions.

The work considered:

a) how the new COPERT 4 profile differs from the current NAEI profile. The profile for diesel exhaust emissions was found to be essentially the same, but those for petrol exhaust and evaporative emissions were different. New VOC profiles were developed using the COPERT 4 data, but including emissions of isoprene based on work done for AQEG. It was found that although the new profiles for petrol exhaust emissions and evaporative emissions are different to the original profiles used by the NAEI, when combined they in fact lead to very similar overall POCP indices. This suggests that use of the new profile in the OSRM is not likely to lead to significantly different ozone predictions.

b) whether the VOC speciation profile is applicable for vehicles and fuels in future years. The most likely cause of changes in the speciation will be the uptake of biofuels stimulated by domestic and EU renewables targets. The increased use of bioethanol will increase emissions of acetaldehyde. However, consideration of the POCP value of acetaldehyde, being close to the weighted average for all VOC exhaust emissions, and the fact that acetaldehyde is formed as a major intermediate in the degradation of many other emitted VOCs means that the increased consumption of bioethanol is not likely to effect peak ozone production and therefore the VOC speciation profile for traffic emissions should still be valid for modelling ozone in future years.

c) whether the VOC profile is being used in the OSRM in the most optimum way. Consideration was given to the way different sub-sector VOC emissions are combined in the main OSRM VOC emission sectors and how changes to these might influence the ozone forming potential of each main OSRM sector in a way that would not be captured by the use of constant speciation factors for each OSRM source sector. Taking traffic emissions as an example, it was shown how increased dieselisation of the fleet will lead to a slight increase in the average POCP of VOCs emitted from traffic. However, as overall VOC traffic emissions will be declining significantly in the future, the increase in ozone forming propensity will have little overall effect on the OSRM predictions of future ozone concentrations. The changes do mean that episodic ozone production will not decline quite as quickly as anticipated by the OSRM through use of a constant speciation profile for traffic emissions, but the difference will be very small.

4.2.2.2 Initialisation Parameters

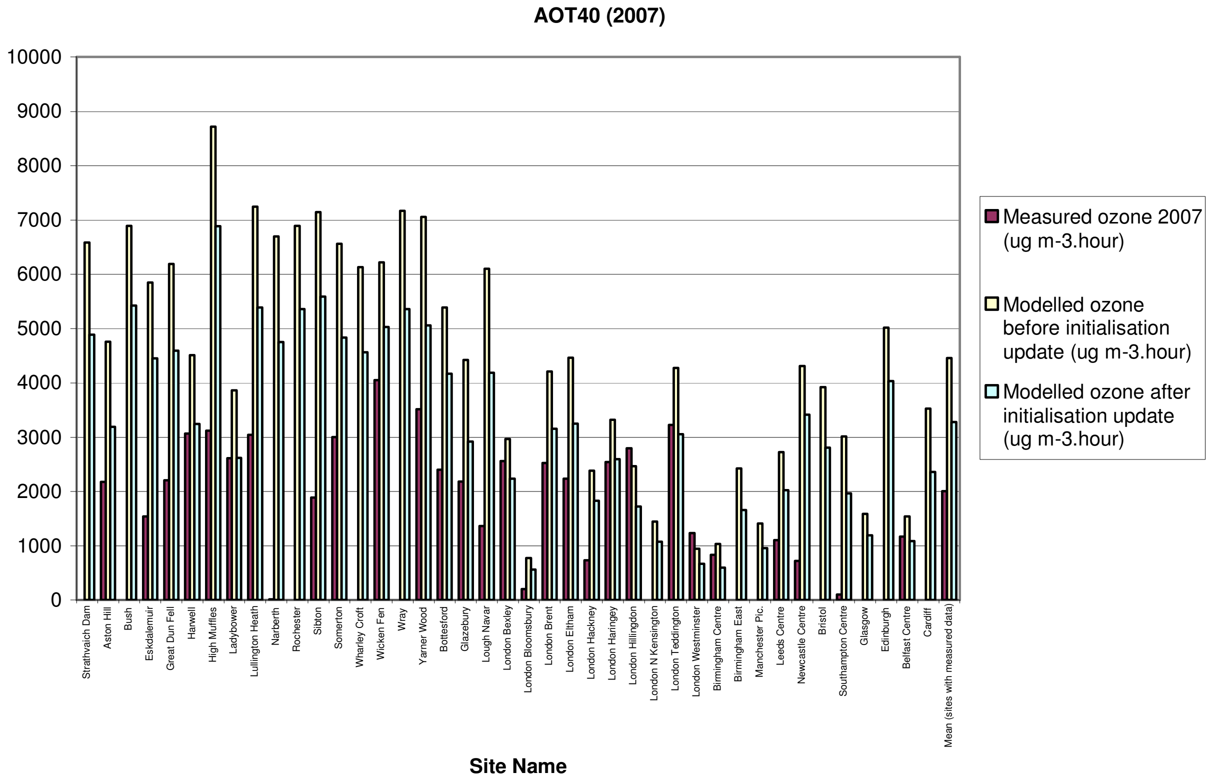
The OSRM currently uses daily concentration fields for ozone and other key species based on the global tropospheric STOCHEM model to initialise concentrations on each trajectory. The initialisation fields represent the climate of the late 1990s and are scaled forward to the relevant model year according to projected concentrations for different global climate and emission scenarios.

To reflect year-on-year variability in baseline hemispheric ozone concentrations, a set of month and year-dependent adjustment factors were applied to the STOCHEM input data based on measurements of ozone at Mace Head. The adjustment factors covered years from 2000 to 2007. The effect of modifying the initialised ozone concentrations was assessed by running the OSRM with 2006 and 2007 meteorology and emissions data and comparing with measured ozone concentrations at different AURN monitoring sites. Modelled ozone concentrations were generally reduced by using the Mace Head adjusted initialised concentrations for these two years.

For 2007, a “low ozone” year where the OSRM had been generally overpredicting ozone concentrations, the performance of the OSRM (after making the Mace Head adjustment) was improved overall when compared with ozone concentrations at the 41 AURN sites. Figure 4.1 shows modelled versus measured ozone for the AOT40 metric with and without the Mace Head adjustment at each site. There is still a tendency for the OSRM to be overpredicting ozone concentrations, but overall the difference between modelled and measured values has been halved. The same trend was observed for the days greater than 120 μgm^{-3} metric. For 2006, a “high ozone” year where the OSRM had been generally underpredicting ozone concentrations, the performance of the OSRM (after making the Mace Head adjustment) was actually worsened overall when compared with ozone concentrations at the 41 AURN sites as this tended to further reduce concentrations.

A more detailed examination was made of predicted concentrations at the Harwell site for each month of 2007. Figure 4.2 shows the monthly average of daily maximum hourly mean concentrations of ozone at Harwell in 2007 calculated by the OSRM with (new initialisation) and without (old initialisation) Mace Head adjustment to initialisation fields compared with observations. For some months, the new initialisation led to better agreement with observations than the old initialisation method and in others the agreement was worse. In the summer months and overall for the year, the agreement was better. The OSRM with the new initialisation method generally performed less well compared with the old initialisation method for the Harwell site in 2006.

