Environment Agency

Evidence

Comparison of Simple and Advanced Regional Models (CREMO)

Model Evaluation: Ground-level Ozone

Report – SC060037/d

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This report is the result of research commissioned and funded by the Environment Agency.

Published by:
Environment Agency, Horizon House, Deanery Road, Bristol, BS1 5AH

www.environment-agency.gov.uk

ISBN:

Further copies of this report are available from our publications catalogue: http://publications.environment-agency.gov.uk or our National Customer Contact Centre: T: 08708 506506
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Dissemination Status:
Publicly available

Keywords:
Ozone, photochemistry, regional air quality models, evaluation, diagnostic, acceptance criteria, metrics, monitoring network, NOx, VOC, precursors

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Project Number:
SC060037/d

Product Code:
LIT

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Miranda Kavanagh

Director of Evidence

Executive summary

Ozone is a secondary pollutant formed in the lower atmosphere from the sunlight-initiated oxidation of volatile organic compounds (VOCs) in the presence of oxides of nitrogen (NOx). Exposure to ground-level ozone has effects on human health, crops and vegetation, and materials such as rubber, paints and plastic. Air quality standards have been established to mitigate effects on human health and vegetation, but these standards are widely exceeded across the UK and Europe.

As part of the CREMO project, a comparison of two modelling systems for ground-level ozone has been undertaken. The two modelling systems were (a) the Community Multi-scale Air Quality (CMAQ) modelling system (versions 4.6 and 4.7), operated by the University of Hertfordshire and (b) the Ozone Source-Receptor Model (OSRM), developed and used by AEA Technology.

Comparison of the annual mean concentrations of ozone and NO_2, especially along a given transect, showed very good agreement between the two modelling systems, both qualitatively and quantitatively. There were almost identical changes in the concentrations of O_3 and NO_2 when the emissions of a representative refinery regulated by the Environment Agency were removed. The response to the reduction in the refinery emissions was dominated by the reduction of the NOx emissions.

Contents

1 Introduction

The overall aim of the CREMO project is to enable the Environment Agency to make an informed decision on the use of advanced regional-scale atmospheric chemical transport models as one of its assessment tools. In particular the project has evaluated the performance characteristics of the Community Multiscale Air Quality (CMAQ) modelling system[1] for real regulatory applications through comparison of CMAQ with existing methods. The project applies CMAQ to a series of assessments including acid deposition, particulate matter, and ozone and tests its capabilities through targeted comparisons with 'simpler' models and with measurements according to agreed model acceptance criteria. This report contains an evaluation of the capabilities of CMAQ to predict regional ozone concentrations in the UK and their response to changes in emissions of nitrogen oxides (NOx) and volatile organic compounds (VOCs).

1.1 Background

The emissions of sulphur dioxide (SO_2), oxides of nitrogen (NOx), volatile organic compounds (VOCs) and ammonia contribute to a number of environmental impacts which affect human health and/or ecosystems: acid deposition/eutrophication, ground-level ozone and particulate matter. These impacts do not necessarily occur in the immediate vicinity of the emission source but often involve long-range transport to the affected areas, a result of the timescales for chemical processing of the emissions in the atmosphere.

The Environment Agency is responsible for the regulation of specific industrial sectors and has long used regional-scale atmospheric chemical transport models to assist in setting emission limits. The Department for Environment, Food and Rural Affairs (Defra) also makes use of such models to assist in the development of policy measures relating to the environmental impacts resulting from such emissions (including provision of input into the UN Economic Commission for Europe Convention on the Long Range Transport of Air Pollutants protocols and EU Directives). A number of different models have been used by Defra and the Environment Agency to cover specific impacts and spatial scales: for example, FRAME for acid deposition, TRACK-ADMS for annual audits and the Ozone Source-Receptor Model (OSRM) for ozone.

Since the late 1990's, a number of 'advanced' models have been developed with the capability to address multi-pollutant issues on multiple scales. The modelling systems included the Community Multiscale Air Quality (CMAQ) modelling system (Byun and Schere 2006), the Unified EMEP model (Simpson *et al*. 2003) and the CHIMERE model (Bessagnet *et al*. 2009 and references therein). These are all available for use by the air pollution research community.

In 2007, Defra commissioned a review of its ozone modelling tools (including the OSRM) (Monks *et al*. 2007), as part of a wider review of its air pollution modelling activities. The review noted that the UK modelling approach differed from other countries in its use of boundary layer trajectory models. One of its key recommendations (R1.1) was to move to a

[1] When the project was commissioned, MODELS3 was the operational version of this community air quality model. MODELS3 comprised the Community Multiscale Air Quality (CMAQ) modelling system and the MM5 mesoscale meteorological model. The MM5 model has since been replaced by the Weather Research and Forecasting (WRF) numerical weather prediction model. All references to MODELS3 have been updated to CMAQ to avoid confusion.

