Review of tools for modelling tropospheric ozone formation and assessing impacts on human health & ecosystems

A report to collate, evaluate and summarise information on tools for modelling ozone (O_3) formation and assessing impacts on human health and ecosystems

prepared for the

United Kingdom Department for Environment, Food and Rural Affairs (**Defra**)

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1. Executive Summary

The work described in this report collates, evaluates and summarises information on tools available for modelling ozone (O_3) formation and assessing impacts on human health and ecosystems within the Defra policy context. Information on the major models used in the UK for ozone prediction is presented in comparison to a number of continental models and a US model.

The major components in chemical modelling systems and the principal sources of uncertainty are reviewed. An overview of the metrics required from ozone models is outlined. The heart of the report is Table 1 (page 36) which summarises the information that has been gathered. The results are discussed in section 5. Then follows a brief discussion of future safety and the report concludes with a set of recommendations for further action by Defra. Appendix B gives all the information obtained from our correspondents, to whom we are very grateful.

The principal recommendations are as follows.

Moving to an Eulerian Model (section 7.1)

R 1.1 Defra should consider moving its ozone modelling activity to an Eulerian basis.

R 1.2 The Eulerian model results should be compared with the results from observations and with those from comparative Lagrangian models to ensure continuity.

R 1.3 Defra should 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.

Tests of Chemical schemes; biogenic species (section 7.2)

R 2.1 Defra should aim to support models which use chemical schemes, tested for ozone, such as the MCM or CBM-IV. However, Defra should explore the use of surrogate schemes which have a firm basis in explicit chemistry and which have been tested by comparison with experimental data.

R 2.2 Defra should use models that have chemical schemes that allow robust coupling between the speciation in the emission inventories and the chemical scheme. This allows specific policy measures to be assessed more clearly and contains less simplifications and tuning of mechanisms.

R 2.3 Defra should require an improved representation of biogenic species in its chosen models, in order to be prepared for likely warmer summer periods in the future and to be able to better assess any biogenic/anthropogenic coupling. (see also R 3.5)

Emission estimates (section 7.3)

R 3.1 Defra should ensure that its chosen models have transparent sources of emission estimates.

R 3.2 Defra should ensure that its chosen models have recognised and realistic schemes for the spatial and temporal disaggregation of emission estimates. Some assessment is also required of how these might change in the future.

R 3.3 Defra should ensure its models are able to use the information in the NAEI.

R 3.4 Defra should investigate the policy need for its chosen models to include improved biogenic emission estimates, or land use data in conjunction with biogenic emission factors.

R3.5 Defra should ensure that the UK biogenic emission inventory is reassessed.

R 3.6 Defra should try to ensure that European and British estimates of emissions are updated as often and as reliably as possible.

Model evaluation and intercomparison (section 7.4)

R 4.1 Defra should ensure:

- any contracts let for ozone modelling include a review of the performance of its chosen models with observations, to ensure their continued performance levels; and
- regular comparisons between UK ozone models choosing, perhaps, periods of peak and background ozone, to ensure that the performance of the Defra chosen models is satisfactory.

R 4.2 Defra should ensure that UK ozone policy models have a strong peer-reviewed evidence base.

R 4.3 Defra should ensure that UK ozone models are taking part in European wide comparisons for policy purposes, to model observations from small groups of high quality stations in chosen countries, to ensure the performance of its own models, and of those used by the EU for regulatory purposes.

R 4.4 Defra should ensure that a chosen model is regularly reviewed for updating. Where a model is a version of a parent model developed elsewhere, the latest version of the parent model should be used.

Model Quality Control (section 7.5)

R 5.1 Defra should require the principal investigators for its chosen models to consider the recommendations of the Royal Meteorological Society (1995) on the use of models and, where appropriate, to follow them.

Extension to other species (section 7.6)

R 6.1 Defra should use a modelling approach that allows a number of policy areas in air quality to be assessed.

Model review and a modelling forum (section 7.7)

R 7.1 Defra should implement a systematic series of peer reviews for its models to ensure their continued satisfactory performance and to facilitate their extension to other appropriate species.

R 7.2 Defra should run a regular modelling forum or actively participate in appropriate Knowledge Transfer networks to ensure community review and awareness of its requirements and performance.

2. Introduction

2.1 Ozone as a pollutant

Ozone (O_3) is a relatively strong oxidising agent which, in sufficient concentrations, can be detrimental to human health and inhibit the growth of crops and damages natural ecosystems.

Photochemical oxidant formation was first recognised as a pollution problem in Los Angeles in the middle of the 20th Century. In Europe the regional trans-boundary nature of ozone pollution was realised in the last quarter of the century as emissions of NO_x and VOC from traffic and industry increased. Photo-oxidant pollution is now a problem throughout the globe, particularly in the tropical conurbations where uncontrolled emissions are subject to intense sunlight.

Ozone is a so-called secondary atmospheric pollutant as it is not emitted but formed photochemically in the lower atmosphere by the chemical reactions nitrogen oxides (NO and NO_2, referred to as NO_x) with volatile organic compounds (VOC) in the presence of sunlight.

While ozone is mainly formed photochemically in the lower atmosphere (the troposphere), there is some transfer down from the stratosphere where concentrations are much higher. The magnitude and impact of S-T exchange is still a matter of debate.

Since ozone has an appreciable lifetime in the atmosphere it can be transported long distances far from source regions or from the site of a transfer from the stratosphere. In the Earth's northern hemisphere, the background concentration is within a range of 40 to 70 $\mu g\ m^{-3}$. (WHO, 2000).

There are two main processes that can remove ozone from the troposphere, photochemical loss routes via photolysis and reaction with HO_x radicals, and (dry) deposition to the Earth's surface.

The concentration increases on normal summer days to levels of 80 to 120 $\mu g\ m^{-3}$ but concentrations can increase much more during ozone episodes. In north western Europe, these usually occur in periods of warm weather which ensue when a zone of high pressure forms over a region and remains nearly stationary. Concentrations can then rise to levels of 300 $\mu g\ m^{-3}$ or more.

Normally ozone concentrations decrease over night as photochemical production ceases and ozone is removed at the ground, so a marked diurnal variation is observed in the concentrations. During episodes the extent of the variation may diminish and the concentrations remain high throughout the night as well.

The major sources of the ozone precursors (NO_x and VOC) are vehicular traffic and industrial processes. The amount of ozone formed depends on the intensity of the light and on the ratio [VOC]/[NOx]. Ratios between 4 and 10 are favourable for ozone formation at appropriate light intensities. In the centre of conurbations, NO_x concentrations are high so little ozone is formed; chemically much of the ozone formed is scavenged by NO. However as an air mass moves out into the countryside the NO_x concentrations fall and more ozone is formed.

Thus high ozone concentrations do not usually occur where one might intuitively expect, in the centre of cities, close to the major sources. The highest concentrations are found in the hinterland of cities – suburbs and rural areas downwind of the city. This is a practical example of the effect of the non-linearity in ozone formation and removal which, together with atmospheric transport, makes it a difficult pollutant to control.

2.2 Ozone control and modelling

The health effects of ozone are more marked during ozone "episodes" when ozone can accumulate over a period of days and concentrations can rise well above the apparently acceptable level of 120 μg m^{-3} (mixing ratio ~60 ppb) for long periods. (WHO, 2000)

Effects on vegetation appear with exposures to ozone at lower concentrations (80 μg m^{-3}, mixing ratio 40 ppb) during the growing season. There will be appreciable economic consequences if background levels rise and crop productivity is affected.

Thus there are two different regimes that legislators must take into account in attempting to limit or reduce ozone concentrations: the general background of ozone which has until recently being rising and is approaching 80 μgm^{-3} in westerly air flows to Europe, and peak levels which mainly occur in episodes.

Being a secondary pollutant, ozone does not lend itself readily to legislative controls. The simple "end pipe" controls, which may suffice for primary pollutants, are inadequate for ozone with its non-linear dependence on VOC and NO_x. What is needed is an air quality strategy, and this was recognised in Europe in the 1999 CLTRAP Protocol to Abate Acidification, Eutrophication and Ground-level Ozone, and the 2002 EU Air Quality Daughter Directive on Ozone. These view ozone as part of a larger air quality problem in which abatement measures may affect the various major pollutants in different ways; they also try to take into account the non-linearity, mentioned above, where measures which, say, reduce NO_x in conurbations may lead to increases in population exposure as more ozone is formed closer to the population centres.

Under various international agreements and also UK legislation, Defra is required both to monitor ozone together with other pollutants, and also to model its formation. Modelling ozone formation is required to assess the current UK situation and so try to ensure compliance with the prescribed exposure limits. Modelling is also needed to produce future scenarios to predict the likely effects of current and proposed air quality legislation in the light of expected economic growth with the consequent growth of emissions.

Defra in common with a number of responsible agencies across the world has conducted a variety of modelling studies in the recent past. There is a constant need to review current modelling activities to ensure that the models used are *fit for purpose.* They should reflect the current state of the art, assess the uncertainties inherent in such modelling studies, and be able to encompass changes both within the modelling art itself and the expected drivers for future policy, such as predicted changes in temperature and weather patterns.

2.3 Review of ozone modelling; the work plan

Objective of work

The objective is to collate, evaluate and summarise information on tools for modelling ozone (O_3) formation and assessing impacts on human health and ecosystems within the Defra policy context.

The Sub-objectives are to:

1. review and evaluate current tropospheric O_3 models utilised or potentially suitable to supporting Defra's policy needs;
2. deliver a workshop to engage users on the outcome of the project;
3. make recommendations on future R & D in the area of tropospheric ozone modelling for evidence-based policy delivery; and
4. deliver a final report by a specified date in 2007.

The models included in this assessment, given the policy focus, are very much of the regional air quality type. These tend to be limited-area models which are of moderate to high spatial resolution with vertical information biased towards the boundary layer.

The Methodological Approach

Objective 1. There are three tasks.

Task 1 - The first task is to identify the candidate models followed by an information gathering phase that will collate and summarise the information such as the description of a model and its uses to date. The basic features of the models will be catalogued as follows.

a. Functional type – Lagrangian vs. Eulerian

b. Spatial scales – grid size, requirements for nesting, vertical extent (urban, regional, global)

c. Meteorology – driving meteorology

d. Chemistry scheme – level of chemical complexity with respect to VOCs

e. Emission schemes – if applicable

f. Timescales accessible – hours to decades

g. Published information – model description and applications

h. Details of use within the UK and users.

Further to the basic model descriptors, information will be collected on whether the candidate model has been used in the UK, EU or international context to support any form of policy development or implementation. As part of this work, a brief review of the available science-sector based models will be provided with a view to an assessment of whether they are likely to become policy relevant models or provide policy relevant input.

The output of the first task will be a small database of the candidate models with a collation of the supporting documentation.

Task 2 - The second task will be to gather quantitative measures of the policy metrics with which to evaluate the candidate models against

* The metrics used for NECD and UNECE reviews and revisions
* Those identified in the Air Quality Strategy and its review
* Those utilised for reporting on compliance with EU Directives (3rd Daughter Directive)

These will be collated into a short quantitative evaluation criteria document to be used in conjunction with task 3.

Task 3 - The third phase (task) of the work will take the candidate models and evaluate them against a series of criteria.

* Is the modelling methodology used appropriate for use in addressing policy related questions (see task 2)?
* Does the methodology incorporate up-to-date principles and science?
* What are the inputs (data sources, parameters *etc*) and outputs from each model (including resolution, run time *etc*)?
* Are the input data streams appropriate for the task and widely available and is the meteorology (resolution and quality) used appropriate for the application?

* How do the outputs support Defra's requirements with respect to European and UNECE policy requirements and metrics (see task 2)?
* Is the model being used outside its current ideal capability?
* What are the strengths and weaknesses of each model?
* What is the potential future capability of the model?
* How well has the model been tested and validated – is it robust?
* Has the model been adequately peer-reviewed?
* What are the most significant areas of uncertainty and sensitivities regarding the model application?
* What is the level of uncertainty in the outputs and can this uncertainty be quantified?
* Can the model be used in forecast mode?
* Are the models well suited to be challenged by the currently available observational datasets?

The evaluation will be systematic and unbiased. The output of the three tasks in objective 1 will be fed to the work in objective 4.

As part of the process of undertaking objective 1, tasks 1 to3, identified modellers will be contacted with a view to inputting information in to the collation phase of the project.

Objective 2

Consultation with the modellers/user community. An important element of the work will be a consultation with the modellers, this can either take the form of an interim workshop to gather information on models and approaches that would engage the modelling community, or a final workshop presentation that would present the draft final results of the project to both the modelling and user community for scrutiny. The required form on any workshop will be agreed with the project officer as appropriate.

Objective 3

The report should make recommendations for future R&D in the context of the models currently available. In order to achieve this we will identify key development opportunities for Defra funding to improve value of each model to Defra's policy needs (as ascertained and quantified in objective 1, task 2) and prioritise the development opportunities identified.

An element of the work in objective 3 will also be future "gazing", looking at such questions as for example:

* Is their a requirement for an AQ forecasting ability?
* What role will data assimilation play in model development?
* What role would satellite data play in any future modelling strategy?
* Can the models be interfaced to cost-benefit analysis?
* Can a single model address the target policy areas?
* Is there a requirement for a hierarchy of models to address problems of scale?
* Should Defra be using an ensemble model approach?
* Can Defra's modelling needs be met by external agencies such as EMEP?

* Could any climate model (*e.g*. nudged) meet the AQ model requirements?
* What role will the climate models play in future policy development?

Objective 4

The final report will synthesise and integrate the findings of each of the work undertaken in objectives one to three. It will make an assessment of the "fitness for purpose" of the models reviewed for delivering Defra policy requirements.

2.4 How the enquiry was conducted

An initial list of possible UK ozone models with contacts was used. Each contact was sent the questionnaire, the returns from which comprise Appendix B. To provide a comparison, we then wrote to colleagues involved in modelling on the continent and in the United States and asked them to help us. Almost all replied and their returns are also given in Appendix B. After studying the replies, we then sent some supplementary questions to all our contacts, to which many replied; the replies have been integrated into the returns in Appendix B.

A list of the contacts is given in Appendix A. The sample was confined to people known to the team personally – there was no attempt to cover all the models in all the countries. One warning and disclaimer – in the report models are frequently referred to by country. This is for convenience – it does NOT imply that the various models are used by the regulatory authorities in those countries.

We are very grateful to our various colleagues for all the information and help, so freely given.

2.5 The organisation of the report

Following this introduction, section 3 provides a brief description of the modelling process, indicating the elements involved. The section attempts to indicate the inherent uncertainties in each element and, if possible, the way in which they affect the model as a whole.

Section 4 lists the various ozone metrics which the ozone models used for policy applications within Defra should provide

The heart of the report is based on the summary table of all the models given in Table 1 (page 36). From this, section 5 draws on the descriptions of the available models, classifying them into their various types, chemistry, emission inventories and so on, drawing attention to the pros and cons of each and attempting to assess whether they are indeed "fit for purpose".

Section 6 outlines potential future developments which will affect air quality and modelling and assesses the resilience of the models in dealing with them.

Section 7 then makes a number of recommendations to Defra about the use of the models and suggests some areas where there should be some further research and development.

Following the thanks and acknowledgements in section 8, the Appendices provide the list of the contacts for the various models (A), the summary table of the model characteristics (B), and the returns from the contacts (C) which make up the database of model characteristics, required in objective 1.

3. Ozone modelling: methods and uncertainties

3.1 Chemical Transport Models: Lagrangian and Eulerian

The modelling of the distribution of ozone in the atmosphere and its evolution with time is achieved with chemical transport models (CTM). These fall immediately, on the basis of fundamental approach, into two classes, Lagrangian and Eulerian.

Lagrangian models follow the trajectories of individual air parcels through the atmosphere, computing the changing chemistry as the parcel moves. The model then calculates the ozone distribution by computing the statistics of the trajectories of a large number of air parcels. A Lagrangian model uses a moving frame of reference as the parcels move from their initial location. In terms of dispersion plumes, it is said that the Lagrangian observer moves with the plume.