Figure 4.1 AOT40 modelled for 41 AURN monitoring sites in 2007 using the OSRM before and after adjusting the ozone initialisation parameters according to monthly data for Mace Head in 2007. The modelled results are compared against monitoring data for each site and for the mean of all sites



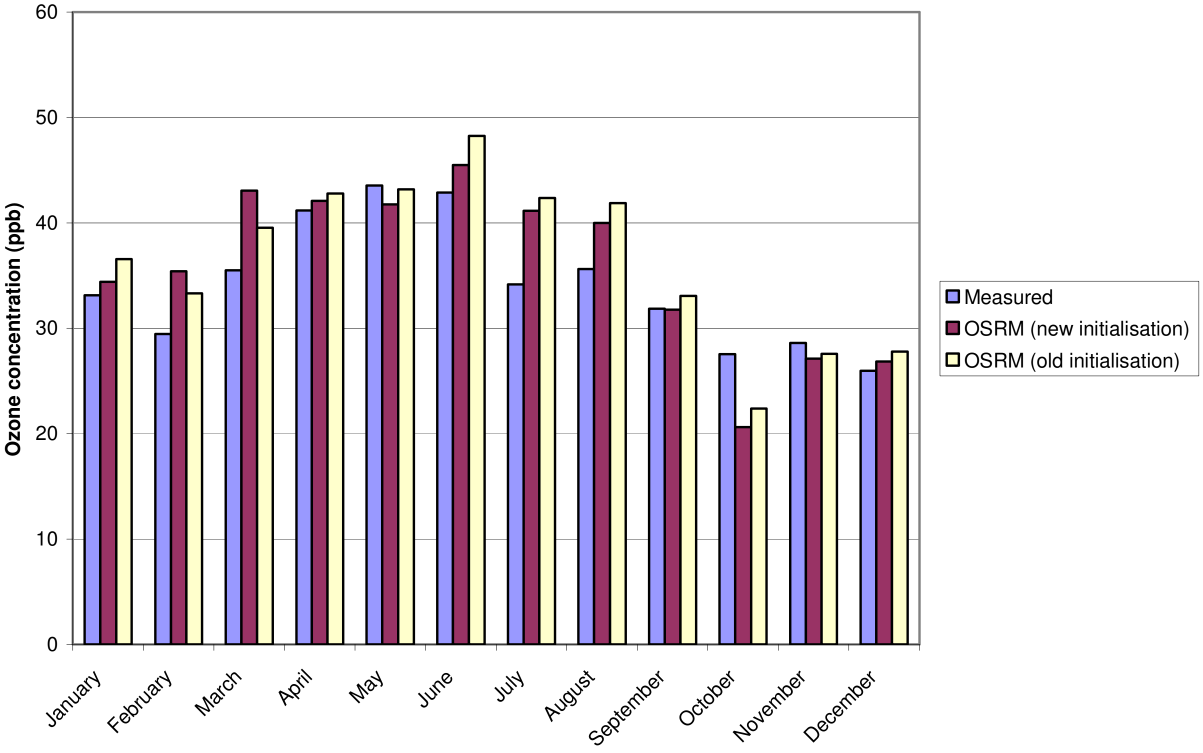
4.2.2.3 Chemical Scheme

The OSRM currently uses a modified version of the chemical mechanism used in the STOCHEM model. This mechanism is not currently traceable to the MCM and therefore has not benefited from the developments made to this scheme during the current contract. The aim here was to incorporate into the OSRM the most condensed version of the CRIv2-R5 chemical scheme, developed in Objective 3, directly traceable to the MCM. This was a major task, involving a considerable amount of re-coding of the model to include the differential rate equations representing the scheme and the re-mapping of new and revised species names to the emission speciation profile. The CRIv2-R5 scheme involves 555 reactions of 196 chemical species, compared to the current 180 reactions of 70 chemical species. An additional advantage of the scheme is that it includes chemistry associated with formation of secondary organic aerosol from emitted VOCs giving the OSRM the potential for modelling this additional secondary air pollutant that contributes to PM_{10} and $PM_{2.5}$.

The implementation of the new scheme was undertaken with the considerable support of Dr Steve Utembe. He has played a major role in the development of the scheme, together with Dr Mike Jenkin, and has successfully implemented it into the STOCHEM model and the PTM.

A new version of the OSRM was created and successfully tested with the new CRIv2-R5 scheme. The original version of the OSRM has been saved for comparison with the new version and for future policy use, should Defra prefer this to be undertaken with a version used for previous policy work.

Figure 4.2: Monthly average of daily maximum hourly mean concentrations of ozone at Harwell in 2007 calculated by the OSRM with (new initialisation) and without (old initialisation) Mace Head adjustment to initialisation fields compared with observations

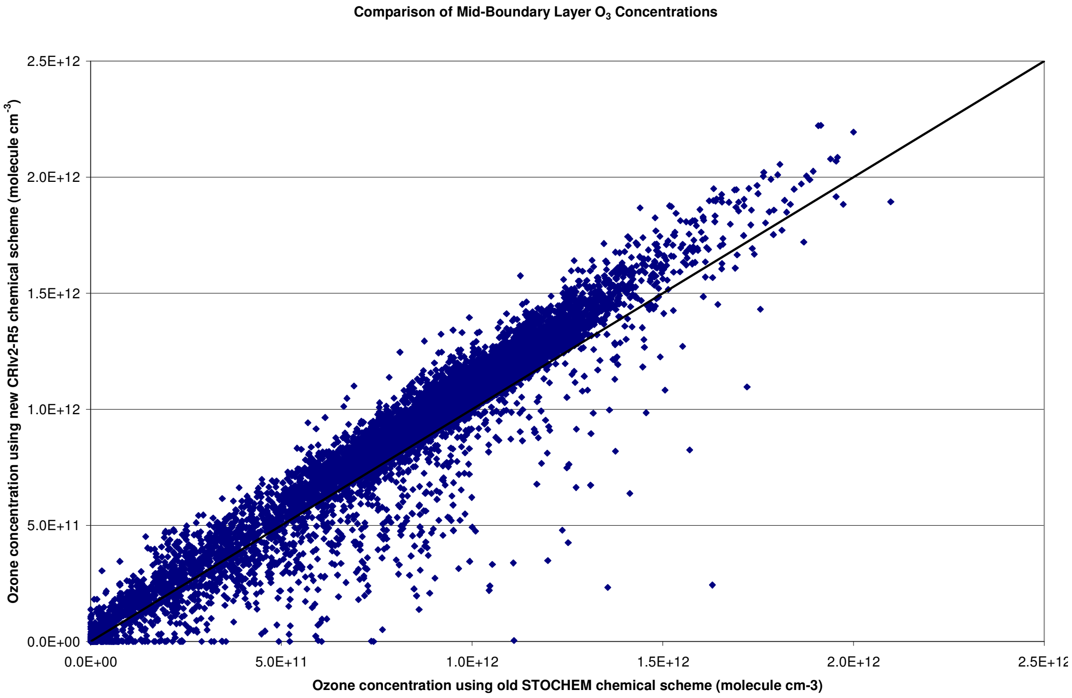


An assessment of how the OSRM performs with the new chemical scheme in comparison with the old chemical scheme was made by modelling the mid-boundary layer concentrations at Harwell for each hour in 2007 (a low ozone year). The results are demonstrated in Figure 4.3 showing ozone concentrations in molecule cm^{-3} modelled with the new scheme plotted against those for the old scheme. There is a very good linear relationship indicating that the OSRM with the new scheme is generally producing sensible outputs. The 1:1 line is also shown. Overall, when averaged over the whole year for this site, using the new scheme leads to around 6.6% higher ozone concentrations than obtained using the old scheme, though there are outliers where the new scheme leads to much lower concentrations. These outliers need to be explored. Since the OSRM was already tending to overpredict peak ozone in 2007 compared with observations at Harwell (and most other sites) then the new scheme effectively worsens the agreement. However, further analysis is required after application of the surface ozone conversion algorithm for this and for other sites and years. Examination of other metrics such as the daily maximum hourly mean concentrations for each month will help to assess the performance of the new scheme in modelling peak ground-level ozone concentrations.

Besides the modelled ozone concentrations, the impact on model run time is an additional aspect of the evaluation of OSRM utilising the new chemical scheme. The greater size and complexity of the CRIv2-R5 scheme inevitably requires additional processing to solve the additional differential chemical rate equations. The OSRM took roughly three times as long to simulate a month and a year when using the new scheme compared with the original scheme. This is roughly in line with the additional number of chemical species and reactions involved in the new scheme.

Further analysis of the test results of the CRIv2-R5 version of the OSRM is currently being carried out.

Figure 4.3: Mid-boundary layer concentrations of ozone at Harwell in 2007 modelled for each hour using the OSRM with the old STOCHEM chemical scheme and the new CRIv2-R5 chemical scheme.