Eulerian framework, as used by advanced models such as CMAQ and EMEP. Other recommendations were:

- To compare Eulerian model results with the results from observations and with those from comparative Lagrangian models to ensure continuity (R 1.2);
- To conduct a model comparison exercise where two of the current Lagrangian-based models are compared to two (or more) regional air quality Eulerian-based models.

As part of the Joint Environment Programme (JEP), the power generators (E.ON and RWE npower) have being using CMAQ to investigate the contribution and significance of the power generation sector (Wright 2008).

1.2 Project aims and objectives

The CREMO project has two main objectives:

1. To provide a technique for assessing the contribution of industrial emissions of NOx and VOC under realistic meteorological conditions to ambient levels of ozone based on CMAQ and involving comparison with simpler methods and observations.
2. To provide a technique for assessing the contribution of industrial emissions under realistic meteorological conditions to ambient levels of PM_{10} and $PM_{2.5}$, based on CMAQ and involving comparison with simpler methods and observations.

This report is concerned with the following specific task:

To evaluate the capabilities of CMAQ to predict regional ozone concentrations and their response to changes in emissions of nitrogen oxides (NOx) and volatile organic compounds (VOCs);

1.3 Structure of document

This document describes the work undertaken under the task above. It is structured as follows:

- Background on ground-level ozone and information on the case study (Section 2).
- Results of the case study. A summary of relevant findings from Defra's regional model inter-comparison exercise (Section 3).

2 Assessment of ground-level ozone

2.1 Background

Ozone (O_3) is a secondary pollutant formed in the lower atmosphere from the sunlight-initiated oxidation of volatile organic compounds (VOCs) in the presence of nitrogen oxides (NOx). The chemistry is very non-linear and ozone concentrations do not respond in a simple manner to precursor emission control. Ozone is also present in the unperturbed atmosphere and ground-level concentrations are influenced by input from the stratosphere and by changes occurring at the hemispheric scale (*e.g.* as a result of climate change) (AQEG, 2009).

While the control of VOCs emissions generally improves ozone air quality, the position is more complex for the emissions of oxides of nitrogen (*i.e.*, nitric oxide and nitrogen dioxide). Oxides of nitrogen are involved in both the production of ozone and, at higher concentrations, the loss of ozone. There is a strong coupling between the concentrations of ozone and oxides of nitrogen (NOx), as illustrated in Figure 2.1 (adapted from Clapp and Jenkin 2001).

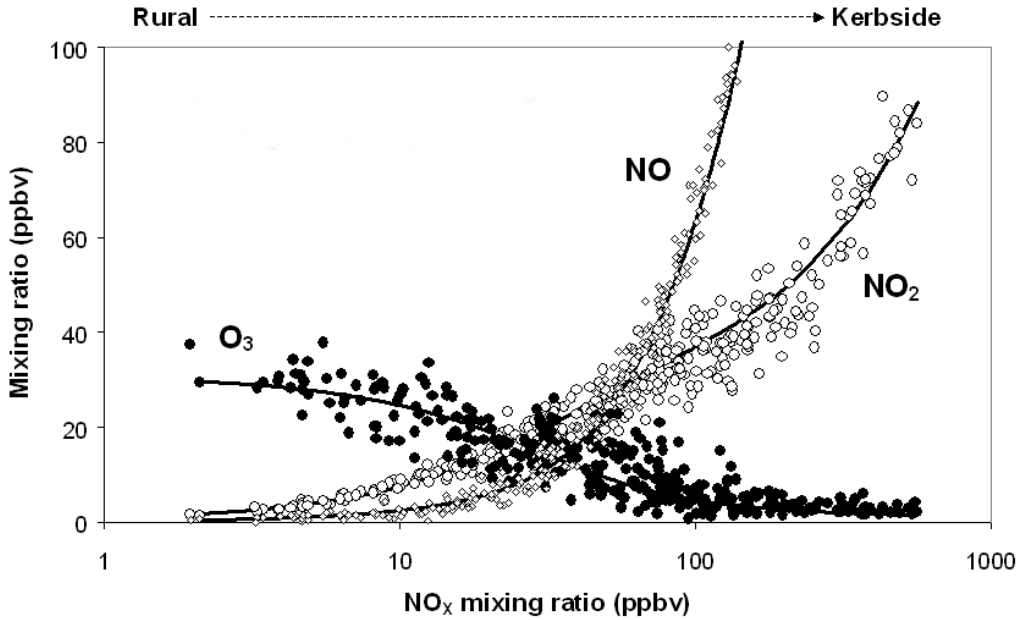


Figure 2.1 Dependence of the observed daylight average mixing ratios of O_3, NO and NO_2 on the concentration of NO_X at six southern UK sites (note that the NO_X axis is logarithmic). The solid lines were calculated with the assumption of the photo-stationary state.