An Eulerian model on the other hand usually uses a fixed three-dimensional Cartesian grid as a frame of reference rather than a moving frame of reference. Starting from initial values of the chemical and physical parameters in each of the grid cells which occupy the space, the conditions and chemcial compositions evolve with time. It can be said that an Eulerian observer watches a dispersion plume go by.

As Stockwell (2002) points out, Lagrangian models provide physically meaningful air trajectories, and so are effective in relating emissions from sources to concentrations at receptor sites. Also Lagrangian models, because they can handle more complex chemical mechanisms, are more suited to the description of ozone formation on the regional scale under low-NO_x conditions (AQEG, 2007).On the other hand it is difficult to encompass chemical interactions between different air parcels (Stockwell, 2002) and some vertical transport processes in many Lagrangian models. There do however exist more computationally demanding Lagrangian models which give good descriptions of chemical interactions between air parcels and full three dimensional transport.

In contrast, Eulerian models allow chemistry, transport and deposition to be treated in a more realistic manner than the majority of Lagrangian models, with good descriptions of the mixing and chemical interactions between different air parcels. They can also include relatively detailed treatments of chemistry, emission, deposition and other processes (Stockwell, 2002). They are well suited to describing the competition between vertical mixing and rapid chemistry that drives urban scale ozone formation (Derwent).

However, with Eulerian models, spatial resolution can be limited (mainly by computer power, but also by knowledge of emissions), actual trajectories can only be indirectly calculated, and it is more difficult to relate the emissions from a specific source to concentrations at a given receptor site. (Stockwell, 2002).

Lagrangian models generally make smaller demands on computing time and so can use much more comprehensive chemical schemes. Eulerian models, providing a more comprehensive picture, demand more computational resources and so can only use simpler chemical schemes. However the difference is diminishing with increasing computational performance and the use of parallel processing.

It is notable that, about 10 years ago, UNECE (EMEP) switched from a Lagrangian to an Eulerian model for their European assessments, following an external review of their capabilities. The major models used in the USA are Eulerian (Stockwell, 2002).

3.2 Model uncertainties

All environmental models contain a large number of simplifications in their formulation which introduce uncertainties. These may be grouped into four main areas or categories - following Oreskes *et al.*, (1994) and AQEG (2007):

* Theoretical aspects of the system that are not fully understood,
* Empirical aspects of the system that are difficult or impossible to measure,
* Parametrical aspects of the system that have been simplified, and
* Temporal aspects of the system that are not stable in time.

The remainder of this chapter deals with aspects of categories which are appropriate to ozone modelling.

The Air Quality Expert Group (AQEG, 2007) point out that there are four major areas of model uncertainty.

> The first concerns the theoretical aspects of ozone formation that are not fully understood. Broadly speaking, two major regimes of ozone formation have been identified: intense VOC-limited ozone formation in urban plumes and steady NO_x-limited ozone formation on the regional and trans-boundary scales. Whilst the extremes of these regimes have been well studied in field studies carried out in Europe and North America, it is not at all clear which regime dominates ozone formation observed in a given UK episode.
>
> The second major area of model uncertainty concerns those empirical aspects of ozone formation that are difficult or impossible to measure or observe and then to represent in ozone models. Many of these empirical uncertainties involve the near impossibility of measuring atmospheric concentrations of the many reactive free radical species, emitted VOCs and their secondary organic reaction products that together control ozone formation over Europe.
>
> The third major area of model uncertainty arises because of the simplifications introduced into the process descriptions in the models. Photolysis rate coefficients are a good example of parametrical uncertainty: these parameters control the rate of photochemical ozone formation and are influenced by cloud cover and photochemical haze formation. Rarely are the large amounts of solar radiation data available used and clear-sky conditions are commonly assumed. Parametrical uncertainties are also introduced into models through the simplified descriptions employed of the natural biogenic emissions of isoprene and other VOCs. As a result, natural biogenic emissions are highly uncertain and hence so too are their contribution to ozone formation in the United Kingdom.
>
> The fourth major area of model uncertainty arises because processes and the parameters that drive them are assumed to be constant in time when in reality they are highly variable or sporadic. Scavenging by precipitation, re-suspension and fires are classic examples of sporadic processes. Man-made emissions are most accurately quantified as annual and national totals. These totals have then to be broken down to an hourly basis and gridded at a spatial scale of 1 km × 1km or down to individual road-links, across the country. In the real world, however, emissions from a single 1 km × 1 km grid square or a single road link are highly variable and unpredictable and this variability introduces large uncertainties in ozone model predictions and their evaluation against observations. (AQEG, 2007)

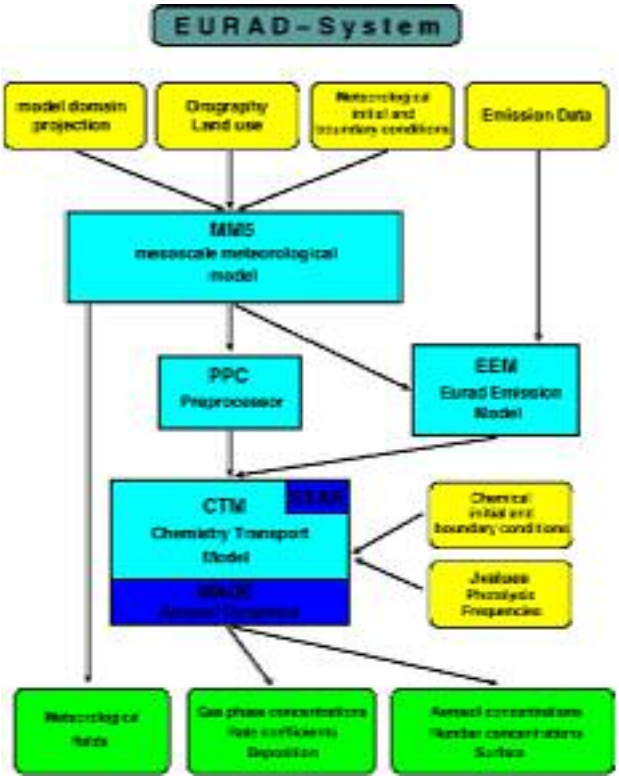

Figure 3.1: A block diagram of a chemical transport modelling system. (Taken from *http://www.eurad.uni-koeln.de/*)

3.3 Model input parameters

Figure 3.1 shows a block diagram of a particular Eulerian model in order to illustrate the input parameters required. A Lagrangian model requires similar input variables.

a. CTM module

The chemical transport module is the heart of the model. It contains a scheme of chemical reactions, which must be self consistent and sufficient to describe chemically the formation and removal of the chemical species being modelled.

Gas phase chemistry

CTMs vary greatly in the complexity of the chemistry they encompass. While the inorganic chemistry scheme involving OH, HO_2, O_3, NO, NO_2 *etc*. is common to all, the means for dealing with the organic chemistry differ widely. For a complete picture, there are simply too many species and far too many reactions to encompass and, furthermore, the parameters for most reactions are unknown. Mechanisms are classified as either explicit or aggregated based on their treatment of the organic reaction.

Explicit mechanisms consist of reactions for individual compounds and these may become very large. The most comprehensive near-explicit scheme is the *Master Chemical Mechanism* (MCM) (Jenkin *et al*., 1997, Derwent *et al,* 2007), first constructed in Leeds, with support from Defra. Version 3 considers the complete degradation of 120 or so organic compounds involving some 4500 chemical species and 12500 chemical reactions. Most of the organic degradation schemes were developed according to theoretical methodologies such as structure-reactivity relationships. The mechanism includes detail that exceeds available laboratory data but uses a well defined protocol to construct the mechanism in a compatible and reproducible way. The MCM is generally regarded as a research tool, since the size precludes its use in most practical models; it serves as a benchmark for other chemical schemes which can be tested against it in chemistry-only box models.

One way to simplify the problem is by using *surrogate species*. The reaction of a particular compound represents a number of homologous compounds, and the rate parameters for the surrogate are used for all. The number of compounds and reactions are very small in comparison with the MCM. A related approach is to use an explicit scheme but limit the number of reactions in it. Thus some species are treated explicitly, some essentially act as surrogates. However the number of reactions depends on the view taken by the modeller. The CHIMERE scheme provides an example, as does the EMEP scheme. (Simpson *et al*., 1993, Andersson-Skold *et al*., 1997)

One surrogate scheme with a more fundamental basis is the Common Reactive Intermediate (CRI) mechanism which is based on the MCM. Again some 120 VOC are included but the number of species is limited to 250 and the reactions to 570.

There are two methods for aggregation: aggregation by molecule and by molecular group. For *aggregation by molecule* the model species "ALD" might represent all aldehydes while "PRO" might represent propane and all less reactive alkanes. In RADM2 for example, this reduces the number of organic species to about forty. The rate parameters are estimated, perhaps from modelling or by smog chamber simulation experiments. (Stockwell *et al*., 1990, Middleton *et al*., 1990, Stockwell *et al*., 1997)

Another example of a mechanism aggregated by molecule is the SAPRC-99. It is the US EPA and California Air Resources Board (CARB) standard for air quality and state implementation plan (SIP) modelling. The mechanism has been evaluated extensively against environmental chamber data and it is widely used (*Carter et al., 1990, 2000*).

The *carbon bond mechanism*, perhaps the most common chemical scheme used, is the only example of aggregation by functional group. The species represent numbers of double bonds, numbers of aromatic rings and other organic functional groups, molecules in the group being assumed to have similar bond reactivities. The number of reactions then becomes manageable (Gerry *et al*., 1989)

The choice of mechanism-reduction scheme for organic compounds initially depended on the intuition of the investigator, but the MCM could providing a useful background against which to test the simpler schemes in the uses to which they are put.

Further schemes of reactions are required for halogens, organo-halogen compounds and for sulfur species, where these species are thought to be of importance.

Aqueous chemistry

Cloud droplets act as temporary miniature vessels in which reactions can take place and photo-oxidation occur. Oxidation of sulfur dioxide to sulfate occurs in clouds and much detailed aqueous chemistry is involved. Again various chemical schemes are employed and again many of the parameters are unknown, so the uncertainties are large.

Also required are Henry's Law coefficients for the gaseous species and, in many cases, these are poorly known. The coefficients are also required for estimating losses from the atmosphere by rain out and so on.

Aerosols

The representation of aerosols presents a large problem since the formation and degradation of secondary aerosols (formed in organic oxidation) is far from understood, and to this must be added the microphysics of condensation, growth and cloud processing. A variety of empirical schemes are in use, but it will be some time before any satisfaction can be felt about the representation of aerosols in chemical models.

Photochemistry

Another area of uncertainty is the photochemistry of most of the species which occur in the atmosphere. Accurate spectra and absorption data together with the variation of quantum yields of decomposition with wavelength are required. The work to obtain these is difficult, and is undertaken in only one or two laboratories world wide. The photolysis radiation can readily be calculated for the time of day, but it varies with cloud cover and haze, which may be difficult to take into account, even if enough information is provided by the meteorological driver. Often, clear sky values are assumed which can introduce a large source of uncertainty (AQEG, 2007).

Surface – atmosphere exchange

Estimates are also required of the loss of species from the atmosphere at the surface. The surface itself needs characterisation, through the use of land use data, before dry deposition rates are applied to determine the deposition to the surface. Much effort has been devoted to determining dry deposition rates for vegetation, but the interactions are complex and much is still being discovered about species which are deposited to the surface under some conditions and emitted under others.

Similar considerations apply to air - sea exchange.

Choice of chemical scheme

Chemical schemes involve reactions with a wide range of rate coefficients and as such, constitute "stiff" schemes for numerical integration. Despite the development of numerical integration, the chemical scheme still constitutes a heavy drain on computer resources, which increases rapidly with the number of reactions. Thus the choice of chemical scheme may well be dictated by the speed with which the answers are required.

b. Meteorological module

The CTM requires as input data meteorological 3D fields of temperature, humidity, and winds, as well as surface fields of pressure, heat flux and surface stress, as a function of time. The meteorological driver provides some or all of these.

Approximations are required for the ground topography (orography), to provide both the correct ground level, and land use data is needed for the surface roughness.

In constructing the driver, the grid size is specified together with the number of height levels. The grid box sizes must be suitable for the problem chosen, but this is often a compromise – while the ideal would seem to be a very small size to accommodate as much variation as possible, there are then large demands on computer resources and it may well be impossible to provide realistic initial conditions and inputs for small cells. On the other hand choice of too large a scale overlooks "sub-grid" phenomena.

One particular problem with the height levels is the height of the atmospheric boundary layer. In much air pollution, the top of the boundary layer is the "lid" of the chemical reaction vessel and the height determines the concentrations at which the species are reacting. How well defined the height is depends on the number of model levels within the lower part of the troposphere, and these are not usually chosen with the concentration problem in mind. The boundary layer itself is subject at times to sharp concentration gradients, convection, turbulence and stratification, which adds further uncertainties to the meteorological input.

c. Emission Data

Anthropogenic Emissions

Accurate emission estimates are hard to obtain and, in early modelling attempts, were thought to be of lesser importance than other aspects. The view has now changed as the importance has been recognised but, it is fair to say, satisfactory emission estimates are still difficult to produce.

Emission estimates are usually made from national economic, industrial and traffic data and combined with a variety of emission factors to convert the indicators to the annual emissions of chemical species for given areas and regions. Questions arise about the partitioning of the emission types and the division of emissions between regions. The scientific problems are exacerbated when political interference takes place, as was the case in eastern Europe in earlier days, and perhaps could be in the future if countries suffer penalties for excessive emissions.

A further major step required is temporal and spatial disaggregation: the conversion of annual emissions to the model timescale and the apportionment of the emissions throughout the area being studied.

While an emissions processor is attached to most models, disaggregation is seen as a valid activity in its own right. Temporal disaggregation should not only take the expected seasonal and diurnal variations into account but also should include social influences which differ from region to region as, for example, between the Mediterranean and northern Europe.

Spatially, emissions must be distributed throughout the region. There are particular problems with point sources such as power stations and line sources such as roads. They can be accurately placed, but the concentration for the whole grid square is certainly imprecise.

Biogenic Emissions and Deposition to the Biosphere

Biogenic emissions refer to the variety trace gases produced by vegetation, bacteria and animals. Most attention has concentrated on emissions of isoprene and other terpenes which can be strongly emitted by many tree species. Much effort has been devoted to elucidating the relations of emissions to species, atmospheric conditions, the nature of the soil *etc.* but while there is some understanding, the production of reliable emission factors is still a difficult task. The factors are then combined with land use data to give the estimate. A comprehensive data base for Europe (PELCOM) was devised to provide land use data on a 1 km grid. It is updatable but the web site appears only to run up to 2001.

The oxidation of some biogenic hydrocarbons are included in the MCM, but the contribution of biogenic emissions to the formation of ozone in UK is still not well known – the contribution is likely to increase as the expected warming in the climate takes place.

Also required for adequate modelling are deposition velocities for all the major species. These can vary with the state of the vegetation and the prevailing environmental conditions. Those for the major inorganic species are reasonably well known, but the problems with ammonia which may be deposited, or released, depending on the conditions, illustrate the general problem and ensuing uncertainties

d. Initialisation and Boundary Conditions

A model run always requires initial values but the importance of these varies with the type of study. It is less for long term studies where the lifetimes of the species are less than that of the period in question, and where the continued diurnal variation in the meteorological and photochemical variables, and in the emission rates, smooths out the initial effects. For short term studies, adequate initialisation is crucial.

Initial values may be obtained from observations, with interpolations between stations. Alternatively the results of previous model runs may be used. In future data assimilation in which model values are *nudged* towards the observed values may provide a better initialisation method.

For limited area models, good boundary conditions are required. These may be provided by a larger area model, or by making assumptions about advection of species into the edge of the area. The inner areas of nested models have an advantage here, since the same model scheme and assumptions are used throughout.