4.3 Assessment of Eulerian Models

Following Defra's independent review of ozone models which recommended moving modelling activity to an Eulerian basis (Monks et al, 2007), Objective 4 involved a screening and initial evaluation of alternative, Eulerian-based chemical transport models for Defra ozone policy applications. The focus was on the two models CMAQ and Chimere.

CMAQ (Community Multiscalar Air Quality) is a community model first developed as part of a USEPA project and supported by CMAS (Community Modelling and Analysis System) and the wider community. It is an open-sourced model, freely available and well supported. Grid resolution is chosen to suit each project with one-way nesting to higher resolution. Most users are in the U.S., but it is widely used in Europe. It uses the Carbon Bond 05 or SAPRC99 chemical schemes, but can be adapted to use different schemes.

Chimere is a similar open source model developed in France by INERIS, but is run by a smaller number of research institutes. It uses the MELCHIOR chemistry scheme.

Both models can run off meteorology data from the weather prediction model, WRF (Advanced Research Weather Research and Forecasting) which is also freely available and well-suited for Eulerian chemical transport models. WRF simulations were themselves driven by historical met data purchased from ECMWF (European Centre for Medium-range Weather Forecasting). The availability of meteorology data from all sources is different for research and commercial organisations, but is was possible to purchase retrospective met data at commercial rates from ECMWF for the whole of 2006 and used to drive WRF on a 6-hourly basis.

A considerable amount of effort was made to optimise WRF parameterisation and the computer systems used to run it to produce met data suitable for running CMAQ at 48km, 12km and 4km resolution. The initial optimisations of WRF and CMAQ were done for one month, June 2006, but once the systems were shown to be stable, an annual simulation was performed while tests on the June 2006 outputs were being carried out.

CMAQ and Chimere both require spatially and hourly resolved emissions data. Gridded EMEP emissions data for Europe and more highly resolved NAEI emissions data for the UK were optimised for running in these models, including those for stack (point) sources. Temporal emission profiles from the NAEI were used to provide the required hourly emissions data. Biogenic emissions are calculated based on the Biogenic Potential Inventory combined with temperature and radiation data.

Exploratory one month runs were performed with CMAQ using two nested grids: the European grid at 48km resolution and a UK grid at 12km resolution. A simulation at 4km resolution was also run for a large part of southern England. An initial evaluation of results for UK ozone and NO_2 concentrations in June 2006 was described in the report of Murrells et al (2009) and in the two quarterly project reports for the January-March and April-June 2009 quarters. The evaluation compared results with measurements at a number of AURN rural monitoring sites using a standard evaluation protocol developed in this project for Objective 8, including diagnostic evaluation.

Figure 4.4 shows a single-sheet Model Performance Summary for ozone using measurements from 11 rural AURN sites around the UK. The results are from a 12km UK run and show paired hourly values (model *vs* observations) for at all sites over all of June and box and whisker plots for each site individually with day-of-week and diurnal profiles. The initial assessment for June 2006 indicated that CMAQ captures many of the features shown by the monitoring data, including the diurnal and day-of-week variations in ozone concentrations, though there were some exceptions at sites such as Rochester which need fuller investigation. Suggestions were made in the last quarterly report as to what might be causing the problems at this site. The most likely cause is the impact of plumes from London, to the west of the site, and local power stations that may require higher resolution simulations to capture the full impact on ozone concentrations at this site.

CMAQ is also operational for PM modelling, though full evaluation of results is still required.

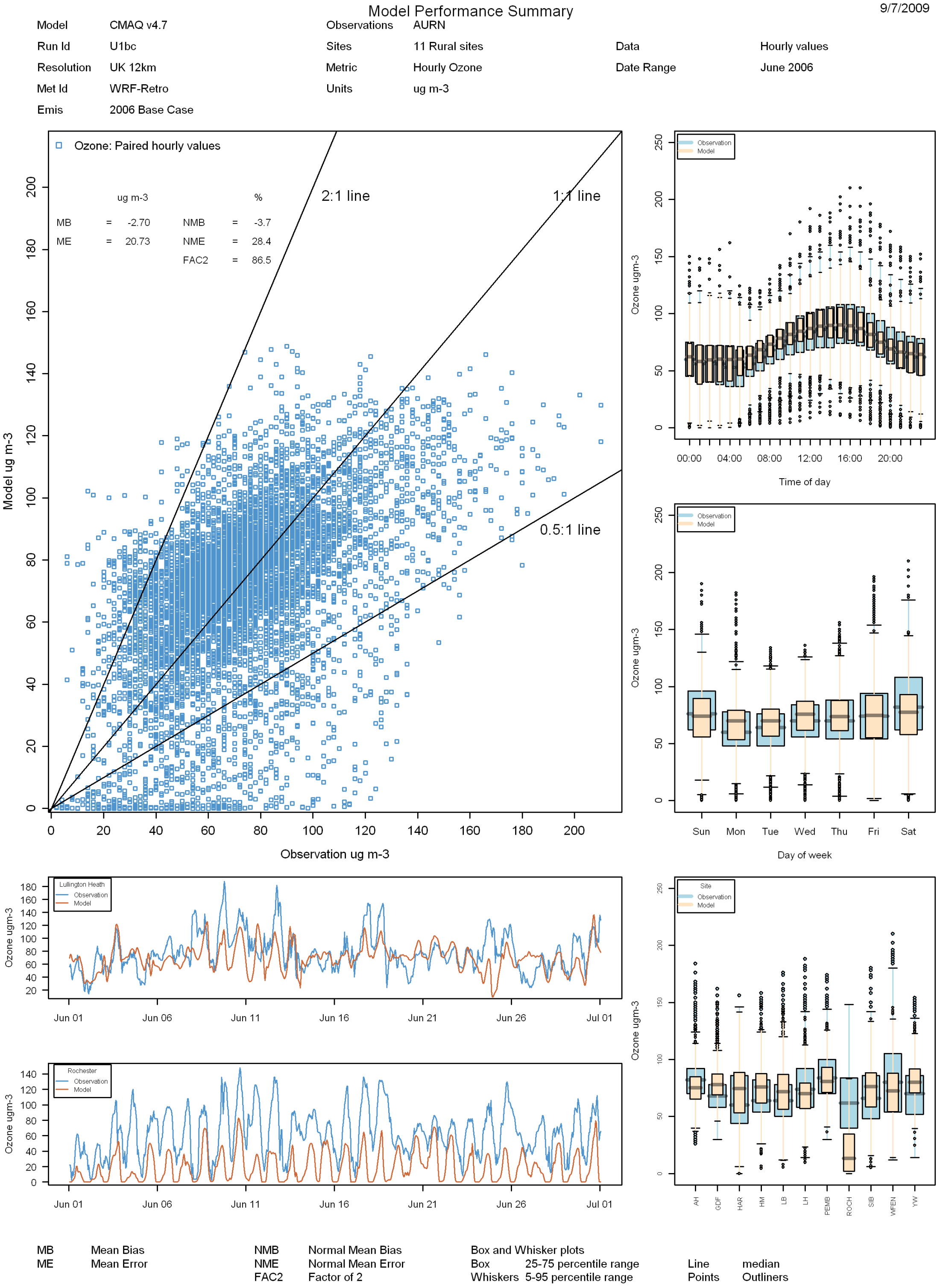
Chimere has been investigated, but is not yet operational. A number of problems have been experienced with running Chimere which are difficult to resolve because it appears to be used by a much smaller community with less experience working on a variety of different computer configurations. Obtaining information from the Chimere help desk in France has been problematic and it appears there are conflicts between configurations available to different users. The CMAQ community and support group, on the other hand, appears to be much more mature. Priority has therefore been given to further exploit and evaluate CMAQ.

4.3.1 Full Annual Assessment of CMAQ Simulations for UK Ozone in 2006

The annual WRF and CMAQ simulation has been completed on the 48km European grid and 12km UK grid. An assessment was made of the two ozone concentration metrics previously used to evaluate the OSRM and for Third Daughter Directive reporting of ozone.