Figure 2.1 shows that concentrations of ozone are generally higher in rural locations compared to urban and, at the opposite extreme, kerbside locations, where the emissions and hence concentrations of oxides of nitrogen are higher. The concentrations of ozone are suppressed through the reaction of ozone with nitric oxide. As the emissions and hence

concentrations of oxides of nitrogen are reduced at these locations, ozone concentrations will rise and tend towards the concentrations observed at surrounding rural sites.

The non-linear nature of these processes requires the use of sophisticated chemical transport models to understand the production of ground-level ozone and its subsequent control.

2.2 Models

The main models participating in the CREMO project were:

- the Community Multiscale Air Quality (CMAQ) modelling system (versions 4.6 and 4.7), operated by the University of Hertfordshire and the power generators (Chemel *et al*. 2010, Wright 2008).
- the Fine Resolution Atmospheric Multi-pollutant Exchange (FRAME) model, developed and operated by the Centre for Ecology and Hydrology (CEH) (Dore *et al*. 2007, Matejko *et al*. 2009, Vieno *et al*. 2010a).
- TRACK-ADMS, developed and operated by AEA Technology (Abbott and Vincent 2006).
- the Ozone Source-Receptor Model (OSRM), developed and operated by AEA Technology (Hayman *et al*. 2010, Hayman *et al*. 2006).

In this assessment (Task (c) in the CREMO project) the relevant simple and complex chemical transport models for ground-level ozone are compared. Specifically, model runs were undertaken using CMAQ v4.6 (University of Hertfordshire) and OSRM (AEA Technology). The CREMO model evaluation protocol (Hayman *et al*. 2012a) has been applied to evaluate the performance of the participating models.

2.3 Selected case study

The assessment for ground-level ozone adopted in the CREMO project was based on the footprint of a large industrial facility regulated by the Agency. In task (a), the footprint produced by a power station had been compared (Chemel *et al*. 2011). This however was not an appropriate installation for the assessment of ozone as power stations are not a major source of volatile organic compounds, a key component of photochemical or ground-level ozone. The Fawley refinery was therefore selected as the installation for this comparison.

The annual emissions of oxides of nitrogen (NOx) and volatile organic compounds (VOC) from the refinery in 2003, the year selected for the CREMO comparison, are summarised in Table 2.1, together with the total UK emissions. The refinery emissions represent 0.4-0.5% of the UK total emissions.

Table 2.1 Emissions of oxides of nitrogen and volatile organic compounds for the UK and the Fawley Refinery in 2003

Pollutant	Total UK emissions ktonnes per annum	Fawley emissions ktonnes per annum	Fawley emissions as % of Total
NOx	1608.7	5.74	0.4
VOC	1199.0	5.55	0.5

Table 2.2 provides a breakdown of the refinery VOC emissions to specific activities (without speciation) and the allocation to the different SNAP (Selected Nomenclature for Air

Pollutants) level 1 source categories (sectors). This breakdown was used to create a set of emission maps where the refinery emissions have been removed from the total.

Table 2.2 Breakdown of the Fawley Refinery VOC emissions by SNAP source sector.

Source Type	SNAP Sector	Emissions tonnes per annum
Combustion	1: Combustion	59
Flaring	9: Waste	3
Drainage	4: Production	1,359
Process	4: Production	4,034
Tankage	4: Production	100
TOTAL		**5,555**

Two runs were undertaken for the year 2003:

1. Base case run – with all emissions (refinery and non-refinery)
2. Footprint run – with all non-refinery emissions (*i.e*. without the refinery emissions)

A third run was also undertaken using the OSRM in which only the refinery VOC emissions were excluded. The model run still made use of the refinery NOx, CO and SO_2 emissions.

3 Results

The assessment of ozone in this report is largely a dynamic evaluation (see Box 1 in the CREMO Model Evaluation protocol (Hayman *et al*. 2012a)):

- *Operational evaluation* is a comparison of model-predicted and routinely measured concentrations of the end-point pollutant(s) of interest in an overall sense.
- *Diagnostic evaluation* entails investigating the atmospheric processes and input drivers that affect model performance to guide model development and improvements needed in emissions and meteorological data.
- *Dynamic evaluation* assesses a model's air quality response to changes in meteorology or emissions, which is a principal use of an air quality model for air quality management.
- *Probabilistic evaluation* strives to characterize uncertainty of the model predictions for model applications such as predicted concentration changes in response to emission reductions.

3.1 Ozone metrics

Many metrics have been used to evaluate the impact of ground-level ozone on human health, ecosystems and materials (see AQEG, 2009). Hayman *et al.* (2012b) undertook a short review and recommended that the following metrics should be used in the CREMO project:

- Annual mean ozone concentration: a general indicator, sensitive to local NOx emissions.
- Annual mean concentrations of NO_2, NOx and Ox = [NOx] + [O_3]: as there is strong coupling between O_3 and NOx.
- Maximum running 8-hour mean concentration: this will be sensitive to peak concentration and the photochemical production of ozone.
- SOMO35: widely used as a metric to assess the impact on human health in policy development. Note that this effectively equal to the UK metric used in the Air Quality Strategy.
- AOT40: widely used as a metric to assess the impact on vegetation in policy development.