In all these processes there are appreciable uncertainties – it is the experience of the modeller concerned which then determines which can be reduced or neglected, or which require further work.

3.3 Model Validation

With the many uncertainties in the model itself and its input data, modellers devote a lot of effort to testing the model results against observations, where these can be made, and to comparing their models with other ozone models. While formal validation of a model is mathematically impossible (too many variable and too few observations), comparisons against observations give a valuable guide to overall model performance.

As the Air Quality Expert Group (AQEG, 2007) point out: policy-makers expect modellers to establish the trustworthiness of their models. For ozone models, this almost always involves some form of comparison of model predictions against network data (see for example, van Loon *et al.,* 2007). However worthy such exercises are for confidence building, they are far from representing model validation of verification. Oreskes *et al.* (1994) suggest that validation and verification of models of natural environmental systems is not possible: there are always poorly known input parameters, fine scale details can be of crucial importance and assumptions and inferences may fail under particular circumstances. That an ozone model reproduces ozone network observations from the past does not guarantee its adequacy for the future or for predicting the response to ozone control strategies. Agreement with observations is inherently partial. Models agree with some observations but not all. A model can certainly perform well against observations and the precision and accuracy of the fit can be quantified. The performance of models can be evaluated relative to observations, relative to other models or against our own theoretical expectations but they cannot be verified or validated (Oreskes *et al.*, 1994). Nevertheless, comparison against observational data remains a good first step in the evaluation of model performance.

4. Ozone metrics

The environmental effects of tropospheric ozone are described in terms of short term peak concentrations and long term exceedances. The economic effects on plants result from long term exceedances of low concentrations of ozone during the growing season. Human health is thought to be affected by high peak values which mainly occur in episodes and also by the exceedance of lower "threshold" values over longer periods. There are thus two sets of metrics.

4.1 Metrics for Health Effects

The table of candidate ozone metrics, 4.1, is taken from contribution by *John Stedman and Tim Williamson* to the forthcoming 5th Report of the Air Quality Expert Group (AQEG, 2007). The table indicates the metric, its relevance to air quality and the key influences on the metric at urban locations.

Several metrics are based on the annual average of the daily maximum of the running 8-hour mean concentration. This has been calculated using cut-off concentrations of zero (that is, including all days), 70 μg m^{-3} and 100 μg m^{-3}. For metrics with cut-offs, the concentration is subtracted from the daily maximum of the running 8-hour mean concentration and the value set to zero if the result is zero or negative. The average across all of the days in the year is then calculated. Such metrics have been recommended as appropriate for the assessment of the impact of the daily variation in ozone concentration on human health. The range of cut-offs reflects uncertainty as to whether there is a threshold for the ozone to have an effect (COMEAP, 1998). The WHO concluded that there was some evidence that associations existed below the current guideline value (60 ppb, 120 μg m^{-3}), but not enough to lower the present cut-off (WHO, 2004). The 70 μg m^{-3} cut-off is recommended (UNECE/WHO, 2004) for use in cost-benefit analysis and integrated assessment modelling on the basis of a combination of the uncertainty in the shape of the concentration response function at low ozone concentrations, the seasonal cycle and geographical distribution of background ozone concentrations and the range of concentrations for which European scale ozone modelling was able to provide reliable estimates.

The metric of the annual average of the daily maximum of the running 8-hour mean with a cut-off at 70 μg m^{-3} is closely related to the SOMO35 metric adopted for European scale integrated assessment modelling. It can be calculated by multiplying by the number of days in the year and the application of a factor to take account of the different units used. SOMO35 is typically quoted in ppb.days or ppm.days. The 70 μg m^{-3} cut-off metric is preferred over SOMO35 because the units are easier to interpret and to compare with other metrics, and the magnitude of the metric is not unduly influenced by low data capture in a particular year.

The metric most sensitive to peak concentrations during photochemical episodes is the maximum 1-hour average during the year. This metric is thus most likely to show a response to reductions in relevant precursor emissions. It is, however, highly variable from year to year and from site to site and is particularly subject to instrument malfunction or interference. High percentiles of the hourly concentration, such as 99.9th or 99th are therefore sometimes preferred for data analysis. (COMEAP, 1998, WHO, 2004, UN-ECE/WHO, 2004).

Table 4.1: The ozone metrics of relevance to human health

Metric	Relevance	Key influences on the values of this metric at urban locations
Annual average	Basic metric used to show long-term trends.	Includes all of the hours in the year. Strongly influenced by the magnitude of local NO_x emissions
Annual average of the daily maximum of the running 8-hour mean	Used as "basic metric" for many of the health metrics. Also used as Defra's air quality indicator.	Strongly influenced by the magnitude of local NO_x emissions
Annual average of the daily maximum of the running 8-hour mean with a 70 µg m^{-3} cut-off	Health impact, related to SOMO35 (below)	Influenced by the magnitude of local NO_x emissions and by photochemical episodes
Annual average of the daily maximum of the running 8-hour mean with a 100 µg m^{-3} cut-off	Health impact	Strongly influenced by photochemical episodes and to a lesser extent the magnitude of local NO_x emissions
Maximum 1-hour average (peak hour in the year)	Used as the basis for some epidemiological studies, although has been suggested that 8-hour is more representative. Also an indicator of short term peaks.	The metric most sensitive to peak concentrations during photochemical episodes and thus likely to show a response to reductions in relevant precursor emissions.
Number of days with daily maximum of running 8-hour mean exceeding 100µg.m^{-3}	Equates to the number of exceedences of the UK ozone standard (AQS objective is no more than 10 exceedences per year)	Strongly influenced by photochemical episodes and to a lesser extent the magnitude of local NO_x emissions
Number of days with daily maximum of running 8-hour mean exceeding 120µg.m^{-3}	Equates to the number of exceedences of the EU Target Value (no more than 25 days, averaged over 3 years) and Long Term Objective (no exceedences) from the 3rd Daughter Directive	Strongly influenced by photochemical episodes and to a lesser extent the magnitude of local NO_x emissions
SOMO35 (sum of means over 35 ppb)	Used as a metric by IIASA, for CAFÉ and NECD revision, related to Annual average of the daily maximum of the running 8-hour mean with a 70 µg m^{-3} cut-off	Influenced by the magnitude of local NO_x emissions and by photochemical episodes
97th percentile of daily maximum of running 8-hour mean	Equates to the removal of the 10 highest vales, this equates to the UK AQS objective for ozone	Strongly influenced by photochemical episodes and to a lesser extent the magnitude of local NO_x emissions

4.2 Metrics for vegetation exposure to ozone

The metrics for vegetation exposure to ozone are shown in Tables 4.2 and 4.3 taken from the ICP mapping and modelling manual (http://www.oekodata.com/icpmapping/index.html). As shown in the tables, three cumulative exposure approaches are used to define critical levels for ozone: stomatal fluxes, ozone concentrations and vapour-pressure deficit-modified ozone concentrations. It is worth noting that concentration-based critical levels that used *AOTX* (ozone concentrations accumulated over a threshold of X ppb) as the ozone parameter have been superseded, as several important limitations and uncertainties have been recognised for using *AOTX*. In particular, the real impacts of ozone depend on the amount of ozone reaching the sites of damage within the leaf, whereas *AOTX*-based critical levels only consider the ozone concentration at the top of the canopy.

Table 4.2: Terminology for critical levels of ozone

	Indicator	Units	Explanation
Terms for concentration-based critical levels			
Concentration-based critical level of ozone	AOTX	ppm h	The sum of the differences between the hourly mean ozone concentration (in ppb) and X ppb when the concentration exceeds X ppb during daylight hours, accumulated over a stated time period. Units of ppb and ppm are parts per billion (nmol mol^{-1}) and parts per million (μmol mol^{-1}) respectively, calculated on a volume/volume basis.
Concentration accumulated over a threshold ozone concentration of X ppb	CLec	ppm h	AOTX over a stated time period, above which direct adverse effects on sensitive vegetation may occur according to present knowledge.
Concentration accumulated over a threshold ozone concentration of X ppb modified by vapour pressure deficit (VPD)	AOTXVPD	ppm h	The sum of the differences between the hourly mean ozone concentration (in ppb) modified by a vapour pressure deficit factor ($[O_3]$VPD), and X ppb when the concentration exceeds X ppb during daylight hours, accumulated over a stated time period.
Terms for flux-based critical levels			
Projected leaf area	PLA	m^2	The projected leaf area is the total area of the sides of the leaves that are projected towards the sun. PLA is in contrast to the total leaf area, which considers both sides of the leaves. For flat leaves the total leaf area is simply 2*PLA.
Stomatal flux of ozone	F_{st}	nmol m^{-2} PLA s^{-1}	Instantaneous flux of ozone through the stomatal pores per unit projected leaf area (PLA). F_{st} can be defined for any part of the plant, or the whole leaf area of the plant, but for this manual, F_{st} refers specifically to the sunlit leaves at the top of the canopy. F_{st} is normally calculated from hourly mean values and is regarded here as the hourlymean flux of ozone through the stomata.
Stomatal flux of ozone above a flux threshold of Y nmol m-2PLA s-1	F_{st} Y	nmol m^{-2} PLA s^{-1}	Instantaneous flux of ozone above a flux threshold of Y nmol m^{-2} s^{-1}, through the stomatal pores per unit projected leaf area. F_{st}Y can be defined for any part of the plant, or the whole leaf area of the plant, but for this manual F_{st}Y refers specifically to the sunlit leaves at the top of the canopy. F_{st}Y is normally calculated from hourly mean values and is regarded here as the hourly mean flux of ozone through the stomata.
Accumulated stomatal flux of ozone above a flux threshold of Y nmol m^{-2} PLA s^{-1}	$AF_{st}Y$	nmol m^{-2} PLA	Accumulated flux above a flux threshold of Y nmol m^{-2} PLA s^{-1}, accumulated over a stated time period during daylight hours. Similar in concept to AOTX.
Flux-based critical level of ozone	level of ozone, CLef	nmol m^{-2} PLA	Accumulated flux above a flux threshold of Y nmol m^{-2} PLA s^{-1} ($AF_{st}Y$), over a stated time period during daylight hours, above which direct adverse effects may occur on sensitive vegetation according to present knowledge.

Table 4.3: Critical levels for ozone

Approach		**Crops**	**(Semi-) natural vegetation**	**Forest Trees**
Stomatal flux based critical level	CLef	*Wheat*: An AFst6 of 1 mmol m^{-2} PLA *Potato*: An AFst6 of 5 mmol m^{-2} PLA	Not available	*Birch and beech*: Provisionally AFst1.6 of 4 mmol m^{-2} PLA
Stomatal flux based critical level	Time period	*Wheat:* Either 970°C days, starting 270°C days before midanthesis (flowering) or 55 days starting 15 days before mid-anthesis *Potato*: Either 1130°C days starting at plant emergence or 70 days starting at plant emergence		One growing season
Stomatal flux based critical level	Effect	Yield reduction		Growth reduction
Concentration based critical level	CLec	*Agricultural crops*: An AOT40 of 3 ppm h *Horticultural crops*: An AOT40 ppm h	An AOT40 of 3 ppm h	An AOT40 of 5 ppm h
Concentration based critical level	Time period	*Agricultural crops*: 3 months *Horticultural crops*: 3.5 months	3 months (or growing season, if shorter)	Growing season
Concentration based critical level	Effect	Yield reduction for both agricultural and horticultural crops	Growth reduction in perennial species and growth reduction and/or seed production in annual species	Growth reduction
VPD modified concentration based critical level	CLec	An AOT30VPD of 0.16 ppm h	Not available	Not available
VPD modified concentration based critical level	Time period	Preceding 8 days	Not available	Not available
VPD modified concentration based critical level	Effect	Visible injury to leaves	Not available	Not available

5. Fitness for purpose: current ozone models overview

The characteristics of the models reviewed in this report are summarised in Table 1 (page 36), which are based upon the individual replies from correspondents. These are shown in full as separate tables in Appendix B. Since the replies were solicited separately there are gaps in the information and the approach is not entirely consistent since correspondents interpreted questions in different ways. Correspondents were given a chance to review their contribution and to provide some extra information, some of which is included in Table 1 (page 36). It should be again emphasised that the information was obtained privately – so that while the models are referred to by country, they are NOT necessarily the models used for ozone evaluation by the regulatory authorities.

Some of the UK models mentioned have been used to support Defra in its policy development and air quality strategy formulation, in particular the OSRM and UK PTM models. The EMEP model is the main tool for policy formulation within Europe through the aegis of the UN ECE and the Commission of the European Communities. (AQEG, 2007)

The following sections review the salient features of the models in the light of the discussion of models and inputs in section 3.

5.1 Lagrangian or Eulerian?

The UK has four Lagrangian-based trajectory models (ELMO, NAME, OSRM, UK-PTM). There are just two Lagrangian models, MOON (DK) and OFIS (GR) among the continental group. The global UK climate model, STOCHEM, included because it finds uses in other UK models, is also Lagrangian.

Abroad, other hand, Eulerian models predominate: EMEP, CAMx (CZ), CAMx (CH), EURAD (DE), REM_CALGRID (DE), 2 Danish models, CHIMERE (FR), LOTOS-EUROS (NL), CHIMERE (RU), MARS, MUSE and three other Greek models, 6 Spanish Models, and CMAQ in the USA. CAMx, an Eulerian model, first devised by Environ in the USA, is used by six continental groups. CMAQ was built in a coordinated US national program.

The UK has effectively three Eulerian ozone models. MODELS-3/CMAQ, which has a number of variants for different chemical schemes; CMAQ (a development of MODELS-3) which has changed its chemical scheme; they are the result of collaborative work between the various groups involved. EMEPUK is an adaption of the EMEP model to UK conditions. Another Eulerian model is apparently being developed (AQUM). UKCA is also an Eulerian model for chemistry and aerosols used to study climate change on regional and global scales.

There are also a diagnostic model (Spain) and a statistical model (Ru) being used for ozone forecasting. Also included in Table 1 (page 36) is a UK urban model, (ADMS-urban) which is a Gaussian model, nested in a trajectory model.

The preponderance of Lagrangian models among the UK modellers is striking, and probably reflects the history of their development and use in this country.

5.2 Chemical schemes

There are a variety of schemes in use and, once again, one has the impression of an independent UK line. Although in the discussion below, particular chemistry schemes are referred to, many workers refer to additions or extensions that they or others have made to the schemes that they use.

The most explicit, but extremely large, scheme, MCM, is used in one UK model, UK-PTM. ELMO uses a scheme derived from the MCM. One of the Spanish models MCM-3i, uses the MCM, presumably as a box model for comparison with the other chemical schemes. An

interesting Spanish development is KINMOD which extends part of the MCM to include secondary organic aerosols.

The commonest chemical scheme is the aggregated CBM-IV, which is used by twelve continental models: CAMx (CH), REM_CALGRID (DE), DEOM and CAC (DK), CAMx aerosols (CZ), LOTOS-EUROS (NL), EPA-UAM-IV, MAP and OFIS (GR), CMAC/CHIMERE, CALGRID, three CAMx models (Spain). MODELS-3/CMAQ in the UK has a variant that uses CBM-IV, as does CAMQ (UK). ADMS-urban (UK) also uses CBM-IV. CBM-V is used in the USA.

Three UK groups use the limited explicit chemistry from the STOCHEM model with added VOC (NAME, OSRM, UKCA). The CRI scheme may be used by UKCA in the future.

The three CHIMERE models use the MELCHIOR chemistry scheme (FR, RU, ES) which is an explicit scheme with, necessarily, a limited (but large) number of reactions.

The aggregated schemes, RACM/RADM are used in one of the UK MODELS-3/CMAQ variants as well by EURAD (DE), MOON (DK), one of the MARS (GK) variants and one of the MUSE (GK) variants. RADM-AQ is used for aqueous components by CAMx (CH).