Figure 4.5 shows the monthly mean of the daily maximum ozone concentrations at the rural Harwell and Yarner Wood sites. The results are compared against the measurements and results from OSRM simulations previously reported in the project report of Murrells et al (2008). Results for the similar metric, the monthly average of the daily maximum 8-hour running mean are shown in Figure 4.6. These show that CMAQ performs well at both of these sites in terms of these metrics. There are differences in the performance of CMAQ compared with the OSRM. August 2006 seemed to show unseasonably low values of peak ozone at both these sites that are not reflected in either the OSRM or CMAQ simulations.

Figure 4.4 An example Model Performance Summary produced using ozone data from the CMAQ model for June 2006.



Model Performance Summary

9/7/2009

Model CMAQ v4.7
Run Id U1bc
Resolution UK 12km
Met Id WRF-Retro
Emis 2006 Base Case

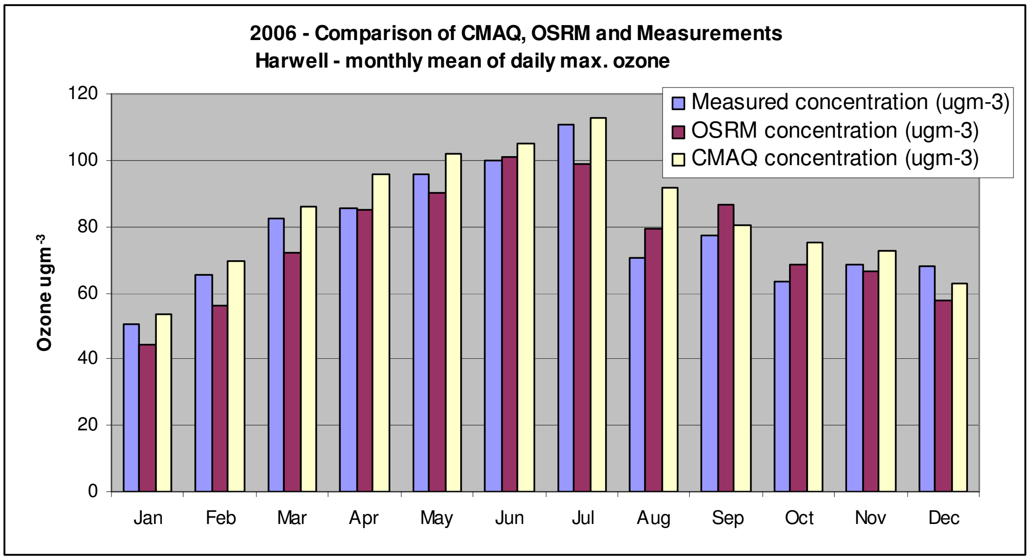
Observations AURN
Sites 11 Rural sites
Metric Hourly Ozone
Units ug m-3

Data Hourly values
Date Range June 2006

	ug m-3		%
MB	= -2.70	NMB	= -3.7
ME	= 20.73	NME	= 28.4
		FAC2	= 86.5

				Box and Whisker plots			
MB	Mean Bias	NMB	Normal Mean Bias	Box	25-75 percentile range	Line	median
ME	Mean Error	NME	Normal Mean Error	Whiskers	5-95 percentile range	Points	Outliners
		FAC2	Factor of 2				

Figure 4.5: Comparison of the monthly mean of the ozone daily maximum at Harwell and Yarner Wood monitoring sites modelled using the OSRM and CMAQ.



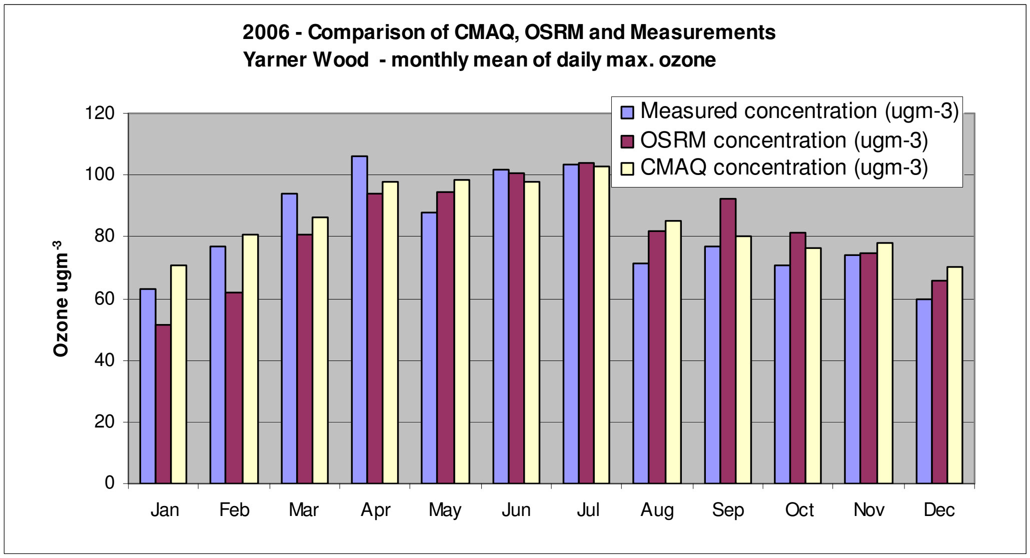
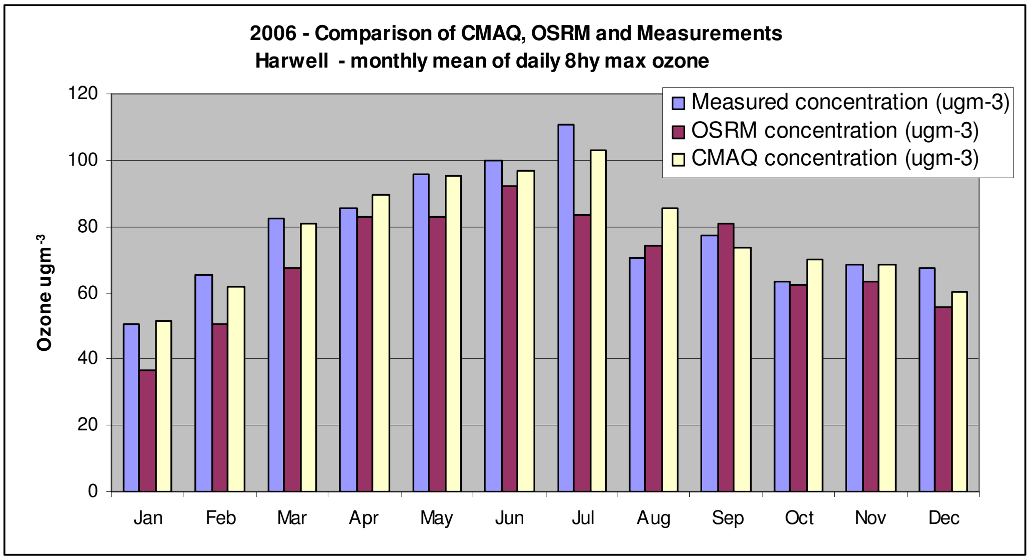
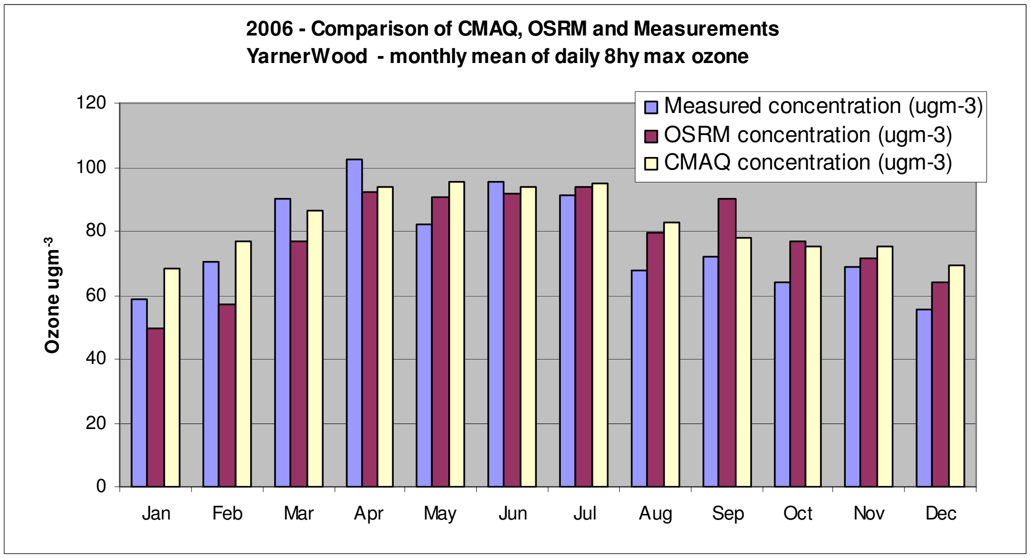