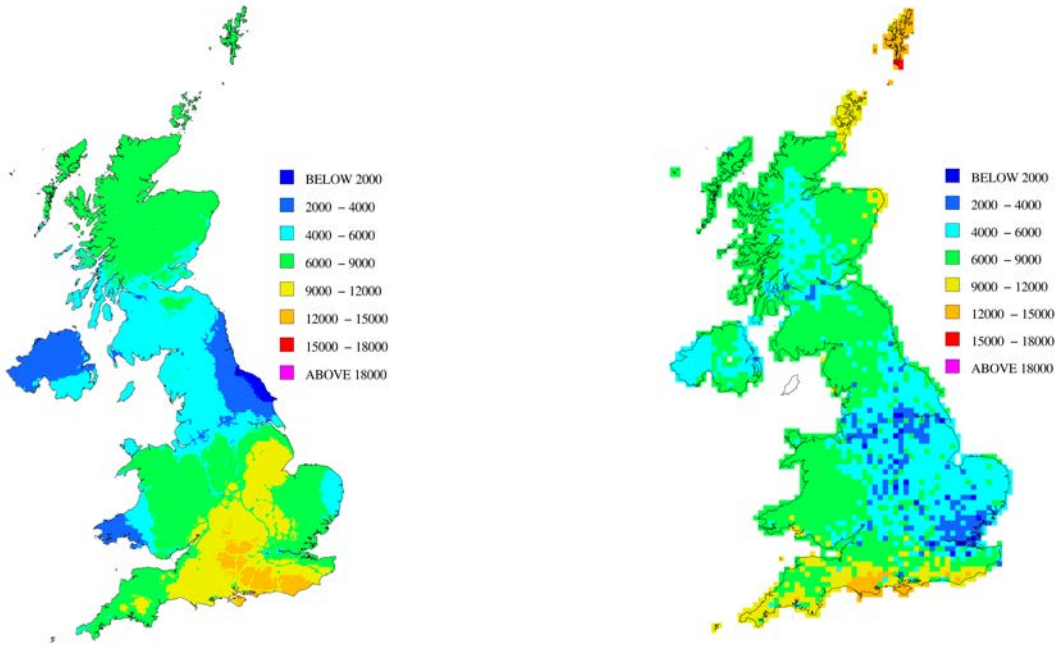
Only one of these metrics focuses explicitly on peak ozone concentrations, the maximum running 8-hour mean concentration. Peak concentrations in all the other metrics are attenuated to some extent by the presence of lower ozone concentrations on days without an ozone episode within the averaging, so that for these metrics the build up of ozone during episodes is not likely to be seen.

3.2 Ozone in 2003

The year 2003 was selected as the one to be used for the CREMO model inter-comparison. It was one of the hottest years on record, with the highest UK temperature (38.1 ºC) recorded at Gravesend in Kent on 10th August 2003. It was a year with marked photochemical activity. Major photochemical episodes occurred in July and August across

the UK and Northern Europe. The peak O_3 concentrations during these episodes were 246 μg m^{-3} at Harwell (15th July), 238 μg m^{-3} at London Brent (6th August), 236 μg m^{-3} at London Brent and Lullington Heath (11th August). These were classical UK photochemical ozone episodes: high pressure conditions existed with easterly airflows bringing polluted air to the UK from Europe. Although ozone concentrations were higher than those recorded in more recent years, the episodes were largely limited to the central and southern parts of the UK, as illustrated in Figure 3.1. The left-hand panel of the figure shows a map of the AOT40 exposure metric for crops (wheat) for 2003 derived using the empirical Pollution Climate Mapping approach (Bush *et al*. 2005).

Figure 3.1 also shows the equivalent map produced by the OSRM. The OSRM underestimates the AOT40 metric. There has been debate in the scientific literature as to the cause of the episodes (forest fires in Portugal (Solberg *et al*. 2005), elevated isoprene emissions (Vieno *et al*. 2010b)). Forest fires and elevated isoprene emissions would not normally be included in the inventories used by the OSRM and CMAQ models.



PCM **OSRM**

Figure 3.1 Maps of AOT40 wheat crops metric (in μg m^{-3} hours) derived for 2003 using the empirical approach of the Pollution Climate Model (left-hand panel) and the Ozone Source-Receptor Model (right-hand panel)

3.3 Case study

The modelled annual mean concentrations of ozone and nitrogen dioxide derived using the OSRM for the base case along a south to north transect that includes the refinery (OS coordinates 445.55 E 103.65 N) are shown in Figure 3.2. The figure also includes the difference in concentrations between the base case and the base case when the emissions of the refinery are removed (*i.e.* the footprint of the refinery). The differences are small (for O_3, a maximum increase of ~1 ppb in 25 ppb in the immediate vicinity of the source but much lower elsewhere).