The Statewide Air Pollution Centre chemistry scheme (SAPRC97 and SAPRC99) is used by CAMx (CZ) and SMOC (ES).

The EMEP chemistry scheme is used by EMEP itself, EMEPUK, DEHM (DK), and a Muse variant (GK).

There are a number of other named chemistry schemes in use: TOMCAT (with small augmentations), KOREM, SORGAM, CF and CMU. It also appears that some models use private chemistry schemes.

A number of models MODELS-3/CMAQ (UK), CHIMERE (RU), LOTOS-EUROS (NL), MARS and MUSE (GK) and two Spanish CAMx models, have the option of using several chemistry schemes, presumably for comparative purposes.

It is evident that the UK modellers prefer either to manufacture their own schemes or use the explicit MCM, while the preponderance of continental modellers seem to prefer well established schemes, usually with a provenance in the USA.

5.3 Anthropogenic emissions

As indicated in section 2, the adequate description of precursor emissions is crucial for successful modelling of air quality. However there are always compromises in the way emissions are used – groups have different methods for tackling temporal and spatial disaggregation, and mismatches in scales between the emission inventories and the models. These are seldom fully explained.

The major source of emission estimates is the EMEP/Corinair emission inventory, which is supported by both the UNECE and the EU. It is updated from time to time. It is the source for five UK models, ELMO, NAME, OSRM, MODELS-3 and CMAQ, the three CHIMERE models (FR, RU, ES), CAMx (CZ), EURAD (DE), MOON, DEHM and DEOM (DK), LOTOS-EUROS (NL) and one of Spanish CAMx models.

Four UK models use the NAEI (National Atmospheric Emission Inventory): NAME, UKPTM, OSRM and CMAQ.

The UBA/FUB/TNO inventory is used by CAMx (CH) together with other inventories Lombardy and Switzerland. REM_CALGRID (DE) uses a variety of national and international emission inventories.

GEMS is used for global emissions by NAME and AQUM in the UK. CAC (DK), EURAD (DE), and LOTOS-EUROS (NL) uses emissions from the TNO (NL). Two models make use of GEIA emissions; UK-PTM, DEHM (DK)

CMAQ (USA) uses SMOKE.

As is apparent from the account above, modellers are not confined to using just one emission inventory; combinations are used to obtain the emission estimates required. Also there is use of local emission inventories where these are appropriate (CH, DE, ES and UK).

5.4 Biogenic emissions

When tropospheric ozone is seen as a product from pollutants, anthropogenic emissions suffice but, in parts of Europe and probably the UK, biogenic emissions play an appreciable role and should be taken into account. The models looked at in this survey appear to deal with biogenics on an *ad-hoc* basis, sometimes including isoprene, sometimes two extra terpenes, and sometimes not at all.

Early experience in the south eastern USA demonstrated that false control strategy can result from a lack of a proper appreciation of the role of biogenics. And global warming may increase the contribution which biogenics make to the mix of VOC and the formation of ozone. It is clearly desirable that inventories of biogenic emissions are both available and used in policy-directed ozone models.

5.5 Chemical initialisation

The individual replies (Appendix B) to the supplementary questions show that the method of initialisation depends on the author. Use is made of nesting within a larger domain model and some use observations from remote sites. For ozone peak values, this is of lesser importance provided the primary pollutant sources are within the studied domain. However for background ozone, then ozone advection into the domain is likely to be of importance and needs to be accounted for in the initialisation. This should be accomplished by nesting, or by use of observations but the scheme used requires detailed scrutiny.

5.6 Evaluation

It was realised that the question on the evaluation of the models would be difficult to answer in a short form, since one is asking the correspondent to summarise what is probably long periods of comparison with observation in a sentence or two. It is equally difficult to summarise the individual replies (Appendix B) here. Those that responded have clearly worked hard on the reliability of their models for ozone prediction. The simple fact that many of the models are in use for policy applications is an indication that evaluation has been done and is satisfactory for the applications.

The USA has adopted standards that air quality models are required to reach. The EPA requires models to have a paired mean normalized gross error of less than 35 % and a paired normalized bias ±15 %.

The US community has an enviable record of comparisons with observations and with intercomparison of models From a North American viewpoint, Europe seems rather backward in model development, as is indicated in the following comment from a peer review (the third!) of CMAQ (Aiyer *et al*., 2007)

> "CMAQ is rather unusual in that it is built in a coordinated national program (Canada has a similar program). By contrast, the EU has a variety of models being developed in and by various countries, and within those countries there are often competing efforts at various institutions, none of which are being conducted in a community approach. Part

of this is driven by the unique mission of CMAQ, which is to be a regulatory/policy tool for use by a number of stakeholders, and that regulatory applications in the U.S are based on specific “demonstration of attainment” requirements of the SIP process."

The present report shows this to be correct.

An interesting evaluation has been carried out between seven regional air quality models (van Loon *et al.*, 2007) for model and measurement ozone data in 2001. It was found that in general the model reproduced the main features of the ozone diurnal cycle (see Figure 5.1) but generally overestimate daytime ozone. Some models suffered from a systematic bias caused by the boundary conditions. Further conclusions were that daily maxima were better simulated than daily averages, and summertime concentrations better than winter. In simulating SOMO35 (see Table 4.1) and the number of days of exceedance of the 120 μg m^{-3} threshold for the daily maximal 8-h ozone concentration, the models produced the frequency well, but the simultaneity of measured occurrence and simulation was not well captured.

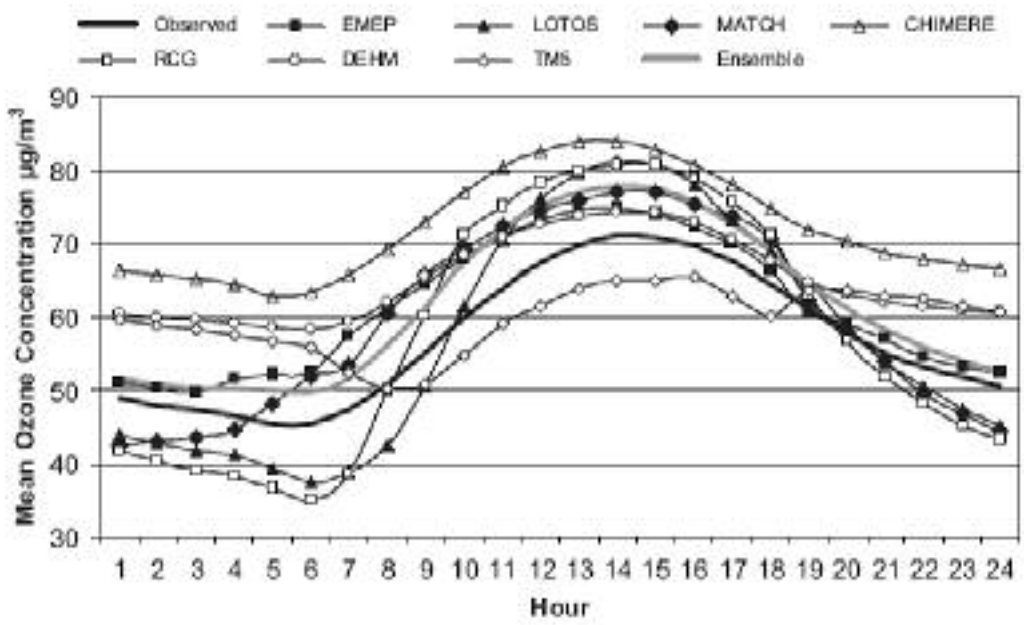

Figure 5.1: Yearly mean diurnal cycle of ozone, in μg m^{-3}, as a function of hour, for seven regional air quality models, averaged over all monitoring stations. (van Loon *et al*., 2007).

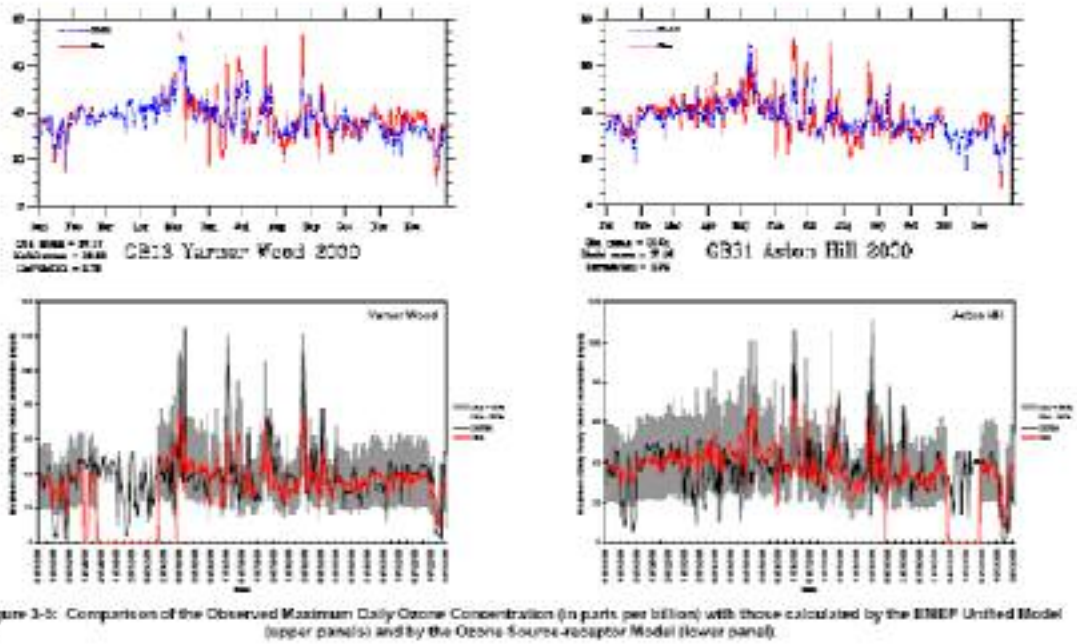

Figure 5.2: Comparison of the observed maximum daily ozone mixing ratios in ppb with those calculated from EMEP unified model (upper panels) and OSRM (lower panels) (Hayman *et al,* AEAT/ENV/R/1858 Issue 2, 2005)

The UK Photochemical Trajectory Model, OSRM, ADMS Urban and the EMEP Model have been compared in the UK context. On a like-for-like basis, the OSRM and UK Photochemical Trajectory Model were found to give identical output and responses. The comparison of the OSRM with the ADMS Urban and the EMEP models (see Figure 5.2) gave similar overall responses, although there were differences, often large, in detail (Hayman *et al,* 2005).
A question does arise about the validity of models imported from North America without modification. However there is some possibility of tuning of both model and chemistry, which may not translate directly to Europe, where the geographical and meteorological conditions are appreciably different.

5.7 Extendibility to other compounds

The individual replies (Appendix B) to the supplementary questions show, as perhaps expected, that the models can be extended to other major pollutants, including NO_2, HNO_3 and SO_2. Aerosols are also mentioned. The model that uses the MCM can deal with PAN, organic nitrates, HCHO, NH_3, particulate nitrate, sulfate and ammonium, multi-functional carbonyls and secondary organic aerosol.

However, while these can certainly be modelled, the reliability of the results for policy purposes maybe questionable. The agreement between model and observations, while far from perfect, has been tested many times over. For most other species, where there have been tests, the agreements are not as good, and the reasons for problems are not easy to discern. This is particularly true for aerosol, secondary organic aerosol and particulates, where it is difficult to represent the processes satisfactorily in the CTM schemes.

5.8 Ozone Metrics

It is hardly surprising that early all the models surveyed, Table 1 (page 36), produce one or more of the metrics mentioned in section 4. Any model which produces hourly ozone values over long periods can be adapted to produce such metrics.

Producing seasonal or annual averages is likely to be less reliable, unless some means is devised to check the intermediate model predictions against observations, and apply corrections if necessary. Data assimilation techniques should be useful in this context.

5.9 Policy applications

As the summary table, Table 1 (page 36) shows, most of the models are said to be used for policy purposes and to provide required information on a national or European scale. As mentioned at the beginning of the report, our contacts are personal and the models mentioned are not necessarily those employed by a particular country for ozone modelling.

5.10 Computer Resources

The replies (Appendix B) show that the models are run on PCs, under Linux or Windows, clusters of PCs, mainframes and workstations, and super computers. The reported running times vary enormously with the task but vary from several hours for a month-long prediction to several weeks for a year's prediction. As no benchmarks were set, it is not possible to compare the efficiencies of the code or the systems used.

6. Future safe?

For policy purposes, stable reliable models are needed so that model results are comparable from year to year. On the other hand, while one wants to avoid continuous tinkering, it is essential that the current version of the model reflects the best accepted science and is provided with up to date information. The purpose of this section is to review briefly the possible updating of the model features which may be necessary in the future.

6.1 Emissions and land use

Emissions change in reality, and the estimates also change with the way in which the economic information is produced and treated. A further dimension is added by the necessary temporal and spatial disaggregation which, as has been suggested, has not had the attention it deserves. Modellers are at the mercy of those compiling emission inventories and can only update when new versions become available. Thus most emission inputs are likely to be appreciably out of date.

It is noticeable in the models considered, that a wide variety of inventories are in use, some used in combination. The actual combinations used depend on the whim of the investigator – and one can imagine this changing during the time period that the model is in use. It is clearly desirable that the way emissions are dealt with in models used for policy purposes should be transparent.

Land use determines biogenic emissions but, if incorporated into the model, is often part of the basic description of the domain. Thus it is probably difficult to change as new estimates from satellites become available.

6.2 Chemical and physical understanding

The physical and chemical framework of the models is reasonably static, but there can be changes in detail, which affect the results and necessitate changing the model.

Changes in rate constant parameters or the inclusion of new reactions are straight forward in explicit CTM chemical schemes but pose problems for aggregated schemes. In this context it should be remembered that even in the MCM, the majority of the reaction parameters are estimated and it is unlikely that they will ever be measured, even if possible to do so. Defra have reviewed the formulation and application of the MCM against a number of other common chemical mechanisms (Derwent *et al.*, 2007). For example, Figure 6.1 shows a comparison between MCM and CBM-IV (Derwent *et al.,* 2007) under specified conditions.

The development of the so-called CRI (common reactive intermediates) mechanism should allow a more economical alternative to MCM which can, nonetheless, provide an adequate treatment of ozone formation from the degradation of a large number of emitted VOC. This would seem essential to understanding the impact of targeted emission reductions. It is clear that CRI provides a direct link through the MCM on which it is based, to lab measurements of kinetics and to structure activity relations based on lab measurements. CRI is therefore more fundamentally based than CBM.

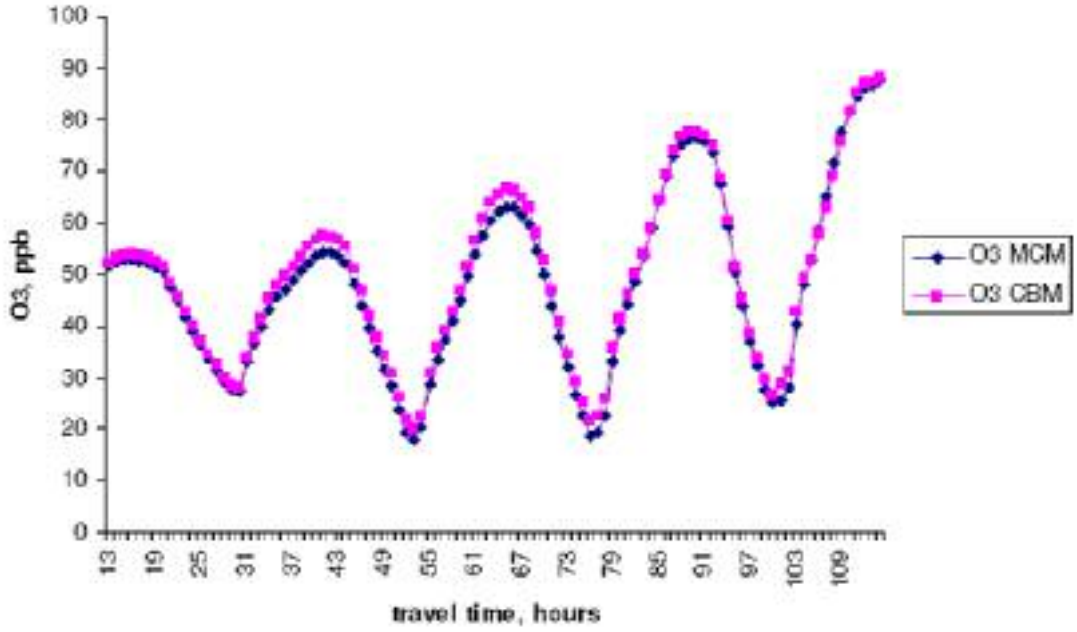

Figure 6.1: Time development of ozone mixing ratios calculated in the UK PTM for the standard trajectory case using the Carbon Bond and MCMv3.1 mechanisms (Derwent *et al.*, 2007).