Figure 4.6: Comparison of the monthly mean of the ozone 8-hourly daily maximum at Harwell and Yarner Wood monitoring sites using the OSRM and CMAQ.



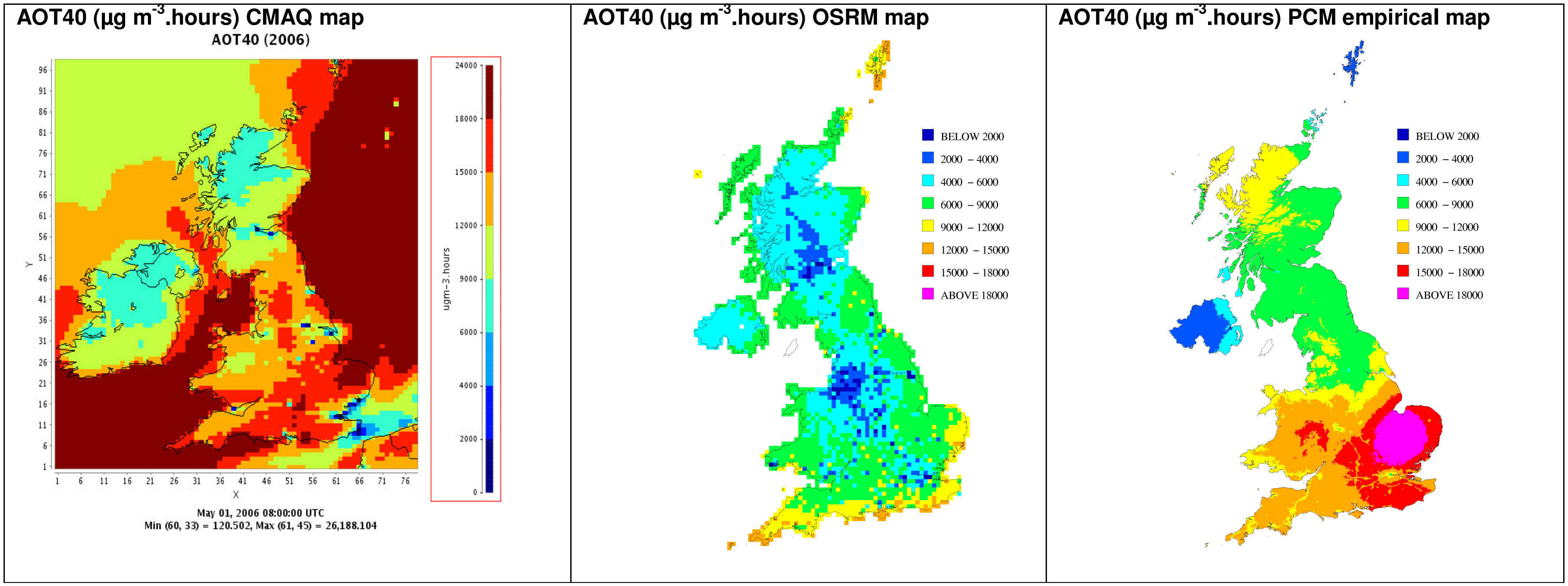


Figures 4.7 and 4.8 show a map of the two Third Daughter Directive ozone metrics for 2006 based on the annual simulation. Figure 4.7 is a map of AOT40 and maps produced from the OSRM and PCM empirical model (previously reported) are also shown. Corresponding maps for the number of days exceeding 120 µg m^{-3} are shown in Figure 4.8.

The spatial distribution of AOT40 for CMAQ is similar to the PCM in the way it shows high ozone levels in the south-east corner of England, but CMAQ also predicts higher AOT40 in the north of England and southern Scotland and lower levels in the north of Scotland compared with the PCM. There are also high levels of AOT40 off the far north-east coast of Scotland, around the Shetlands, a feature displayed by the OSRM. The spatial distribution of the number of days exceeding 120 µg m^{-3} predicted by CMAQ is very different to the PCM, with generally much lower values resembling the results from the OSRM.

Figure 4.9 shows the AOT40 and number of days exceeding 120 µg m^{-3} ozone metrics calculated by CMAQ at over 70 network monitoring sites and compares with results from the OSRM and with monitoring data. The sites are ranked with the remote sites first and the most polluted roadside and industrial sites last. There are many differences in terms of performance of the models at the different

Figure 4.7: AOT40 (µg m^{-3}.hours) 2006 for ozone modelled by CMAQ, OSRM and PCM

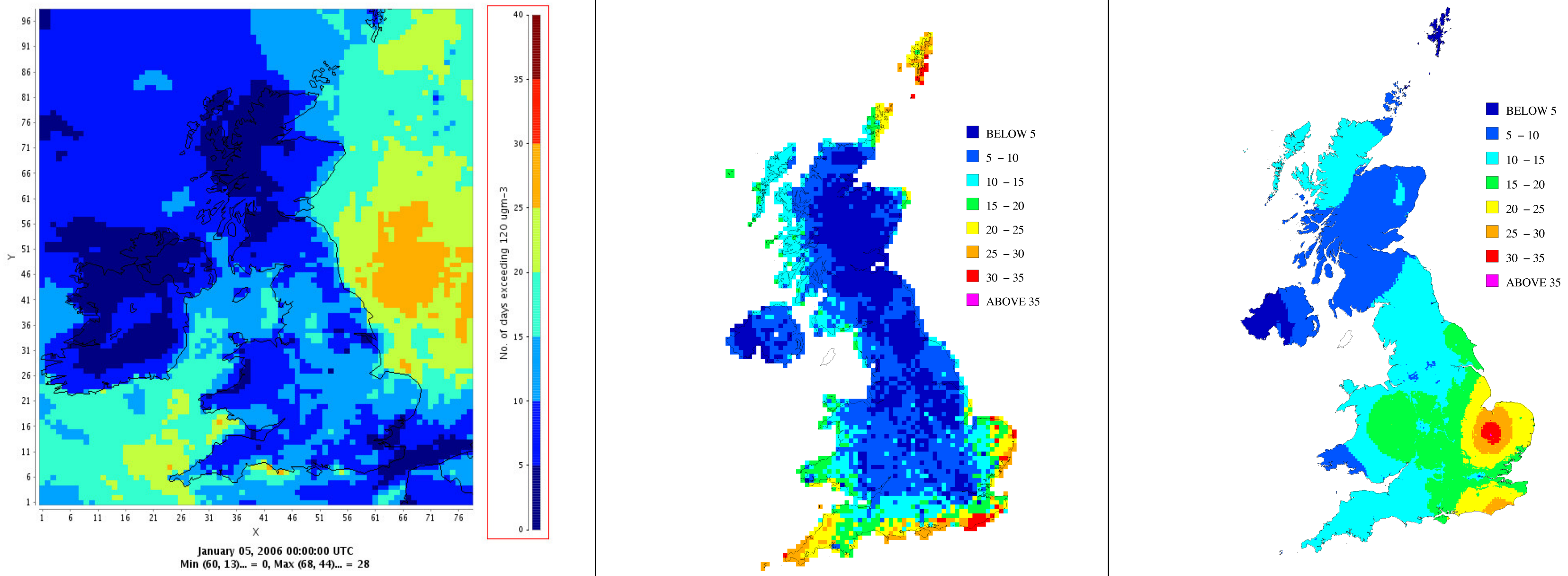


AOT40 (µg m^{-3}.hours) CMAQ map

AOT40 (µg m^{-3}.hours) OSRM map

AOT40 (µg m^{-3}.hours) PCM empirical map

Figure 4.8: Number of days exceeding 120 µg m^{-3} for ozone in 2006 modelled by CMAQ, OSRM and PCM