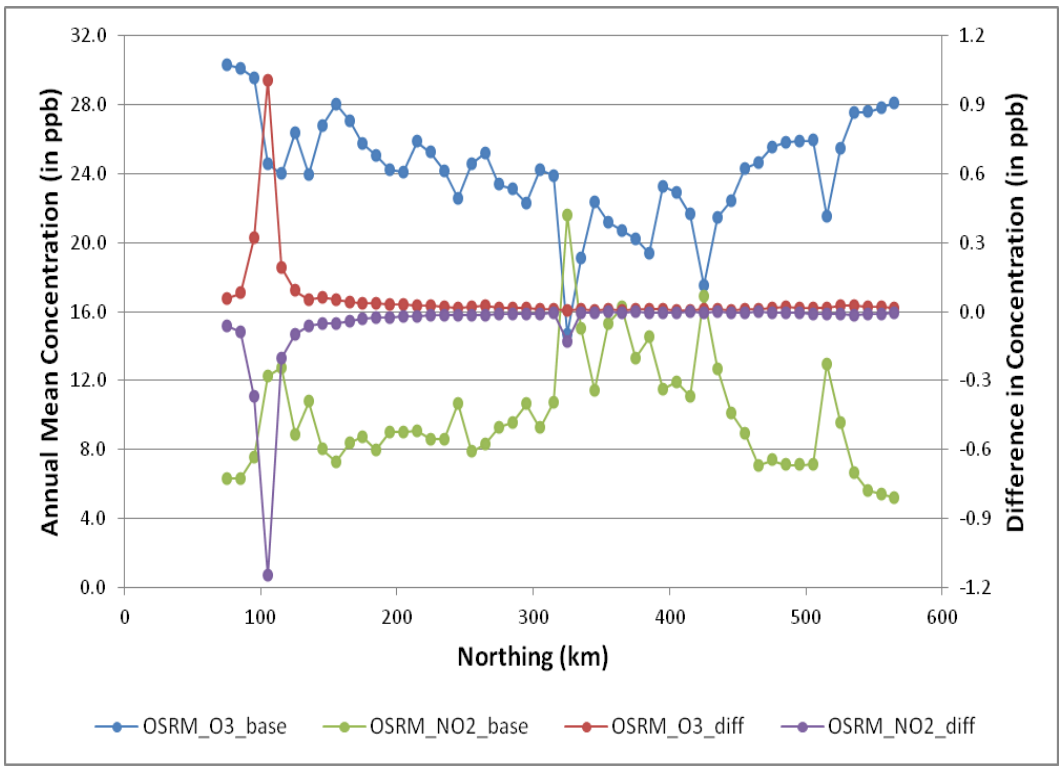
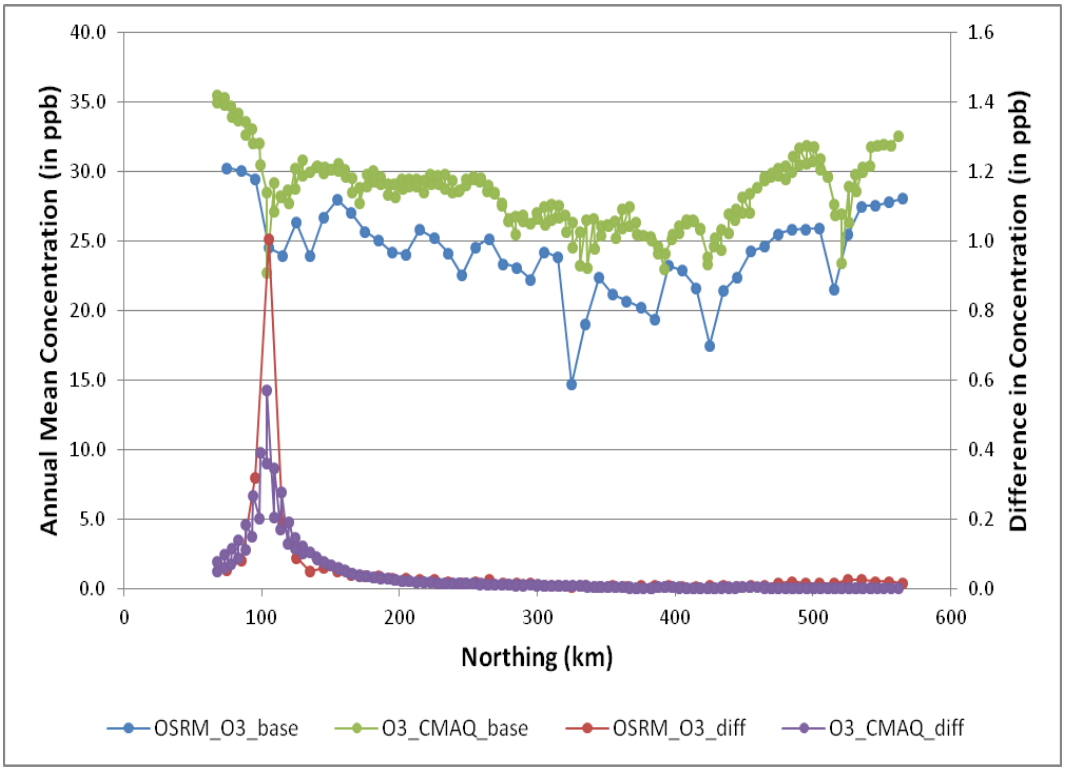