While having less of an effect in ozone modelling, the gradual advances in understanding the role of aerosol, secondary organic aerosol and particulates will require substantial changes to chemical and physical schemes. It is interesting to see that one of the Spanish groups is experimenting with this in one of their chemical box models (KINMOD).

Attention has already been drawn to the problem of photochemical parameters – not only fundamentals such as spectra and quantum yields but also atmospheric conditions which reduce the clear sky values so often used. Improvements in these will necessitate changes within the models.

6.3 Meteorological inputs

The meteorological inputs for state-of-the-art regional air quality modelling should be linked to the large national/international efforts in the production of these fields. In a sense, meteorological fields taken from the major European models *e.g.* ECMWF, UKMO, MeteoFrance would seem have the most utility if available at suitable grid sizes. The scaling of these to regional grid scales requires suitable mesoscale models.

6.4 Data assimilation

In the future, models may well make use of data assimilation to improve the quality of their forecasts, and for the reanalysis of past surveys. While data assimilation is widely used in meteorological forecasting, Hov (2006) has pointed out that the needs of chemical data assimilation differ substantially from those in meteorology so, while there is much activity in this field, it will be some time before data assimilation is a requirement for routine ozone modelling. Some opportunities now exist both with the real time EEA ozone data (http://www.eea.europa.eu/maps/ozone/map) and the advent of the GEMS project (http://www.ecmwf.int/research/EU_projects/GEMS/). In GEMS a number of regional air quality models such as EURAD, BOLCHEM, MOCAGE and CHIMERE are assimilating surface and satellite data with a view to developing a regional air quality forecasting and reanalysis service. The utility of this approach needs investigating though it most likely to be of application in forecast mode.

6.5 Quality Control in Models

One aspect of modelling which attracts little attention is the correctness of the model itself. Errors, simple or fundamental, can occur anywhere – in the input data, in the parameters used, in the parameterisations and modelling fundamentals, and even in the coding. Clearly the models here all "work" and all give reasonable results – but are they error free?

This problem has been considered in detail for small scale dispersion models where there are regulatory implications. Early studies showed that simple coding errors were not uncommon, and the realisation resulted in the guidelines for modelling produced by the Royal Meteorological Society (1995) in conjunction with the then Department of the Environment (DoE). There is clearly still a need in this field, as shown by recent conference on Harmonisation in Atmospheric Dispersion Modelling, and is exemplified in a paper by two of the main protagonists, Britter and Schatzmann (2007).

It would be reassuring if the models used by Defra were subject to similar rules.

6.6 Resilience to Climate Change

The principal short term effects of climate change are likely to be a gradual increase in average temperature and changes in the frequencies and intensities of meteorological events. For ozone modelling these should be taken care of by the meteorological drivers which provide the prevailing conditions under which the chemical transformations take place, but it would be reassuring to know that the various effects are being considered.

Changes in temperature will affect the chemical rates slightly – but should have an appreciable effect on biogenic emissions, particularly if prolonged hot periods are to be experienced. These in turn will have a direct effect on ozone formation. It is essential therefore that the temperature dependences of biogenic emissions are well understood and that the various biogenic emissions and parameters are properly included in the models.

The social responses to climate change must also be taken into account – the emission mix should change appreciably and there may well be large changes in land use in the long term. Models will have to show that these can be encompassed to give good estimates, if the models are to be resilient to the changing conditions.

7. Recommendations

For ozone modelling, Defra requires a model which reliable, well tested, as precise as possible, readily updatable and, as far as possible, future safe. The following recommendations are intended to suggest a way forward towards this ideal.

7.1 Lagrangian or Eulerian?

As indicated in section 5, UK modellers largely prefer a Lagrangian approach. On the continent and in the US, Eulerian models are used exclusively. EMEP switched from Lagrangian to Eulerian some ten years or more ago. The issue is not black and white, with respect to choice, but the main reason for using an Eulerian approach is that atmospheric wind-systems are 3-D. For example it is not unusual for winds at the surface to be quite different to winds at say 300 m, 1 km or 2 to 5 km. This is challenging to deal with in a Lagrangian framework. It is worth noting that Lagrangian models do differ in type. While the majority are 2-D, there are more sophisticated Lagrangian models which are capable of dealing with 3-D winds in similar detail to Eulerian models – however the extra processing required diminishes the processing advantage over Eulerian models.

In general, Eulerian models make it easier to use fine resolution in both the vertical and horizontal. This in turn gives better physics, and allows a better chance to compare with ground-level measurements given the opportunity to have smaller surface layers.

The fine resolution in one direction (*e.g.* vertical) can match with similar resolution in the other (*e.g*. horizontal). The finer the resolution, the more mixing there should be between neighbouring air parcels, so the harder it is to accept the idea of an isolated air mass which is assumed in the simpler Lagrangian models.

Further, transport of SO_4^{2-} for example occurs above the boundary layer, but is then brought down by wet scavenging. Again, such transport can be quite different to that below the planetary boundary layer, and the treatment of clouds is much more natural in a 3-D framework. Some other advantages offered by Eulerian models include the following.

- The meteorology is Eulerian and can be mapped without unnecessary approximation.
- Eulerian models offers better possibilities for nesting and hence for dealing with boundary conditions.
- Eulerian models offer the future possibility of data assimilation.

Table 5.1. Comparison of Selected UK Models

Model Type	Type a)	Policy Relevance b)	Up-to-date methodology	Met Data	Horizontal Resolution c)	Vertical Resolution	Chemical Scheme	Strengths	Initialisation	Weakness	Peer reviewed/ Validated
UK-PTM	L	Currently used	E vs. L?	UKMO NAME	10x10km	Whole of BL	MCM	Ability to handle VOCs and link to NAEI Met variability	STOCHEM	BL model Lagrangian	Heavily/Yes
OSRM	L	Currently used	E vs. L?	UKMO NAME	10x10km	Whole of BL	STOCHEM	Biogenics	STOCHEM	BL model Lagrangian Empirical surface layer conversion	-/Some
MODELS-3/CMAQ	E	Extensively used in US	Yes	UKMO UM	4x4km	12 layers below 1600m	CBM4	Third party provision of model	STOCHEM		Not in UK context/Yes
EMEP4UK	E	Currently used for deposition in UK	Yes	WRF/ECMWF	5x5km	20 layers with 10 in boundary layer	EMEP unified	Link to EMEP programme			In European context/ Limited UK

a) E – Eulerian, L- Langrangian
b) Only ozone considered
c) In UK

Table 7.1 lists four candidate UK models and attempts to look at an evaluation against the criteria listed in Task 3 in section 2.1. The models were chosen to represent the current portfolio of models used in the UK for policy purposes with respect to ozone, and two models that are representative of the major classes of current models used in the USA and EU (EMEP).

All the models have been used in a general policy context and have heritage in this area with varying levels of application in the UK context. It is clear that the major difference in scientific approach, as previously noted, is the use of the Lagrangian vs. Eulerian approaches. This has a number of knock-on effects, such as the vertical resolution and the need, for example, for OSRM to have surface layer conversions. All models on the whole use state-of-the art meteorological fields. The application of chemical schemes reflects the purpose these models have been used for. It is clear that initialisation is a key issue, which is sometimes swept under the carpet and the sensitivity to initialisation has not been assessed. The models have varying levels of peer review and validation.

R 1.1 Defra should consider moving its ozone modelling activity to an Eulerian basis.

R 1.2 The Eulerian model results should be compared the results from observations and with those from comparative Lagrangian models to ensure continuity.

It is not possible to recommend a particular Eulerian model without testing in more detail – however two UK groups are using MODELS-3/CMAQ and it would be worthwhile capitalising on the third party investment already made. Models of US provenance are widely used in Europe, CAMx being the most common. Both CAMx and CMAQ are used extensively by the individual States in the USA to meet the EPA requirements for State Implementation Plans (SIPs) (Stockwell, *private communication*). There has been some investment in EMEP4UK although it has mainly been used to investigate deposition. There are some preliminary runs for ozone and this model should perhaps be investigated further (Defra, CPEA27). The EMEP model is used by the UN-ECE for compliance work and by the EU for prognostics – it has the advantage that it is regularly tested against a range of EMEP stations throughout Europe and tested similarly for SO_2 and NO_2. CHIMERE, the French model, is used in several countries.

R 1.3 Defra should 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.

The result of such an exercise would allow both the chemical performance to be assessed as well as highlighting any practical implementation issues (*e.g.* run-time, availability of meteorology, sensitivity to initialisation)

7.2 Chemical Scheme

UK groups favour limited explicit schemes rather than the aggregated schemes largely used on the continent and in the USA (section 5). The advantage is the updatability and the potential reference back to the MCM and therefore the primary literature. EMEP uses a surrogate scheme. The traceability of chemical schemes to an explicit basis is a more robust methodology than the use of tuned generic schemes and the MCM should be used as a reference benchmark for this process. The CRI offers a different, more linked way forward in that a large number of VOC (>100) are represented so that the reactivity range is preserved and there is minimal emissions lumping. The performance of CRI (in terms of ozone formation) using the NAEI VOC speciation has been shown to agree very well with MCM for a range of 32 in VOC/NOx.

Biogenic species are often limited to isoprene, with perhaps an extension to a couple of terpenes.

R 2.1 Defra should aim to support models which use chemical schemes, tested for ozone, such as the MCM or CBM-IV. However Defra should explore the use of surrogate schemes which have a firm basis in explicit chemistry such as CRI and which have been tested by comparison with experimental data and are tested over the appropriate range of VOC/NO_x ratios.

R 2.2 Defra should use models that have chemical schemes that allow robust coupling between the speciation in the emission inventories and the chemical scheme. This allows specific policy measures to be assessed more clearly and contains less simplifications and tuning of mechanisms.

R 2.3 Defra should require an improved representation of biogenic species in its chosen models, in order to be prepared for likely warmer summer periods in the future and to be able to better assess any biogenic/anthropogenic coupling. (see also R 3.5)

7.3 Emission estimates

As already indicated (section 5), the most common source of estimates for Europe is EMEP, but there are a variety of other schemes, together with combinations, in use. Modellers use what is available and convenient. There are few details about the methods of temporal and spatial disaggregation used to obtain the values necessary for the models, and it is seldom clear how estimates for biogenic emissions are obtained. Biogenic emission estimates are seldom mentioned though they may become crucial in peak ozone episodes in the future.

R 3.1 Defra should ensure that its chosen models have transparent sources of emission estimates.

R 3.2 Defra should ensure that its chosen models have recognised and realistic schemes for the spatial and temporal disaggregation of emission estimates. Some assessment is also required of how these might change in the future.

R 3.3 Defra should ensure its models are able to use the information in the NAEI.

R 3.4 Defra should investigate the policy need for its chosen models to include improved biogenic emission estimates, or land use data in conjunction with biogenic emission factors.

R3.5 Defra should ensure that the UK biogenic emission inventory is reassessed.

R 3.6 Defra should try to ensure that European and British estimates of emissions are updated as often and as reliably as possible.

7.4 Model evaluation, comparison and updating

As indicated in section 5, many models considered have undergone evaluation and presumably all in practical use are compared regularly with observations at a number of stations. Nevertheless there is always a case for evaluation and comparison. As the AQEQ (2007) points out:

> "There is no consistent and comprehensive understanding of model performance and the uncertainties that constrain them. Research is required to understand the policy significance of the different chemical mechanisms and parameterisations that have been adopted, to evaluate the relative importance of man-made and natural biogenic sources,

to harmonise model performance evaluation and to assemble information on uncertainties.

There are three general questions to be answered when evaluating environmental models (Beck, 2002) and these apply equally well to ozone models:

- Is the scientific formulation of the model broadly accepted and does it use state-of-the-art process descriptions?
- Does the model replicate observations adequately?
- Is the model usable for answering policy questions and fulfilling its designated tasks?

It is apparent that, for any comparison exercise, there is a requirement for carefully designed protocols to ensure the correct features of any model are tested. For example, indicator relationships can provide insight into the performance of models in respect of NO_x/VOC sensitivities and the chemical scheme.

R 4.1 Defra should ensure:

- any contracts let for ozone modelling include a review of the performance of its chosen models with observations, to ensure their continued performance levels; and
- regular comparisons between UK ozone models choosing, perhaps, periods of peak and background ozone, to ensure that the performance of the Defra chosen models is satisfactory.

R 4.2 Defra should ensure that UK ozone policy models have a strong peer-reviewed evidence base.

R 4.3 Defra should ensure that UK ozone models are taking part in European wide comparisons for policy purposes, to model observations from small groups of high quality stations in chosen countries, to ensure the performance of its own models, and of those used by the EU for regulatory purposes.

It is important that models are reviewed for updating regularly. This seldom poses a problem where the user is also the developer. However it is essential that modellers using models developed elsewhere have access to, give feedback to and make use of the newest version of the parent model.

R 4.4 Defra should ensure that a chosen model is regularly reviewed for updating. Where a model is a version of a parent model developed elsewhere, the latest version of the parent model should be used.

7.5 Quality control of models and output

As pointed out in section 6, quality control for models has attracted little attention and this seems remiss when models are used for regulatory and compliance purposes.

R 5.1 Defra should require the principal investigators for its chosen models to consider the recommendations of the Royal Meteorological Society (1995) on the use of models and, where appropriate, to follow them.

7.6 Extension to other species

As mentioned in section 5, most models can predict the boundary layer concentrations of other pollutant species such as NO_2 and SO_2. There is almost certainly a need to deal with aerosols, secondary organic aerosols and particulate matter. There should be some

consideration of what these model systems offer beyond the prediction of ozone. There is likely to be a future requirement in terms of multi-pollutant multi-effect and the models used should have some utility in this area.

R 6.1 Defra should use a modelling approach that allows a number of policy areas in air quality to be assessed.

7.7 Model review, and a modelling forum

As mentioned in section 6, US models used for regulatory purposes are subject to frequent peer review as well as comparisons. The reviews lead to detailed improvements in the model itself and increased confidence in the use of the model. The AQEG (2007) recommended the establishment of a modelling forum to exchange experiences with different chemical mechanisms and model parameterisations, to investigate central policy issues such as the relative importance of man-made and natural biogenic sources of VOCs, to assemble information on uncertainties and to lay out a protocol for a model comparison activity. This would be a desirable development, and our recommendations go some way towards meeting the desire. However our view is that more is needed than an informal forum – Defra should lay down firm requirements for its chosen models and ensure that they are met by having regular constructive peer reviews

R 7.1 Defra should implement a systematic series of peer reviews for its models to ensure their continued satisfactory performance and to facilitate their extension to other appropriate species.

R 7.2 Defra should run a regular modelling forum or actively participate in appropriate Knowledge Transfer networks to ensure community review and awareness of its requirements and performance.

8. Thanks and acknowledgements

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Table 1: Summary Table of Ozone Models Considered with their Principal Properties

The table gives a summary of the main answers given by our correspondents.