Number of days exceeding 120 µg m^{-3} CMAQ map)

Number of days exceeding 120 µg m^{-3} OSRM map

Number of days exceeding 120 µg m^{-3} PCM empirical map

Figure 4.9: Comparison of AOT40 (µg m^{-3}.hours) and Number of days exceeding 120 µg m^{-3} for ozone at a number of national network monitoring sites in the UK.

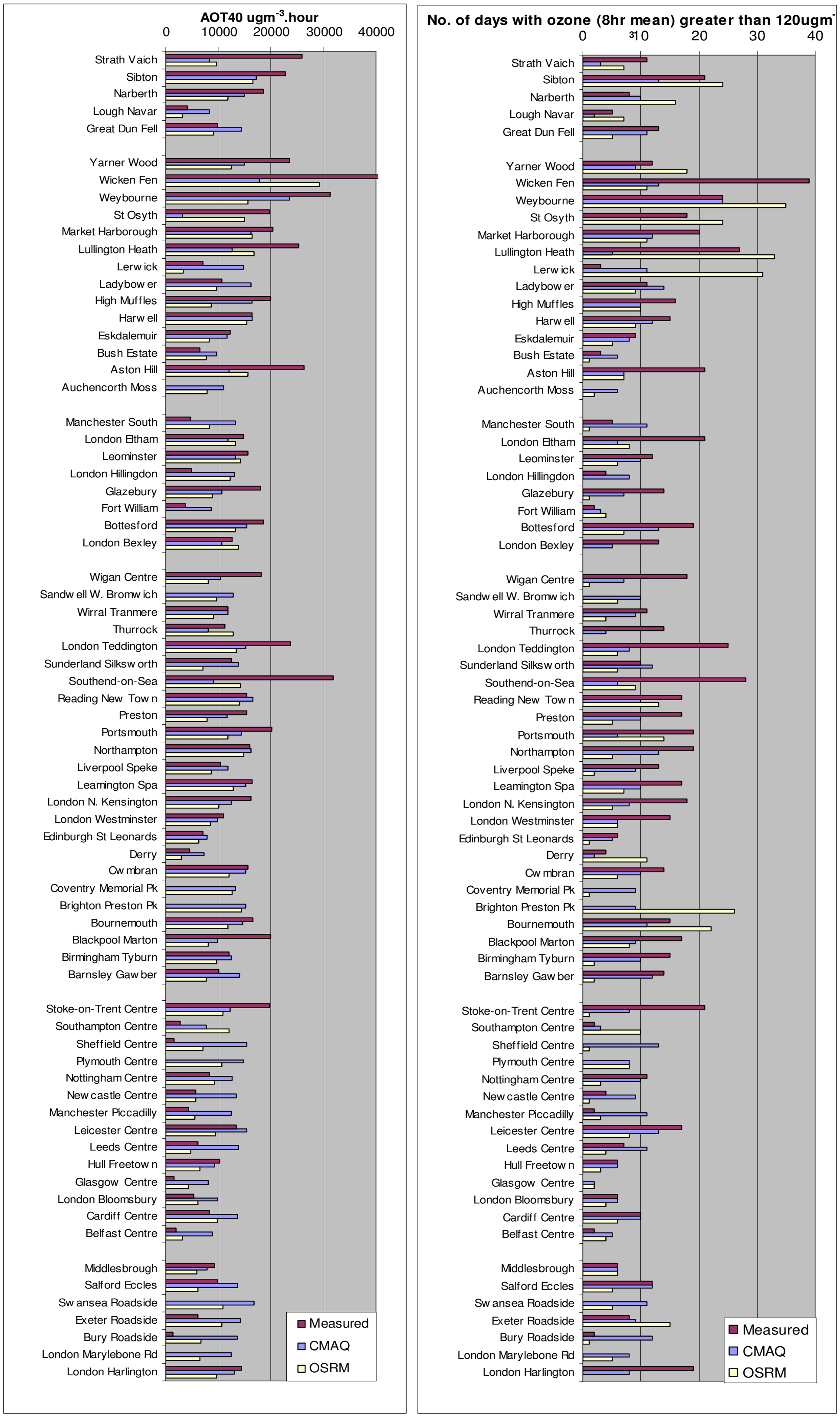
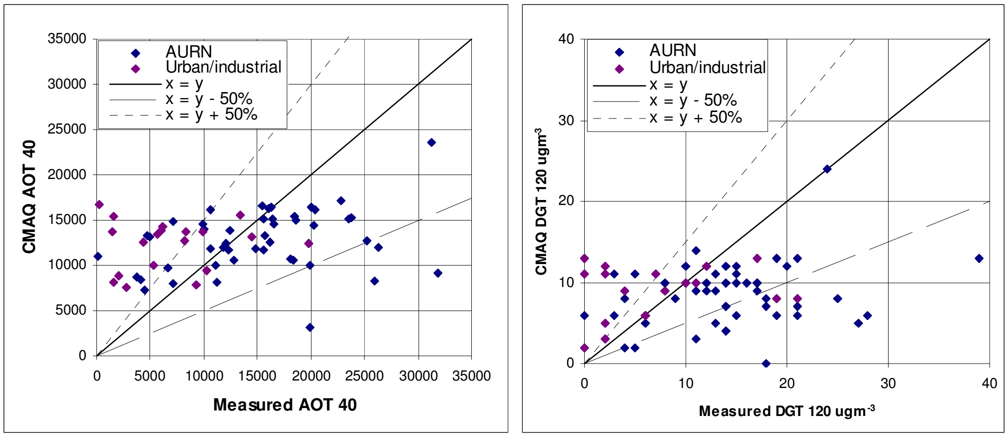


Figure 4.10: Evaluation of CMAQ with measurements of AOT40 (µg m^{-3}.hours) and Number of days exceeding 120 µg m^{-3} for ozone at a number of national network monitoring sites in the UK.



sites in terms of reproducing observations. The scatter plots in Figure 4.10 summarise the performance of CMAQ at all the sites for the two Daughter Directive metrics. Most of the sites where the metrics are overestimated are the urban centre, roadside and industrial sites which are plotted in purple. At these sites ozone is strongly influenced by local emissions.

The results presented here have provided a fairly comprehensive screening assessment of CMAQ in terms of its ability to predict UK ozone concentrations across a range of conditions and sites for one year. A more quantitative and detailed evaluation could be performed following the Model Intercomparison Protocol developed in Objective 8 which would show whether CMAQ meets a minimum set of criteria for it to be considered a truly satisfactory (or better) model for use in UK ozone policy development and assessment. Application of the Protocol would also enable a more rigorous intercomparison between the performance of CMAQ and OSRM (and potentially other models) in predicting ozone. A comparison and evaluation of CMAQ should be extended to another year, preferably one characterised by a different ozone climate to that experienced in 2006, e.g. 2007, and ideally to other ozone episode conditions.