Figure 3.2 The modelled annual mean concentrations (in ppb) of ozone (blue) and nitrogen dioxide (green) along a south to north transect through the refinery, as derived using the OSRM for the base case scenario. The difference in the modelled annual mean concentrations (in ppb) of ozone (red) and nitrogen dioxide (purple) along the same transect between the base case scenario and no refinery emissions.

The concentration along a transect is a diagnostic related to the distance dependence along a radial trajectory illustrated in Fisher (2012). Much of the decrease in annual average concentration is related to the effect of the spread of trajectory end points with distance travelled. One expects a $(\text{distance})^{-1}$ dependence within the concentration along a transect from this effect.

A comparison of the modelled annual mean concentrations of O_3 and NO_2 calculated using the OSRM and CMAQ models along the same south to north transect through the refinery is shown in Figure 3.2. As the OSRM and CMAQ model runs used different model grids and spatial resolutions (OSRM, 10 km and CMAQ, 5 km), the CMAQ grid was first converted to

Ordnance Survey coordinates and values within ±5 km of the selected south to north transect were taken. The results are both qualitatively and quantitatively similar, although it can be seen that CMAQ has higher O_3 concentrations.



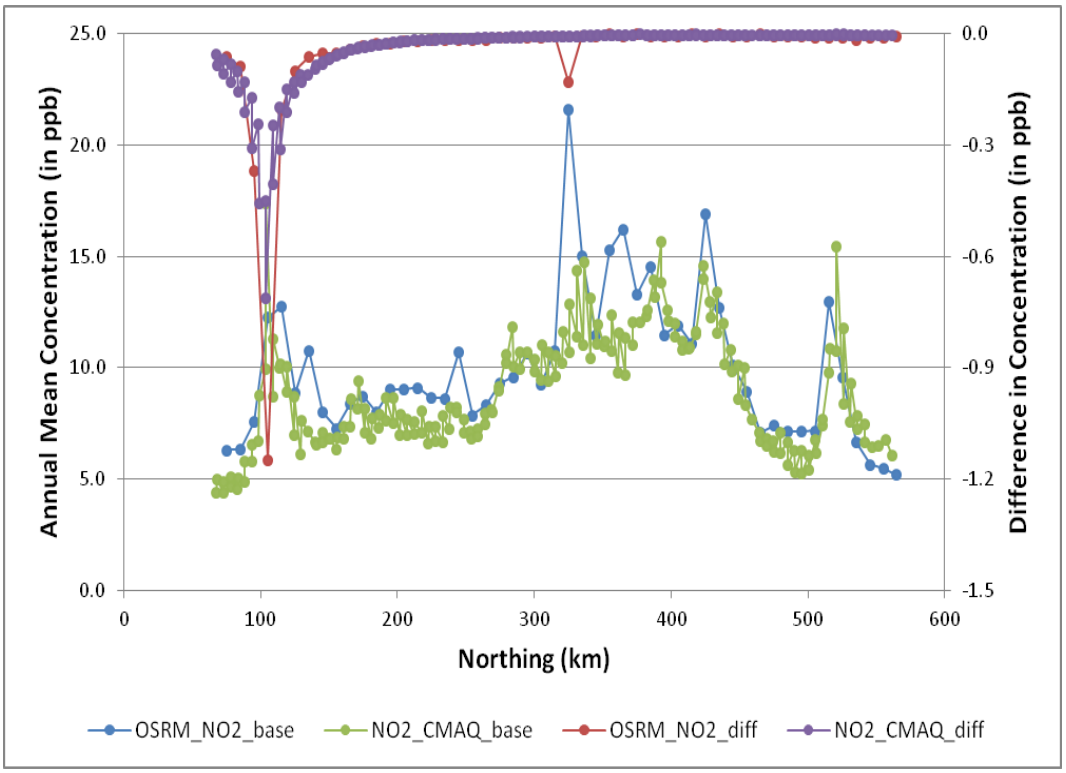


Figure 3.2 Upper panel, modelled annual mean concentrations (in ppb) of ozone along the south to north transect through Fawley derived using the OSRM (blue) and

CMAQ (green) models for the base case scenario. The difference in the modelled annual mean concentrations (in ppb) of ozone along the same transect between the base case and the base case when the emissions of the refinery are removed as calculated using the OSRM (red) and CMAQ (purple) models are also shown. The lower panel shows the corresponding plots for nitrogen dioxide.