Kindly note:

- *many of the responses have been shortened*
- *the responses for Evaluation, Computer Resources, Extension to other species, Published reports and Comments are not included in the table*

The full response from each correspondent is given under the appropriate model and are shown in Appendix B

One warning and disclaimer – in the report models are frequently referred to by country. This is for convenience – it does NOT imply that the various models are used by the regulatory authorities in those countries.

UK models

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
ELMO Uni- Nottingham Uni-Lancaster **United Kingdom**	Lagrangian trajectory Receptor-specific for episode analysis & source attribution 10km grid for UK	Derived from the Master Chemical Mechanism 70 species +SOA VOC: 12 man-made + isoprene, terpenes	HYSPLIT/NCEP Initialisation	UK: NAEI. non-UK: EMEP Biogenic. EMEP, NAEI & Stewart.	EU & UNECE assessments NEGTAP (2001). Defra: SOA estimates Scottish assessments metrics: AOT40, AOT60, EPAQS, WHO
NAME UK Met. Office **United Kingdom**	Lagrangian dispersion Source or receptor oriented	STOCHEM + reactive VOCs VOC: 7 man-made + isoprene	UK Met Office NAME archive 1995-2007 ECMWF 1957-onwards Initialisation Ozone: background field from STOCHEM - but low values in winter. New method will use values from Mace Head. No ozone advection into the domain.	NAEI, EMEP, GEMS	DEFRA air quality forecast model (except for ozone). Emergency response (NAME without chemistry): RIMNET (DEFRA), Volcanic Ash; Foot & Mouth and Blue Tongue (DEFRA) metrics: all
OSRM AEA Technology& Environment **United Kingdom**	Lagrangian trajectory with surface post processing. 10km x 10km (UK), 10km x 10km (London) 50km x 50km EMEP model Domain	STOCHEM 70 species, 200 reactions VOC: 12 man-made + isoprene	UK Met Office NAME archive Initialisation O_3, CO, CH_4, C_2H_6, HNO_3 and PAN are initialised on each OSRM trajectory using output from the STOCHEM model. Initial ozone concentration can be modified to take account of trends in from Mace Head	UK: NAEI 10 km x 10 km non- UK: EMEP 50 km x 50 km Biogenic:bespoke	UK policy applications Curren Defra ozone tool Used for scenarios the Review of the Air Quality Strategy metrics: many produced by post processing, together with maps

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
STOCHEM Met Office, rdscientific, U. of Edinburgh **United Kingdom**	Lagrangian parcel 1.875° x 1.25° Global	72 species including , SO_2, DMS, NH_3 VOC: <=C4 + isoprene, generic terpene	Met Office climate model Initialisation: from previous runs. Typically spun up for 1 year after initialisation	IIASA + interactive biogenics	Transboundary pollution, climate change. metrics; AOT40, stomatal uptake, eight hourly max, SOMO35, monthly, seasonal
UK PTM rdscientific; Imperial College Uni-Birmingham **United Kingdom**	Lagrangian trajectory 10km x 10km	MCM: 4,414 species, 12,871 reactions Carbon Bond Mechanism version 4: 36 species, 93 reactions VOC:175 man-made + isoprene, α-pinene, β-pinene	UK Met Office NAME archive HYSPLIT/NCEP BADC/UK MO Initialisation O_3, CO, CH_4, H_2 SO_2, NO_x, part. sulfate, part. nitrate and part. ammonium from Mace Head or Valencia; HCHO from North Atlantic	UK: NAEI 10 km x 10 km non-UK :EMEP 50 km x 50 km Biogenic: EMEP isoprene, GEIA: terpenes	UK policy applications metrics: Maximum hourly mean ozone; Annual mean of the daily maximum ozone
EMEPUK Univ Edinburgh CEH Edinburgh **United Kingdom**	Eulerian Grid 20km x 20km with 5km x 5km nested for UK 20 vertical layers (10 in BL)	EMEP Extensively verified 80 species, 140 reactions 15 man-made VOCs + O_3, PAN, MPAN	Weather Research Forecast model (WRF version 2.2), ECMWF ERA40 (interpolated).	NAEI over the UK, EMEP everywhere else	Policy formulation for UN ECE LRTAP Input to RAINS, CAFÉ and NEC From hourly to yearly. AOT40
MODELS-3/CMAQ v. 4.3, 4.4 Uni- Manchester Uni-Edinburgh Uni-Hertfordshire Eon **United Kingdom** *Combined work with CMAQ below*	Eulerian, fully nested Inner: 240x170 cells, 5km x 5km, Outer: 45x45 cells, 45 km x 45 km	a. CBM4 36 species, 93 reactions b. RADM2 57 species, 157 reacts. c. SAPRC-99 40 species, 290 reactions VOC: included in SAPRC lumped in RADM2 bonds in CB4	MM5 – 5th Generation. 3D meteorological fields initialisation:	EMEP & NAEI	Most heavily used research an d policy model in USA. metrics: monthly runs of CMAQ provide 6-hourly pollutant concentrations and deposition fluxes

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
CMAQ v 4.5.1 Imperial College **United Kingdom** *Combined work with MODELS-3/CMAQ above*	Eulerian, nested European grid - 48x48km, 70x60 cells England and N. Europe – 12x12km 90x60 cells South East England – 4x4km 64x48 cells	RADM2 for V4.5 CB05 51 species and 155 reactions. From V4.6 switchable modules for aerosol and aqueous VOC: CMB 4 with ALD2, ETH, FORM, OLE, PAR, XYL, TOL, ISOP, TERB .	UKMO UM data stored on BADC Initialisation: STOCHEM data for initial and boundary conditions Europe, inner grids nested	EMEP, NAEI inventories and a Biogenic potential inventory	In the UK CMAQ has been used in the power industry to study power station footprints metrics: Standard model output is hourly ppm, Can be used to produce most other metrica
AQUM (*under development)* UK Met. Office **United Kingdom**	Eulerian, on-line, global/regional	*Not yet decided* *Not yet decided*	Unified model	GEMS 2003, 5km resolution	possibly case studies metrics: *Not yet decided*
UKCA UK Met. Office **United Kingdom**	Eulerian global/regional 1.875° x 1.25° x L38 (12km x 12km x L38)	a) TOMCAT b) TOMCAT + isoprene c) TOMCAT + Sulfur In implementation d) STOCHEM e) CRI mechanism *VOC*: (a) & (c) C_2H_6 & C_3H_8 (b) with isoprene as well (d) & (e) more species	Climate Model or operational models (with data assimilation) *Initialisation*: previous runs or nesting	IPCC (2001) OxCOMP or GEMS 2003, 5km resolution IIASA	Met Office & Defra *metrics* Potentially: AOT40, cumulative stomatal uptake, eight hourly max, SOMO35, monthly, seasonal, annual

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
ADMS-Urban CERC, Cambridge **United Kingdom**	Gaussian model nested in trajectory model. Variable resolution down to 10m Local to large urban areas (*e.g* London area) and small regional	CB4 95 reactions and 36 species Or GRS 6 reactions VOC CB4 7 man-made VOCs +isoprene GRS – 1 surrogate VOC	Standard met data from one measurement site or mesoscale model Initialisation: Flexible. Able to make use of monitored data and/or regional model output..	Flexible. Gridded emissions or explicit source information for individual sources (*e.g* point or road sources)	Influences policy development in London especially the impact of future NO_x concentrations on urban ozone. The impact of VOCs is small at urban scale so this aspect has not fed into policy. Full range of ozone metrics may be calculated.
		Overseas	**Models**		
EMEP MSC-W **UN-ECE**	Eulerian grid 50km x 50km 4km x 4km local grid Global grid being tested	EMEP 80 species, 140 reactions alpha-pinene chemistry in research SOA. Aerosol dynamics in research version	HIRLAM-PS	CAFE and NEC Anthropogenic emissions from official data supplied to EMEP where possible, otherwise estimated Biogenic emissions calculated from landuse and model temperature & radiation.	Policy formulation for UN ECE LRTAP Input to RAINS, CAFÉ and NEC.Hourly to yearly outputs of any gas or particle concentration. Seasonal outputs AOT40, SOMO35, flux indices, and of S and N deposition. Deposition outputs available for each land
CAMx Academy of Sciences Prague, **Czech Republic**	Eulerian, 2 domains Europe, Czech Rep. horizontal. res. 27 km resp. 9 km	SAPRC 99 ozone, 56 species CBM-aero – for aerosols VOC not specified	MM5	EMEP	outputs (images) free for noncommercial use metrics: hourly ozone

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
DEHM (Danish Eulerian Hemispheric Model) NERI, Aarhus University **Denmark**	Eulerian 3-D model with two way nesting hemisphere 150 km x 150 km Europe: 50 km x 50 km N. Europe 16.67 km x 16.67 km	Modified EMEP scheme 63 species, 130 reactions. VOC: 10 + isoprene	Eta/NCEP MM5v3/ECMWF MM5v3/NCEP	Geia/EMEP/DK	DK monitoring forecasting; policy DK and EU AMAP; NECE HTAP metrics: all possible
DEOM (Danish Eulerian Operational Model) NERI, Aarhus University **Denmark**	Eulerian model Europe 50 km x 50 km resolution 3 vertical layers.	CBM-IV with 35 species. VOC: CBM-IV	Eta/NCEP	EMEP/DK	Air quality forecasting metrics: all
CAC Danish Meteorological Institute (DMI) **Denmark**	Eulerian 0.2º×0.2º (*ca* 11 km x 7 km @ 50ºN) 40 vertical levels	CBM-IV + aerosol species 49 species + 11 aerosol 105 reactions. VOC: 67 + isoprene, α-pinene, β-pinene.	HIRLAM / ECMWF	TNO	Public Information metrics: hourly ozone
MOON Danish Meteorological Institute (DMI) **Denmark**	Lagrangian trajectory 5km×5km	RACM 77 gas-phase species 237 reactions VOC: 67 + isoprene, α-pinene, β-pinene	HIRLAM / ECMWF	EMEP	Public information metrics: hourly ozone
CHIMERE INERIS, Paris **France**	Eulerian grid From 2km x 2km to 0.5º x 0.5º (*ca* 55 km x 35 km @ 50ºN)	MELCHIOR 80 species, 300 reactions or reduced 44 species 110 reactions 6 aerosol species,POPs VOC: 12 +isoprene	MM5, ECMWF/IFS, ARPEGE Initialisation:	EMEP, local inventories	Most accurate ozone daily maxima forecast model in Europe, and among most accurate models for daily average PMs metrics: all possible

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
EURAD Rhenish Inst. Env. Research Univ. Cologne, **Germany**	Hemispheric to regional/urban background, troposphere (and partially stratosphere) Horizontal grid sizes: 1 – 250 km Hemispheric, Europe, urban as Berlin, Rhein-Ruhr (1 km grid)	RADM2, RACM-MIM 60 -70 species, 200 reactions 15 lumped species, isoprene, α-pinene, β-pinene	MM5, driven by ECMWF, NCEP	EDGAR, EMEP, TNO, IER-Stuttgart, local inventories	Daily chemical weather forecast used by several local environmental agencies (including data assimilation, daily evaluation) Used for Emission scenarios Metrics: Hourly, 180 µg/m^3 threshhold,
REM-CALGRID (RCG) Free University Berlin, Institute for Meteorology, **Germany**	Eulerian grid model for regional- through urban-scales Europe: 0.5° Lon, 0.25°Lat Germany, of 0.25° Lon, 0.125°Lat urban areas approx. 1 km x 1 km	CBM-IV including a 1-Product Isoprene scheme VOC: Individual VOCs are assigned to 6 Carbon Bond classes	Diagnostic meteorological analysis system based on an optimum interpolation procedure on isentropic surfaces utilizing all available observed synoptic surface and upper air data Initialisation European: monthly climatological background from observations National, local scale: taken from RCG runs for the next larger grid (one-way nesting)	International, national, local inventories	National and local applications (Germany) to predict the impact of air quality action plans International applications within the framework of the EURODELTA and CITYDELTA exercises metrics: hourly, eight-hourly, daily, seasonal, AOT40, AOT60, SOMO35
CAMx Atm. Phys. Aristotle Uni. Thessaloniki, **Greece**	Eulerian photochem. dispersion combined with meteorological prognostic Mesoscale, Urban	CBM-IV VOC: not specified	MM5	Inventory with 10km spatial resolution Atm. Phys. Lab. NOx, NMVOCs and CO monthly variations	regulatory assessments in the U.S. metrics :hourly average concentrations

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
EPA-UAM-IV N.C.S.R. Demokritos, Athens, **Greece**	Eulerian photochem. Mesoscale and urban	Carbon-Bond IV 81 reactions, 33 species VOC: Anthropogenic and biogenic	not specifed	not specifed	not specifed metrics: not specifed
MAP Nat. Tech. Uni., Athens, **Greece**	Prognostic, Lagrangian Urban, local scales	Carbon-Bond IV QSSA; 81 reactions 93 species VOC: not specified	not specified	not specified	not specified metrics: pollutants concentrations for each grid-cell
MARS LHTEE , Aristotle Uni. Thessaloniki, **Greece**	3D, photochemical Eulerian, Mesoscale, urban scale Horizontal resolution Domain size: 50-500 km Grid cell size: 500-10km Vertical resolution Domain height: to 10 km Grid cell height: 20-500 m (varying with height)	Various KOREM 20 species, 39 reactions EMEP 66 species, 139 reactions RADM2 56 species, 156 reactions RACM 72 species, 234 reactions VOC: are split into CH_4 and other 42 NMVOCs	MEMO mesoscale Eulerian model initialisation: Regional background concentrations of NO, NO_2, O_3, PM_{10}, $PM_{2.5}$ and all other species included in the chemical reaction mechanism either from measurements of from large scale model application.	3-D gridded emission inventory of 47 species. Emission values are provided in kg/h/cell area for each grid cell	Policy uses - Summer smog - Winter smog - Air toxics - Urban air quality - Industrial pollutants metrics: Concentrations of chemically reacting pollutants for each grid location.
OFIS LHTEE , Aristotle Uni. Thessaloniki, **Greece**	Two-layer 2-D Eulerian photochemical dispersion model Urban scale	EMEP MSC-W 66 species, 139 reactions VOC: not specified	MEMO mesoscale Eulerian model	not specified	metrics: Concs. of pollutants for each grid location. Annual av. concs; percentiles; exceedance probabilities of threshold values

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
MUSE LHTEE, Aristotle Uni. Thessaloniki, **Greece**	Photochemical Eulerian (with 5, time dependent layers) Local to regional	Various: KOREM 20 species, 39 reactions EMEP 66 species, 139 reactions RADM2 56 species, 156 reactions RACM 72 species, 234 reactions SORGAM 8 organic aerosol species, 16 oxidation reactions (appended to RACM) VOC: split into CH_4 and other 42 NMVOCs	MEMO mesoscale Eulerian model initialisation: Regional background concentrations of NO, NO_2, O_3 and all other species included in the chemical reaction mechanism either from measurements of from large scale model application.	3-D gridded emission inventory of 50 species. Emission values are provided in kg/h/cell area for each grid cell.	Policy uses - Summer smog - Winter smog - Air toxics - Urban air quality - Industrial pollutants metrics: concs. of pollutants for each grid location.
LOTOS-EUROS TNO, RIVM **Netherlands**	Eulerian grid model European 3.5 km height 0.5x0.25 long.- lat. zooming available	CBM-IV: 28 species and 66 reactions CB99: 42 species and 95 reactions VOC: 8 (CBM-IV) or 10 (CB99) species, + isoprene and terpene (α,β)	Either FUB (Freie Universität Berlin) or ECMWF	TNO or EMEP	EU and NL application metrics: all possible hourly concs + deposition fluxes;
CAO-HMC statistical model CAO, Dolgoprudny, and HMC, Moscow **Russia**	Statistical for Moscow city and its suburbs (to 100 km)	Uses current O_3 and NO_2 measurements VOC: not applicable	Russian HydroMetCentre Iniatialisation Observations and predictions of some meteorological parameters including Meteorological Potential of Pollution – MPP	not applicable	forecasting maximal one-hour ozone concentrations in Moscow Moscow policy application metrics: daily 1hr mean