4.3.2 Suitability of CMAQ for Simulating Scenarios for UK Ozone Policy

In supporting any regional transboundary air pollution model, Defra would expect the model to be a reliable and practical tool for assessing alternative policy scenarios in the context of ground-level ozone concentrations in the UK and their responses to precursor emission changes in Europe and the UK. It goes without saying that the preferred model should be able to provide a realistic description of the UK's ground-level ozone climate across a range of spatial scales and time periods, capturing both episodic events and concentrations averaged over longer term periods. But that model would be of little use for ozone policy if it cannot easily be set to run with alternative emission scenarios nor if the computational time to re-run an annual simulation is significantly longer than current models used for Defra ozone policy such as the OSRM.

As anticipated the WRF-CMAQ system is both time and computationally intensive and requires a significant amount of computer resource and storage. The performance of this type of model is dependent on the number of cells (horizontal and vertical) and the complexity of the meteorology and chemistry. WRF is best run with as many layers as possible. This slows the processing time but improves the physical dynamics. In CMAQ, generally more layers are introduced below the boundary layer with fewer layers above reflecting the region of interest.

During this evaluation phase WRF-CMAQ was run on two 'mid range' computers, each with 4 physical and 8 virtual processors. In order to optimise the overall elapsed time, most of the time two jobs were running simultaneously.

Table 4.1 shows the minimum run-time for CMAQ based on the current computer configuration. During the current project, the WRF model has had to be run simultaneously and this has slowed down the CMAQ simulations, but for further 2006 CMAQ simulations, further WRF model runs will not be necessary.

Table 4.1: CMAQ computer run-times (days) for simulations on the European and UK grids

Modelling period	European 48 km grid (days processing)	UK 12 km grid (days processing)
Month	2.5	3.3
4 months	7	10
Year	19	29

The current minimum elapsed time for an annual simulation would be 19 days and 29 days for the European and UK annual simulations, respectively. These can run simultaneously with a total elapsed time being around 30-32 days as a minimum.

Run-times are variable depending on the chemistry and meteorological conditions being experienced and so different months in the year may take different run-times. The minimum run-time rate was experienced frequently during the 2006 annual simulation, when only CMAQ jobs were running, but this could alter if additional WRF simulations are required.

The above estimates are based on the existing grids. Further investigations would be needed to optimise both the horizontal and vertical grids, but this may significantly reduce the overall processing times.

The time required to evaluate different policy scenarios is dependent on the size of the grid and the time period required. The time required may be reduced from a whole year depending on the specific policy requirements, for example by using either representative seasonal months for winter, spring, summer and autumn (January, April, July, October) or looking at the effect of different abatement strategies over a specific pollution episode.

Using the four seasonal months for an evaluation of the effect of a reduction in precursor emissions will provide sufficient information about the performance of CMAQ at different times of year. These will no longer need to run sequentially and by utilising other computers already identified as being available for CMAQ the elapsed time could be as low as 5 days to model the four seasonal months.

Further efficiencies could be obtained by using freed computer capacity used for modelling in the forecasting contract. In order to complete the higher resolution air pollution forecasting runs by 10:00am each day (as required for the forecasting contract), a more extensive network of computers is being established. This will have spare capacity for over half the day when the forecasting runs are complete. This will be available for the evaluation of policy scenarios or the continuous preparation of WRF-CMAQ for the current year enabling the data to be analysed as the year proceeds.

One of the advantages of a single atmosphere model is that whilst the primary objective of a policy scenario may be the change in ozone, the additional effects on NO, NO_2 and PM can be evaluated simultaneously.

The accuracy of the emissions data used in CMAQ and the flexibility for potential scenarios are dependent on the flexibility of the emissions processor. At present the 2006 NAEI emissions as available from the internet are used as the UK source. These are converted to hourly emission using standard factors.

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4.3.3 Conclusion

This initial appraisal shows that CMAQ can provide a realistic description of the UK's ground-level ozone climate in 2006 in terms of the Third Daughter Directive metrics and the monthly mean of the daily maximum ozone concentrations. However, a more in-depth evaluation and comparison with the

OSRM is required following the guidelines in the model intercomparison protocol developed in Objective 8.

Like other models of this kind, CMAQ is computationally more expensive, with longer operational times, but being a 'one-atmosphere' model it does have the advantage of simultaneously modelling secondary PM and other air pollutants, so the effect of a precursor reduction measure can be considered across a range of pollutants. The CMAQ development team in the U.S. are aware of the need to reduce run-time to make the model more useful for common applications. From a current users point of view reducing the number of layers would reduce run-times, but this could be at the expense of model performance.

4.4 Development of a Model Intercomparison Protocol

An additional **Objective 8** was requested by Defra to support the development of a model intercomparison protocol that could be used for an evaluation and comparison of the performance of all air quality models currently used for Defra policy.

A report was prepared providing basic advice to Defra's contractors concerning what should be considered as 'best practice' for air quality model evaluation. A model intercomparison protocol was laid out to provide a framework for Defra to conduct a review of its current modelling activities and to ensure that the models used are fit-for-purpose and reflect current state-of-the-art.

After consultation with the modelling community on an initial draft of the protocol, the final report was prepared providing some background to air quality models and discussing a number of issues that are central to air quality model evaluation (Derwent el al, 2009). A critical step in the evaluation of model performance is the comparison of model results with observations. Annexes are provided in the report giving detailed advice on the selection and availability of network data and the influence that the choice of chemical mechanism, dry deposition parameterisation, emissions and meteorological data can make on model comparisons with observations. However, models must be right for the right reasons and this implies further evaluation beyond a simple comparison with observations.

Protocols are provided in the report for ground-level ozone, acidification and eutrophication and urban air quality modelling. Each evaluation protocol poses three general questions:

- Is the scientific formulation of the model broadly accepted and does it use state-of-the-art process descriptions? This is the scientific evaluation question;
- Does the model replicate observations? This is the operational evaluation question; and
- Is the model suitable for answering policy questions and fulfilling its designated tasks? This is the diagnostic evaluation question.

The protocols do not in themselves answer these questions but exist merely to elicit information from each air quality modelling team to allow Defra to form a view on whether a particular model is fit-for-purpose or not.

A key part of the study was the pilot demonstration of a Model Performance Summary sheet developed using the R statistical and graphics package, freely available as open-source software, to compare modelled results with measurements data. The demonstration focused, as an illustrative example, on a series of plots demonstrating the main evaluation metrics for ground-level ozone, as shown in Figure 4.4 for CMAQ.

5 Other Project Activities

A range of other activities were carried out in this project including the following:

Defra's External Review of Tools for Modelling Tropospheric Ozone – the project consortium supported the group led by Professor Paul Monks (University of Leicester) to undertake an independent review of tools for modelling tropospheric ozone formation and assessing impacts on human health and ecosystems (Monks et al, 2007). Support was given by providing information and advice on the OSRM and PTM and taking part in the User's Workshop at Defra organised by Monks and coworkers.

Support to the **Royal Society Initiative "*Ground Level Ozone in the 21st Century*" -** The Royal Society launched a study to assess and synthesise existing information on ground-level ozone and its impacts, and their coupling to climate change. The study assessed the potential impacts of ground-level ozone concentrations on human health and the environment over the next century, identified options for reducing emissions and mitigating impacts and identified gaps in policy and research. This project supported the contribution by Prof Derwent to this assessment.

Air Quality Expert Group (AQEG) Report on "*Ozone in the UK*". Professor Pilling (Chair), Professor Derwent, Dr Jenkin and Dr Murrells (*ex-officio*) were members of Defra's Air Quality Expert Group (AQEG) that prepared a report on "Ozone in the UK". These members of the project consortium contributed in various ways to the report building on research carried out in this project. The project was used to support Jenny Young (University of Leeds) in providing the secretariat for completing the consultation draft of the report.

Review of Transboundary Air Pollution (RoTAP). Members of the project team have made contributions or assisted other members on text for the Defra Review of Transboundary Air Pollution (RoTAP). This review is including a chapter on ozone modelling. In particular, the OSRM has been used to provide surface ozone flux metrics on a 10x10km grid covering the UK for wheat, potatoes and beech in 2003 and 2020.

The University of Leeds managed the MCM website (http://mcm.leeds.ac.uk/MCM/).