To provide further insight, an additional run was undertaken using the OSRM in which only the VOC emissions from the refinery were switched off. Figure 3.3 shows the modelled annual mean concentrations of O_3 and NO_2 for the base case scenario and the difference in the modelled concentrations between the base case and the emission reduction scenarios. The figure is equivalent to Figure 3.2 except that *only* the refinery VOC emissions have been switched off. It can be seen that the VOC emission reduction scenario is little different from the base case run. This is in contrast to the larger response in the vicinity of the refinery when all the emissions are removed. Again, the VOC emission reduction run provides further confirmation that the NO_x emissions from the refinery account for the behaviour when both NO_x and VOC emissions were switched off.

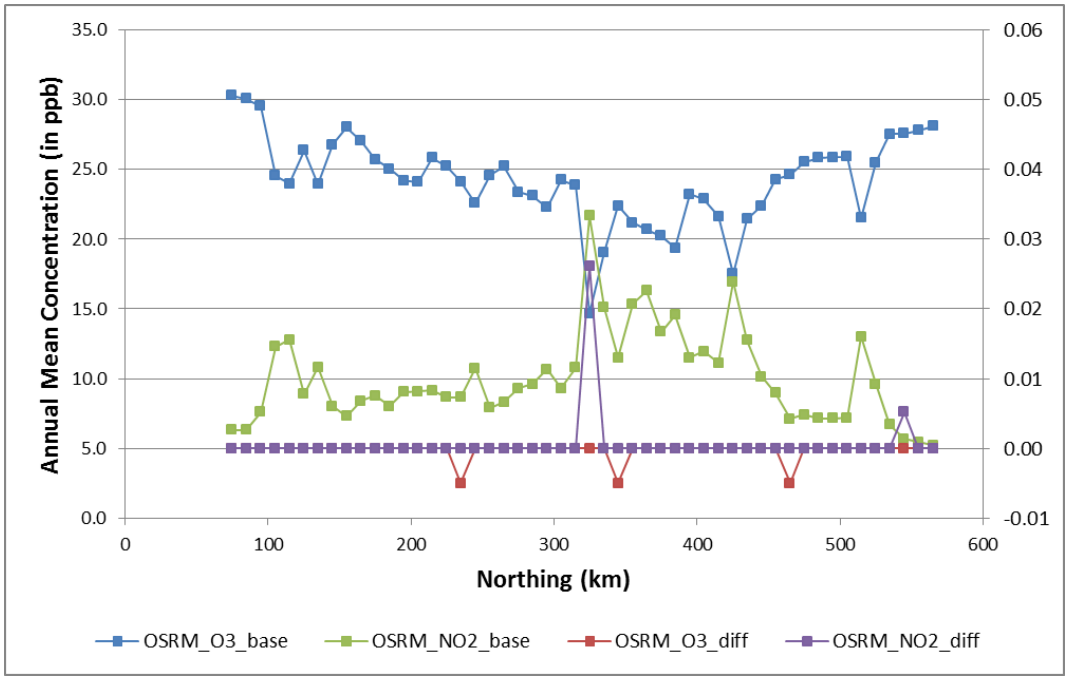


Figure 3.3 The modelled annual mean concentrations (in ppb) of ozone (blue) and nitrogen dioxide (green) along the south-north transect through Fawley as derived using the OSRM for the base case scenario. The very small differences in the modelled annual mean concentrations (in ppb) of ozone (red) and nitrogen dioxide (purple) along the same transect between the base case scenario and no refinery VOC emissions are also shown. See scale on the right hand side.

There is some evidence of a small increase which may reflect a subtle change in the 'reactivity' of the VOC emissions when the refinery emissions are removed. The OSRM uses different VOC speciations for each SNAP sector, which were derived from the NAEI speciated VOC inventory of Passant (2002).

3.4 Defra Model Intercomparison

The Department for Food, Environment and Rural Affairs (Defra) is undertaking a model inter-comparison exercise (MIE) to assess the capabilities of the models, that the Department uses to assess air pollution, and of the other models used by the UK air pollution research community. The OSRM model and the CMAQ model of the University of Hertfordshire are both involved in the regional MIE, which considers the models used for photochemical or ground-level ozone production[2].

The first phase, which was largely an operational evaluation, has been completed (Carslaw, 2011). A second phase is currently in progress. The evaluation has focused on several key areas (i) observed and modelled ozone metrics at a location where 'baseline' or 'background' O_3 dominates (Mace Head), (ii) the ability of the models to predict specific O_3 metrics of relevance to air quality policy, (iii) the effect of precursor (NOx and VOC) emission reductions at a UK and European scale and (iv) the performance of the models in predicting common meteorological variables measured at Met Office surface stations in the UK. The year 2006 was selected as the year of interest (compared to 2003 in CREMO).