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
CHIMERE (extended) Academy of Sciences, Nizhny Novgorod **Russia**	Eulerian 3D model, Europe: 0.5^0x0.5^0 (*ca* 55 km x 35 km @ 50ºN) or 1^0x1^0 + nested domain (Central Russia, including Moscow conurbation) 0.25^0x 0.125	MELCHIOR2 44 species 120 reactions or MELCHIOR1 80 species >300 reactions VOC: aggregated into 9 classes + isoprene and α-pinene	MM5 initialised with NCEP data	EMEP	Currently, used in scientific studies metrics: hourly ozone – all possible
CAMx Iberinco **Spain**	Eulerian Many scales sub-urban to continental	CBM-IV, SAPRC99 and user defined CBM-IV: 38-47 species, 96-110 reactions SAPRC99: 76 species 217 reactions VOC: as in the models.	MM5, RAMS, WRF	emission processors SMOKE, CONCEPT, EPS, EMS	Regulatory assessments and general research throughout the U.S. metrics : hourly
CAMx CEAM **Spain**	Eulerian photochem. dispersion model	Multiple options. CBM4 & SAPRD Aerosol Chemistry VOC: not specified	MM5, RAMS and WRF	not specified	Impact assessment & prognostic metrics : hourly, eight hourly, daily, seasonal, AOT, source-receptor, etc
CAMx Uni. Santiago de Compostela **Spain**	Eulerian model regional to mesoscale 27kmx27km, 9kmx9km	CBM-IV with aerosol chemistry VOC: CAMx default	PSU-NCAR MM5	EMEP & Galician Industrial	Research metrics : hourly
CALGRID Iberinco **Spain**	Eulerian grid-based Mesoscale and regional 5 to 20 km Domain: 20 to 1000 km	CBM-IV & 1990 SAPRC 54 species, 129 reactions VOC: not specified	CALMET gridded fields	Point, mobile and area source emissions	Research metrics : hourly

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
CMAQ and **CHIMERE** Centro Nacional de Supercomputación, Barcelona **Spain**	Eulerian local: 1km x 1km, 2km x 2km Iberian Pen.: 4km x 4km Europe: 12km x 12km, 20km x 20km, 50km x 50km	CMAQ: CBM-IV with aerosols and heterog. chemistry 36 species, 96 reactions CHIMERE: MELCHIOR2 with aerosols and heterog. chemistry, 44 species, 120 reactions VOC: CMAQ: 10 + biogenic isoprene and terpenes CHIMERE: 10 + biogenic isoprene and α-pinene	MM5, WRF-ARW and WRF-NMM	HERMES, EMICAT and EMIVAL at BCNS (specifically for the Iberian Peninsula) EMEP	Scientific, regulatory, policy, environmental impact assessment, air quality forecasting metrics : Hourly, 8-hr, daily, seasonal, annual, AOT40, statistical and categorical evaluation
KINMOD CEAM **Spain**	Secondary organic aerosols only	MCM (as previous) with adaptations for SOA etc. :	not applicable	not applicable	not applicable
MCM v3.1 CEAM **Spain**	Chemical mechanism only	degradation of 135 VOC 12871 reactions; 4414 species. VOC: not applicable	not applicable	not applicable	not applicable
MDpA Modelo Diagnóstico por Análogos Meteológica S.A **Spain**	Empirical model using observed non-linear relationships between today's O_3 and today's: 1. Wind direction and speed, 2. Max. temperature 3. Day of the week and calendar & yesterday's maximum O_3 concentration	not applicable	Uses forecasts of wind and temperature	not applicable	none metrics : daily maximum & no. of hours above threshold

Model	Model Type Scale	Chemistry Treatment of VOC	Meteorology Initialisation	Emission Inventories	Policy relevance Metrics produced
SMOC System for Modelling tropospheric Ozone in Catalonia Uni. Barcelona, Depts Astronomy & Meteorology **Spain**	Eulerian and Lagrangian 20km x 20km (Eulerian column) 3km x 3km (emissions) OZIPR (Ozone Isopleth Plotting Program Research)	SAPRC97 12 hydrocarbon groups 140 reactions VOC: not specified	MASS: 3-D mesoscale Blackadar and Transilient: microescale boundary layer models	MECA (Emission Model for Catalonia)	Directive 02/03/CE metrics :hourly ozne values
MM5-CAMx PSI Villingen **Switzerland**	Eulerian meso-scale model. Domains: Europe to parts of Switzerland. Grid cell size: 27, 9, 3 and 1 km	CBM-IV (gas-phase) RADM-AQ (aqueous) CF and CMU (aerosol chemistry) VOC: Lumped according to CBM-IV + Isoprene, biogenic olefins	MM5 driven by assimilated data of the Swiss forecast model (aLMo)	Europe: UBA/FUB/TNO Lombardy: CityDelta Switzerland, various from the Swiss FOEN	not specified metrics: hourly ozone
CMAQ Howard University **USA**	Eulerian (adjustable) with multi-nesting available. 4 km is the typical lower limit Used for modelling the entire U.S.; Regional scales and Urban scales	RADM2 to V4.5. CB-05 52 species; 156 reactions. SAPRC available. RACM2 for research vers. All can be used with/without modules for aqueous and aerosol chemistry. VOC: CB-05 lumped; RADM2, SAPRC and RACM2 are all lumped	MM5 or WRF ; WRF is the standard for NOAA's air quality forcasting program. Available climatological data and simulation of extra 'spin-up" days are most typically used. Formal data assimilation methods using satellite data and global scale models are under investigation at NOAA and NASA.	SMOKE	Model output is hourly ppm (at end of timestep), average hourly ppm is available. Hourly 3-D gridded chemical concentrations of ozone, nitrogen oxides, CO, PM, mercury, VOC and most other air pollutants and 2-D fields of acid deposition.

10. Appendices

Appendix A. Contacts for model information

Model	Correspondent	
ELMO (UK)	Sarah Metcalfe	Sarah.Metcalfe@nottingham.ac.uk
NAME (UK)	Alison Redington	alison.redington@metoffice.gov.uk
OSRM (UK)	Tim Murrells Gary Hayman	Tim.P.Murrells@aeat.co.uk garry.hayman@npl.co.uk
STOCHEM (UK)	Bill Collins	bill.collins@metoffice.gov.uk
UK-PTM (UK)	Dick Derwent	r.derwent@btopenworld.com
EMEPUK (UK)	Massimo Vieno	mvieno@staffmail.ed.ac.uk
Models3-CMAQ (UK)	Rognvald I Smith	ris@ceh.ac.uk a.fraser@imperial.ac.uk
CMAQ (UK)	Andrea Fraser	a.fraser03@imperial.ac.uk
AQUM (UK)	Paul Agnew	paul.agnew@metoffice.gov.uk
UKCA (UK)	Paul Agnew	paul.agnew@metoffice.gov.uk
ADMS-Urban	David Carruthers	David.Carruthers@cerc.co.uk
EMEP (UN-ECE)	David Simpson	david.simpson@met.no
CAMx (Czech Republic)	Krystof Eben	eben@cs.cas.cz
DEHM (Denmark) DEOM (Denmark) CAC (Denmark) MOON (Denmark)	Joergen Brandt	jbr@dmu.dk
CHIMERE (France)	Laurent Menut	Laurent.menut@lmd.polytechnique.fr
EURAD (Germany)	Michael Memmesheimer	mm@riu.uni-koeln.de
CALGRID_RCG (Germany)	Rainer Stern	rstern@zedat.fu-berlin.de
CAMx (Greece) EPA-UAM-IV (Greece) MAP (Greece) MARS (Greece) OFIS (Greece) MUSE (Greece)	John Douros	jdouros@aix.meng.auth.gr
LOTOS_EUROS (Netherlands)	Michiel Roemer	michiel.roemer@tno.nl
CAO-HMC (Russia) CHIMERE (Russia)	Oksana Tarasova	tarasova@mpch-mainz.mpg.de
CAMx (Spain) CAMx (Spain) CALGRID (Spain) CMAQ-CHIMERE (Spain) KINMOD (Spain) MCM (Spain) MDpA (Spain) SMOC (Spain)	Jose Luis Palau	jlp@confluencia.biz
CAMx (Switzerland)	Johannes Keller	johannes.keller@psi.ch
CMAQ (USA)	William Stockwell	wstock@dri.edu

Appendix B. Model information sheets

Model	***ELMO (UK)***
Institution/s	University of Nottingham Lancaster University
Possible contacts email	Prof. Sarah Metcalfe, University of Nottingham Dr. Duncan Whyatt, Lancaster University. Prof. R.G. Derwent, rdscientific sarah.metcalfe@nottingham.ac.uk d.whyatt@lancaster.ac.uk r.derwent@btopenworld.com
Type & scale	Lagrangian trajectory Receptor-specific for episode analysis & source attribution 10km grid for UK assessment (scenarios & source attribution) Full domain = EMEP, UK nested at finer resolution
Chemistry	Derived from the Master Chemical Mechanism (70 species used in ELMO) + secondary organic aerosol formation
Treatment of VOCs	12 man-made VOCs + isoprene, terpenes C_2H_6, C_3H_8, nC_4H_{10}, C_2H_4,C_3H_6, C_7H_8, C_8H_{10}, CH_3OH, acetone, MEK, HCHO, CH_3CHO
Meteorology	HYSPLIT/NCEP
Emission Inventories	European Inventories: NOx, NMVOC and CO from EMEP. Isoprene from David Simpson. Terpene from GEIA (resampled). Nested UK Inventories: NOx, NMVOC and CO from the NAEI. Isoprene and monoterpene from Stewart (see reference, below), Other natural sources of NMVOC from NAEI.
Chemical initialisation and model boundary ozone advection	Global background for model boundary conditions set at 1990 values for NO, NO_2, CO, CH_4 and O_3
Evaluation: (comparison with observations)	For the evaluation: choose two periods – "peak" which should include an appreciable number of days with observed peak ozone above 200 μg m^{-3} (*ca*. 100ppb) "background" which should only include values less than 100 μg m^{-3} (*ca*. 50 ppb) For each: the no. of days, the no. of observation stations simultaneously covered, and an overall rating of general goodness of

	fit on the scale: 1 (middling); 2 (good); 3 (excellent) Original model (Metcalfe *et al*., 2002) modelled weighted mean peak ozone compared with measured 90th, 95th, 98th percentiles of hourly maximum ozone from UK rural O_3 monitoring network sites (15 sites). Revised model (Strong *et al.,* 2006) as above. Best fit to 98th percentile (15 stations) Latest version (using HYSPLIT trajectories), modelling to single sites compared with 3-hrly ozone at monitoring sites (rural network and some campaign sites) over chosen period.
Computer Resources (*super; mainframe; PC*) and typical run time	SUN Workstation (SunBlade 100) < 2 minutes per run for site-specific studies based on single trajectories derived from HYSPLIT. For a typical 5 day ozone episode running every 6 hours, run time 5 to 9 minutes per receptor point. 18 hours for regular spaced array of 10km grid cells across the UK. Multiple runs may be performed on high performance clusters at either Nottingham or Lancaster.
Policy relevance	Used in assessment of EU National Emissions Ceiling Directive and the UNECE Protocol to Abate Acidification, Eutrophication and Ground Level Ozone. Major contributors to NEGTAP (2001). Secondary Organic Aerosol estimates incorporated into UK maps of particulate matter (*e.g*. http://www.airquality.co.uk/archive/reports/cat09/0610161501-416_dd12004mapsrep_v1e.pdf). Has also been used (*e.g*. re Gothenburg, PVR). SOA output currently used in UK mapping of particulate matter. ELMO was applied in consultations over Stage II PVR, initially for the Scottish Executive and then nationally.
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly, eight hourly, daily, seasonal, annual and derivatives of exceedance (AOT40, AOT60, EPAQS, WHO).
To what other species can the model be reliably extended?	Aerosols (SIA and SOA), oxidised S and N, reduced N *etc.*
Comments	As well as ozone concentrations, HARM-ELMO models mass concentrations of a range of PM components: SIA, SOA, PM_{coarse}, PM_{fine}. The models have also been subject to uncertainty analysis at regional and national scales. Engaged in re-analysis of TORCH campaign data (with Nick Hewitt, Lancaster).

Model	***NAME (UK)***
Institution/s	MET OFFICE
Possible contacts email	Alistair Manning, Alison Redington alistair.manning@metoffice.gov.uk
Type & scale Model domain	Lagrangian dispersion Source or receptor oriented National & Europe
Chemistry	STOCHEM + reactive VOCs (not evaluated)
Treatment of VOCs	7 man-made VOCs + isoprene Formaldehyde (HCHO), ethylene (C_2H_4), propylene (C_3H_6), o-xylene (C_8H_{10}), toluene (C_7H_8), 1,3 butadiene (C_4H_6), acetaldehyde (CH_3CHO) & isoprene (C_5H_8)
Meteorology	UK Met Office NAME archive 1995-2007 ECMWF 1957-onwards Single site met data Ensembles
Emission Inventories	NAEI, EMEP, GEMS
Chemical initialisation and model boundary ozone advection	There is no chemical initialisation for any species other than ozone – the model is just allowed to spin up over a number of days (time required is dependant on size of model domain). For ozone a background field from the global STOCHEM model is used to initialise. This method needs revising however and appears to give quite low values in winter. A different method using monthly baseline values from Macehead is planned. There is currently no representation of advection of ozone into the domain at the boundaries.
Evaluation (comparison with observations)	Full evaluation of the ozone scheme is yet to be carried out. Please note that the Met Office supplies NO_2, SO_2, PM10 and CO to DEFRA for the air quality forecast, but NETCEN currently provide the daily ozone predictions. The NAME model has been run for 2003 – time series results from a number of sites attached. NAME modelling of ozone is still under development. The NAME scheme does not yet include biogenic emissions of isoprene which is no doubt contributing to the under-prediction seen in August 2003. The deposition scheme currently used for ozone is simplistic and its improvement is part of a current research project. Assessment

	of the chemical scheme used in NAME is also being undertaken at Bristol University. As mentioned above the current initialisation is going to be changed to use monthly baseline values from Macehead.
Computer Resources (*super; mainframe; PC*) and typical run time	PC Huge variation in run time depending on application, chosen grid scales, domain etc A typical full chemistry run over one year at 20x20km resolution, domain 15W to 15E, 45N to 65 N, using a combination of NAEI and EMEP emissions would take approximately 8 weeks using a single processor (4 processor PC = 2 weeks).
Policy relevance Is the model actually used for policy applications?	NAME chemistry model used as DEFRA air quality forecast model (except for ozone which NETCEN currently supply). Emergency response (NAME with no chemistry): RIMNET (DEFRA), Volcanic Ash Advisory Centre (VAAC), RSMC, CTBTO. Foot & Mouth and Blue Tongue modelling (DEFRA) Dust modelling, volcanic ash, aerosols, ozone and inversion modelling. oOo The NAME model is used extensively for policy applications but not for direct ozone forcasting. Some examples are: - Greenhouse gas and ozone emission and baseline estimates, - Source attribution studies to understand particulate episodes, - Air quality forecasting (NO_2, SO_2, PM_{10}, CO), - Saharan dust modelling.
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	All
To what other species can the model be reliably extended?	
Comments	The NAME model has been used extensively for modelling atmospheric transport. The chemistry scheme has been evaluated against the PUMA data set and is used routinely for air quality forecasting. A new ozone scheme has been developed and will be tested in the air quality system. A selection of references are given below which can be provided if required, along with other publications. If a more detailed explanation of the current status of NAME with regard to ozone modelling is required please contact us.