Besides project meetings and other meetings directly related to the project, members of the consortium attended a number of other workshops, conferences and seminars:

A presentation was also given by Dick Derwent at the *International Aerosol Modelling Algorithms Conference* at University of California, Davis during December 2007.

Andrea Fraser attended a conference on developments of CMAQ at the USEPA, Chapel Hill, North Carolina, USA in October 2008.

Sally Cooke and John Abbott from AEA attended the *MESO-NET CREMO* Workshop held in June 2008 in London. The workshop was organised by the Environment Agency and NERC and the purpose was to explore how potential users can benefit from comprehensive model calculations and to identify realistic case studies to demonstrate the feasibility of CMAQ, which could be integrated into the CREMO/MESO-NET programme. Potential applications of CMAQ were discussed.

Mike Holland (EMRC) gave a presentation on the work undertaken in Objective 7, "*Modelling solvent dispersion, chemistry and health impacts to inform policy development on VOC control*", (M Holland, T Murrells, D Derwent and M Jenkin) at the Eleventh Annual UK Review Meeting on Outdoor and Indoor Air Pollution Research, 15-16 April 2008 at Cranfield University

Andrea Fraser and Dick Derwent attended the MESO-NET Uncertainty and Model Evaluation Specialist Topic Meeting at the University of Hertfordshire in April 2009.

6 Technical Reports and Publications

Besides the regular quarterly reports and two annual reports, the following specialist technical reports and publications in the peer-reviewed literature resulted from this project:

6.1 Reports

"***A Review of the Master Chemical Mechanism***". R.G. Derwent, M.E. Jenkin, T.P. Murrells, M.J. Pilling and A.R. Read. Report to Defra, July 2007.

"***Climate Change Consequences of VOC Emission Controls***". T Murrells and RG Derwent. Report to the Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland. AEA Report AEAT/ENV/R/2475 - Issue 3, September 2007.

"***Emission Sensitivities for PM Components for Harwell, Oxfordshire Estimated Using a Photochemical Trajectory Model for 2006***". RG Derwent. Report by rdscientific, September 2007

"***NAME Modelling to Support Empirical Modelling of Secondary PM Projections***". A Redington. Report by the Met Office, November 2007

"***UK air quality modelling for annual reporting 2006 on ambient air quality assessment under Council Directives 96/62/EC and 2002/3/EC relating to ozone in ambient air***". A.J. Kent and J.R. Stedman (2008). Report to the Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland. AEA Report AEAT/ENV/R/2499 (2008).

"***Performance of the Ozone Source Receptor Model Against Recommendations of the DEFRA Review on Tools for Modelling Tropospheric Ozone***". T P Murrells, S. Cooke and R.G. Derwent. Report for the Department for Environment, Food and Rural Affairs and the Devolved Administrations. AEA Report AEAT/ENV/R/2653, July 2008

"***Costs, benefits and trade-offs: Volatile organic solvents***". Final report by Mike Holland and Joe Spadaro (EMRC), with contributions from: Dick Derwent, Mike Jenkin and Tim Murrells, August 2009.

"***Evaluating the Performance of Air Quality Models***". RG Derwent, A Fraser, J Abbott, ME Jenkin, P Willis and T Murrells. Report to the Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Executive and the Department of the Environment for Northern Ireland. AEA Report AEAT/ENV/R/2873 - Issue 2, September 2009

6.2 Research Publications

"***Modelling the impact of elevated primary NO2 and HONO emissions on regional scale oxidant formation in the UK***". Jenkin M.E., Utembe S.R. and Derwent R.G. Atmospheric Environment, 42, 323–336 (2008).

"***Up in the air***" Derwent, D., Jenkin, M., Passant, N., Pilling, M. (2008). Chemistry and Industry, 26 May 2008

"***Trends in ozone concentration distributions in the UK since 1990: Local, regional and global influences***" Jenkin, M.E. (2008) Atmospheric Environment 42 (2008) 5434–5445

"***A Common Representative Intermediates (CRI) mechanism for VOC degradation. Part 1: Gas phase mechanism development***" Jenkin M.E., Watson L.A., Utembe S.R. and Shallcross D.E. (2008).. Atmospheric Environment, 42, 7185-7195.

"***A Common Representative Intermediates (CRI) mechanism for VOC degradation. Part 2: Gas phase mechanism reduction***." Watson L.A., Shallcross D.E., Utembe S.R. and Jenkin M.E. (2008). Atmospheric Environment, 42, 7196-7204.

"***Detailed chemical analysis of regional-scale air pollution in western Portugal using an adapted version of MCM v3.1***". Pinho P.G., Lemos L.T., Pio C. A., Evtyugina M. G., Nunes T.V. and Jenkin M. E. (2009).. Science of the Total Environment, 407, 2024-2038.

"***Particulate matter at a rural location in southern England during 2006: Model sensitivities to precursor emissions***". Derwent R., Witham C., Redington A., Jenkin M., Stedman J., Yardley R. and Hayman G. (2009). Atmospheric Environment, 43, 689–696.

"***A Common Representative Intermediates (CRI) mechanism for VOC degradation. Part 3: Development of a secondary organic aerosol module***". Utembe, S.R., Watson, L.A., Shallcross, D.E., Jenkin, M.E., 2009. Atmospheric Environment, 43, 1982–1990.

"***Secondary organic aerosol formation from a large number of reactive organic compounds under European conditions***". Derwent RG, Jenkin ME, Utembe SR, Shallcross DE, Murrells TP and Passant NR. Submitted to Atmospheric Environment, May 2009

7 Conclusions and Recommendations for Further Work

The project has continued to use the OSRM and PTM to model the impact of emission scenarios on ground-level ozone in the UK across a range of temporal and spatial scales. These models are the current “work-horses” for evaluating the effects of emission reduction policies on UK ozone on behalf of Defra.

The project has also enhanced the understanding of the atmospheric chemistry involved in formation of ozone and secondary organic aerosol and has led to the further development of explicit photochemical reactions schemes of various levels of size and complexity that can be used in chemical transport models to model the contribution of different precursor VOC emissions to formation of these air pollutants. Particular enhances were made in the Master Chemical Mechanism and associated condensed codes, including the treatment of biogenic VOCs and formation of Secondary Organic Aerosols, leading to the development of the Secondary Organic Aerosol Potential as a useful concept for policy in describing the propensity for different VOCs in formation of organic aerosols, analogous to the Photochemical Ozone Creation Potential (POCP) concept for ozone.

The project has also enhanced our understanding of the complex coupling between ozone, NO and NO_2 leading to improved semi-empirical relationships for assessing the hemispheric, regional and local contributions to ozone and NO_2 in different UK environments.

Following the recommendations of Defra’s independent review of ozone models, the project has demonstrated the application of an alternative Eulerian-based model, CMAQ, for modelling ozone on a national scale in the UK over a time-period from a month to a year. Although a computationally more expensive model, CMAQ can provide a realistic description of the UK’s ground-level ozone climate in 2006. A more in-depth evaluation of the model is required. A protocol has been developed and demonstrated for evaluating and comparing the performances of this and other air pollution models.

The research consortium involved in this project has recommended a research programme to build on the progress made to date whilst maintaining an ozone modelling service using existing tools. The core programme proposed includes:

- the application of current models in support of Defra policy on ozone and secondary PM, including the modelling of UK ozone in 2009 and 2010 with emission uncertainty and sensitivity analyses
- further improvements to photochemical reactions schemes used in models relating to the role of biogenic and solvent emissions in ozone and Secondary Organic Aerosol (SOA) formation.
- further assessment of background and urban-scale oxidant through analysis of ambient data to further improve local effects in models used for Defra policy.

However, we have also proposed the further optimisation, assessment and application of a Eulerian-based model to assist with Defra ozone and secondary PM policy, building on the experiences of the current project, combined with the further development and application of the model intercomparison protocol to give a rigorous assessment of the performances of CMAQ, OSRM and PTM as tools for Defra ozone policy assessment.

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