The initial set of results from the second phase (Carslaw 2012) indicates that there was no single model which out-performed the others. Indeed different models performed better for the different metrics. Of more relevance to the CREMO project are the four emission reduction scenarios that were investigated:

- Scenario S1 — reduction of total anthropogenic NOx and VOC by 30% across the UK + Europe,
- Scenario S2 — reduction of total anthropogenic NOx and VOC by 30% across the UK only,
- Scenario S3 — reduction of total anthropogenic NOx by 30% across UK + Europe,
- Scenario S4 — reduction of total anthropogenic VOC by 30% across UK + Europe.

These are similar in magnitude to the reductions in NOx and VOC emissions agreed recently under the Gothenburg Protocol (UNECE 2012), which sets limits on the percentage reduction in these pollutants and SO_2, ammonia and $PM_{2.5}$ in European countries between 2005 and 2020. These scenarios are therefore of actual policy relevance, pointing to the kind of reductions in concentrations one might expect by 2020.

One of the key summary points in the draft report (Carslaw 2012) noted that there was a very wide range of responses produced by the participating models for the emission reduction scenario runs considered, for both metrics sensitive to long-term (*e.g*. annual means) and episodic exposure. For annual average ozone, the result from the OSRM model for 2006 lies within the range of variation of three versions of the CMAQ model used in the MIE. The normalised bias is slightly positive (indicating over-prediction) but is generally less than 0.1 averaged over rural sites for all four models. Urban sites should be excluded as one does not expect good predictions in Eulerian models with coarse grid resolutions larger than the emission variations which arise within urban conurbations.

Results could be dominated by the boundary conditions at the edge of the model domain. The magnitude of the relative change in the annual average ozone at rural sites resulting from the emission reduction scenarios S1, S2, S3 are slightly positive. Only a reduction of

[2] The other participating models are: CMAQ models operated by AEA Technology and King's College London, the NAME and AQUM models of the Met Office, EMEP4UK from the Centre for Ecology and Hydrology, the Photochemical Trajectory model and the WRF-Chem model operated by the University of Manchester.

total anthropogenic VOC by 30% across UK + Europe leads to a reduction in annual average ozone and then by values that are all less than 1 μg m^{-3}. This suggests that the relative change in *annual average* ozone concentrations in the UK at rural sites from the emission changes within the Gothenburg Protocol would not be significant.

The change in the maximum daily ozone concentration, an indicator of the ozone concentrations reached during episodes over the UK, does show a reduction in all four models in scenario S1 across all *rural* sites for OSRM and the three versions of CMAQ, but an increase in scenario S2 (Carslaw 2012). Aggregating ozone concentrations over a network of monitoring sites may not be a good idea as episodes may not cover the whole country. Aggregating ozone concentrations over sites at a fixed hour of the day may further attenuate any episodic signal in a dynamic system varying in space and time. So identifying the ozone signal during an episode can be difficult. For S3 the response is a reduction in two models and an increase in the other two. For scenario S4 there is a reduction in concentrations in all models. The relative response is largest for S1 but even then less than 2%. There is an indication from the study of Derwent (2012) that the response in ozone to changes in emission does not depend on details of the chemistry. Different chemical schemes would produce broadly the same conclusions.

It is difficult to obtain a definite conclusion about the performance of ozone models during episodes from this preliminary analysis, though this is one of the key, desirable outcomes of the CREMO project (Fisher 2012). One should compare performance only when rural sites are included. At the site at Harwell (Carslaw 2012) in July 2006, a month with a number of ozone episodes, a reduction in VOC emissions, scenario S4, always brought a small relative reduction in ozone in all four models (OSRM and three versions of the CMAQ). The relative response to a reduction in NOx, scenario S3, brought a mixed (sometimes positive, sometimes negative) change in ozone.

4 Conclusions

The assessment of regional ozone concentrations was based on the footprint of a large industrial facility regulated by the Environment Agency. The Fawley refinery was selected as the installation. The comparison is effectively a dynamic evaluation.

The assessment has been undertaken according to the model evaluation protocol developed for the CREMO project (Hayman *et al*. 2012a). As ground-level ozone has multiple impacts and a number of metrics have been developed to assess the impacts (see for example AQEG (2009)), Hayman *et al.* (2012b) undertook a short review and recommended that the following metrics should be used in the CREMO project:

- Annual mean concentrations of ozone and NO_2,
- Maximum running 8-hour mean concentration,
- SOMO35,
- AOT40.

Comparison of the annual mean concentrations of ozone and NO_2, especially along a given transect, showed consistent agreement between two modelling systems (OSRM and CMAQ), both qualitatively and quantitatively. There were almost identical changes, but of opposite sign, in the concentrations of O_3 and NO_2 when the refinery emissions were removed. The response to the reduction in the refinery emissions was dominated by the reduction of the NO_x emissions. This was further confirmed by the fact that the largest changes occurred in the vicinity of the installation.

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