Model	***OSRM (UK)*** **Ozone Source-Receptor Model**
Institution/s	AEA Energy & Environment
Possible contacts Email	tim.p.murrells@aeat.co.uk garry.hayman@npl.co.uk
Type & scale Domain	Lagrangian trajectory model (EMEP domain) 10km x 10km (UK-scale runs), 1 km x 1 km (London runs), 50km x 50km. Uses a Surface Conversion Algorithm in OSRM post-processor to convert hourly mid-boundary layer concentrations to surface concentrations with corrections allowing for local NO_x emission rates. EMEP Model Domain
Chemistry	STOCHEM (not evaluated) with additional reactions added to represent (i) HONO chemistry; (ii) reactions of peroxy radicals with NO_3 and (iii) formation of organic nitrates [70 species, 200 thermal and photochemical reactions]
Treatment of VOCs	12 man-made VOCs + isoprene C_2H_6, C_3H_8, nC_4H_{10}, C_2H_4, C_3H_6, C_7H_8, C_8H_{10}, CH_3OH, acetone, MEK, HCHO, CH_3CHO
Meteorology	UK Met Office NAME archive (1999-2005)
Emission Inventories	(a) NAEI 1 km x 1 km emission inventories aggregated to 10 km x 10 km for the UK by sector, with representative temporal profiles applied for each pollutant and sector (diurnal, day of week, month of year) (b) EMEP emission inventories at 50 km x 50 km for the non-UK emissions (c) Bespoke emission potential inventory for biogenic VOC emissions comprising 8 emission potentials for isoprene and terpenes from deciduous and evergreen trees (50 km x 50 km).
Chemical initialisation and model boundary ozone advection	The concentrations of O_3, CO, CH_4, C_2H_6, HNO_3 and PAN are initialised on each OSRM trajectory using output from the STOCHEM model. This allows the seasonal cycle in ozone to be represented in the model and couples regional scale ozone production to the hemispheric circulation. A full set of daily concentration fields were

	provided for 2 calendar years, one representing the climatology of the late 1990's (actually 1998) and the second a future atmosphere (IPCC SRES scenarios for 2030). Depending on the option used, the initial ozone concentration can be modified to take account of trends in hemispheric ozone concentrations at Mace Head. Using the output of STOCHEM model runs undertaken by Dick Derwent [see project reports for details], monthly trends in ozone at Mace Head were derived for a number of climate-related emission scenarios. For the Business-as-Usual with Climate Change scenario, this would cause changes from 2003 concentrations ranging from –0.8 to +1.6 ppb on the initial daily ozone concentrations by 2010 and –1.9 to +3.8 ppb by 2020.
Evaluation: (comparison with observations)	Comparison of modelled hourly O_3, NO and NO_2 concentrations have been made against observations at 41 UK and 22 EMEP O_3 monitoring sites for the calendar years 1999-2005 (UK) and 1999-2002 (EMEP). The UK sites comprise 20 rural, 10 London urban and suburban background and 11 other urban background sites. The model performs better for the UK sites, with typically 60-80% of the hourly concentrations at rural sites within ±50% of the measured concentration. The corresponding figure for the London and other urban sites is 40-55%. The OSRM calculates a wide-range of metrics, which can be compared against values derived from measurements. Not unexpectedly, the model generally performs better for metrics less sensitive to elevated concentrations or those without thresholds/cutoffs. Examples of comparisons against measurements are shown in the attached Annex (these Figures are taken from a draft of a paper that is being prepared for publication). A detailed comparison against observed values at UK monitoring sites was undertaken for the metrics used in the 3rd Daughter Directive (AOT40 Crops and Number of Days with exceedances of 120 μg m^{-3}) to assist the selection of the supplementary assessment method (project reports available). Although the OSRM has not yet been involved in a model intercomparison exercise, the OSRM outputs have been compared against the outputs of other models (Quantitatively: UK Photochemical Trajectory Model, Pollution Climate Model, ADMS-Urban; Qualitatively: EMEP Unified Model). The AQEG report on Ozone will include a comparison of the OSRM against the Pollution Climate and ADMS-Urban models in terms of urban

	ozone decrements. Overall, the model performance would be assessed as between 2 (good) and 3 (excellent).
Computer Resources (*super; mainframe; PC*) and typical run time	Cluster of dual-processor workstations 4.5 days for a UK-scale model run to a 10 km x 10 km grid covering the UK (~3,000 receptor sites). This typically involves a total of ~26 million trajectories to simulate each hour in a calendar year.
Policy relevance used?	UK policy applications and regulatory impact assessments (*e.g.* EU Decorative Paints and Petrol Vapour Recovery Directives, Vehicle Emission Directives) Yes. The OSRM was used to model the ozone response to a number of transport and non-transport emission reduction measures in the Review of the Air Quality Strategy. It has been used in various regulatory impact assessments (examples already given) and for modelling the impacts on ozone of changes in European VOC emissions with the uptake of bioethanol as a transport fuel.
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	A post-processor code is used to process the hourly concentrations generated by the OSRM and to calculate a large number of metrics for ozone and nitrogen dioxide (see Annex). The code also produces output datafiles for generating maps of these metrics.
To what other species can the model be reliably extended?	The hourly concentrations of NO and NO_2 (and derived metrics) are a routine output and used in policy applications. SO_2 is also calculated although the model does not treat plume rise or near-field dispersion. There is a very simple description of photochemical production of sulphate and nitrate (basically that used in the Photochemical Trajectory Model). This could in principle be replaced by a more sophisticated treatment.
Comments	The OSRM is currently the Defra tool for assessing ozone control policies. The model was extensively used to assess future ozone concentrations and the effectiveness of measures for the Review of the Air Quality Strategy. Would benefit from use of a reduced chemical mechanism that can be directly traceable to the Master Chemical Mechanism

Annex - Metrics Calculated by the OSRM

Ozone:

(1) annual mean concentration
(2) AOT30 for the protection of crops (EU and UN ECE[1])
(3) AOT30 for the protection of forests (EU and UN ECE)
(4) AOT40 for the protection of crops (EU and UN ECE)
(5) AOT40 for the protection of forests (EU and UN ECE)
(6) AOT60 for the protection of human health (EU and UN ECE)
(7) maximum hourly concentration in the year
(8) maximum 8-hour running mean concentration in the year
(9) annual mean of the maximum of the 24 possible 8-hour running mean concentrations in each day
(10) number of days when the maximum of the 24 possible 8-hour running mean concentrations in each day exceeds 100 μg m^{-3} (metric in the UK Air Quality Strategy)
(11) number of days when the maximum of the 24 possible 8-hour running mean concentrations in each day exceeds 120 μg m^{-3} (metric in the EU 3rd Daughter Directive)
(12) AOT30 for the protection of horticulture (EU and UN ECE)
(13) AOT30 for the protection of semi-natural vegetation (EU and UN ECE)
(14) AOT40 for the protection of horticulture (EU and UN ECE)
(15) AOT40 for the protection of semi-natural vegetation (EU and UN ECE)
(16) annual mean of those maxima of the 24 possible 8-hour running mean concentrations in each day > 35 ppb
(17) maximum hourly concentration in the summer
(18) annual mean of the difference between the maximum of the 24 possible 8-hour running mean concentrations in each day and 35 ppb (or 70 μg m^{-3}) for the protection of human health
(19) annual mean of the difference between the maximum of the 24 possible 8-hour running mean concentrations in each day and 50 ppb (or 100 μg m^{-3}) for the protection of human health

Nitric Oxide:

(20) annual mean concentration

Nitrogen Dioxide:

(21) annual mean concentration
(22) maximum hourly concentration in the year

[1] The EU methodology uses fixed hours (08:00-20:00 Central European Time) during the relative accumulation period, whereas the UN ECE calculation uses daylight hours, defined by the incident UV radiation being greater than 50 mW m^{-2}.

Figures

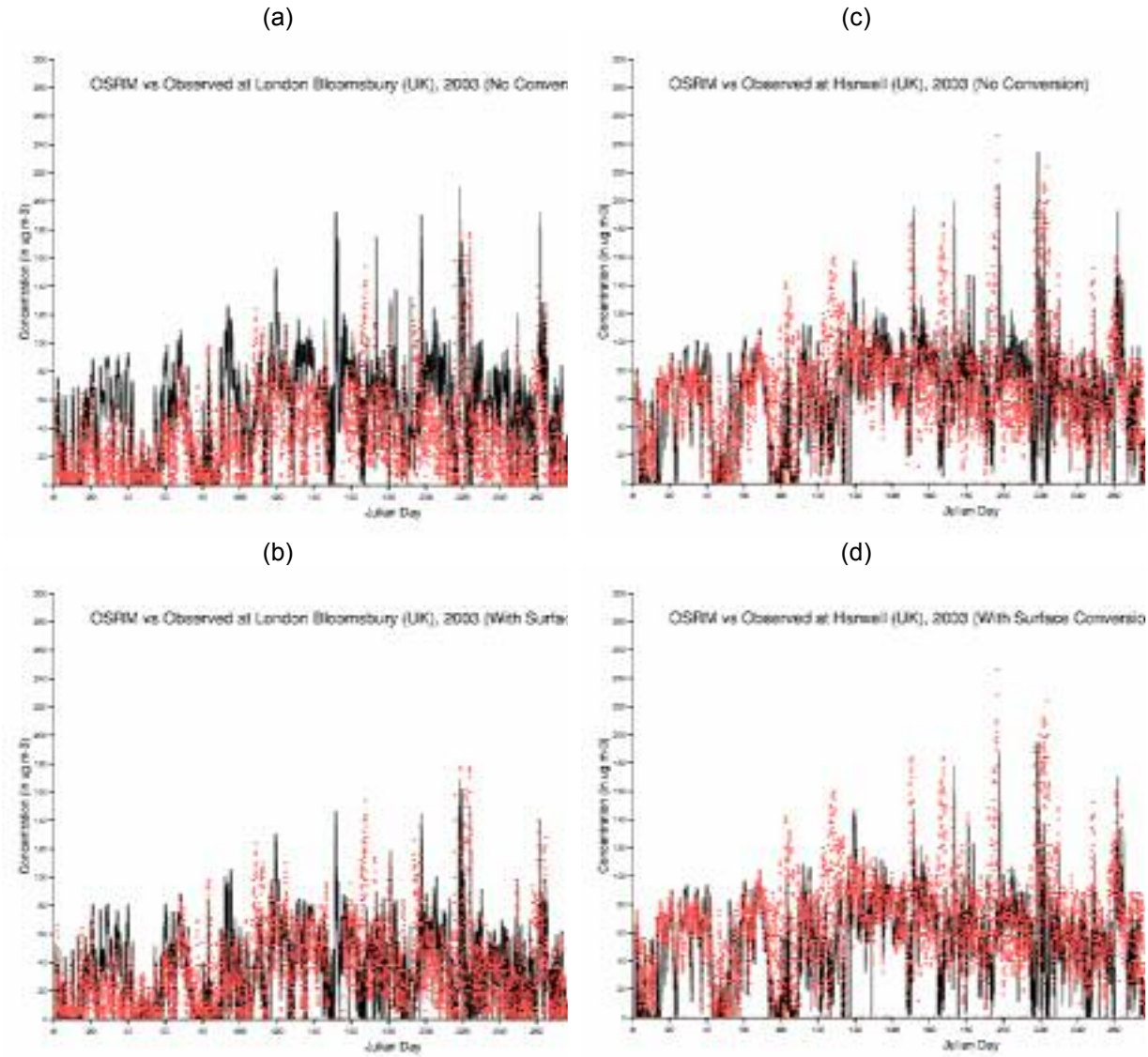

Figure 1: Comparison of Observed and Modelled Hourly Ozone Concentrations at London Bloomsbury (Panels a and b) and Harwell (Panels c and d) in 2003. The Upper Panels show Modelled Concentrations with No Surface Conversion. The Lower Panels are Modelled Concentrations ith the Surface Conversion Algorithm Activated.

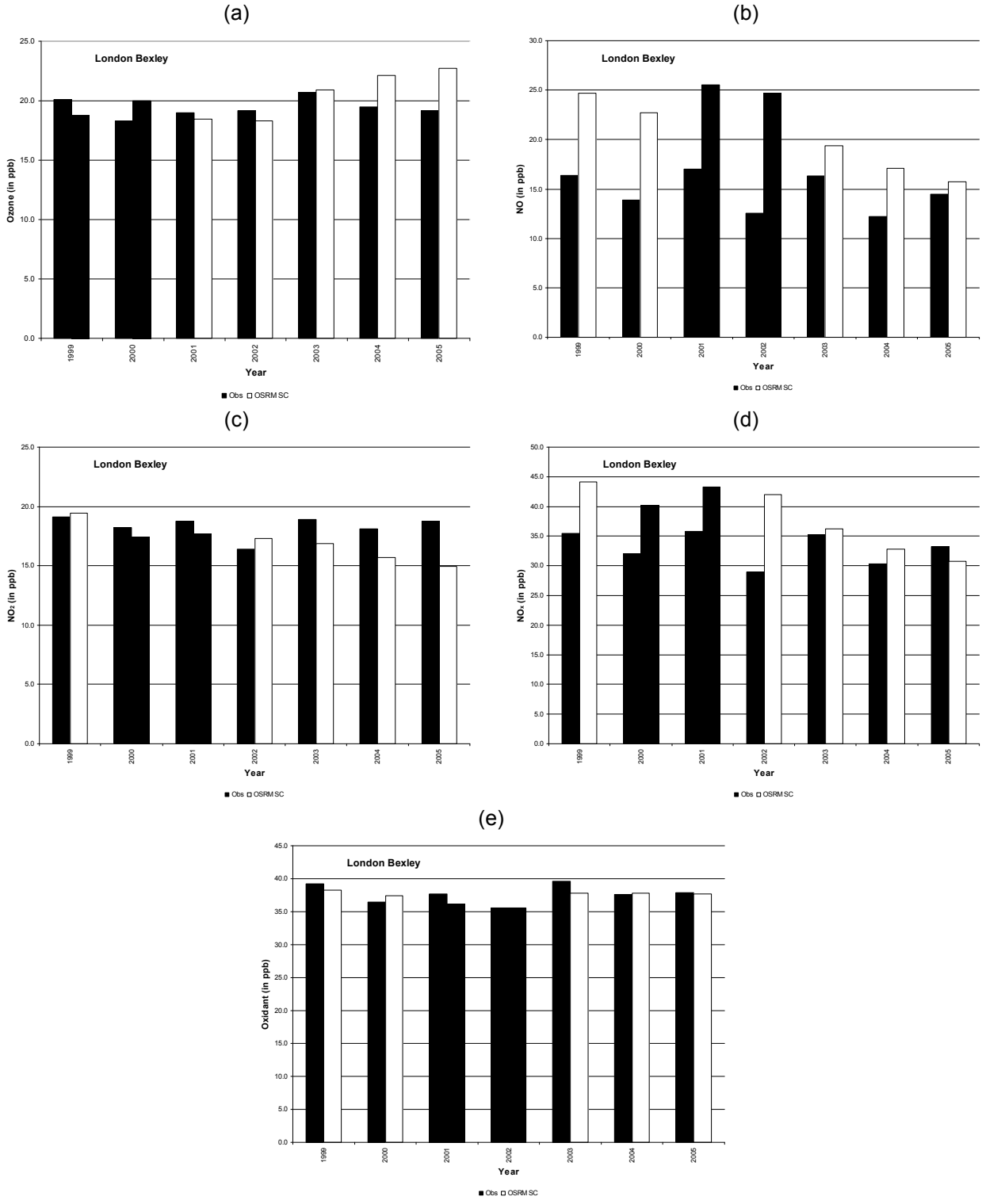

Figure 2: Observed and Modelled Annual Mean Concentrations (in ppb) of Ozone (Panel a), Nitric Oxide (Panel b), Nitrogen Dioxide (Panel c), Oxides of Nitrogen (Panel d) and Oxidant (Panel e) at the London Bexley Site for the Years 1999 to 2005.

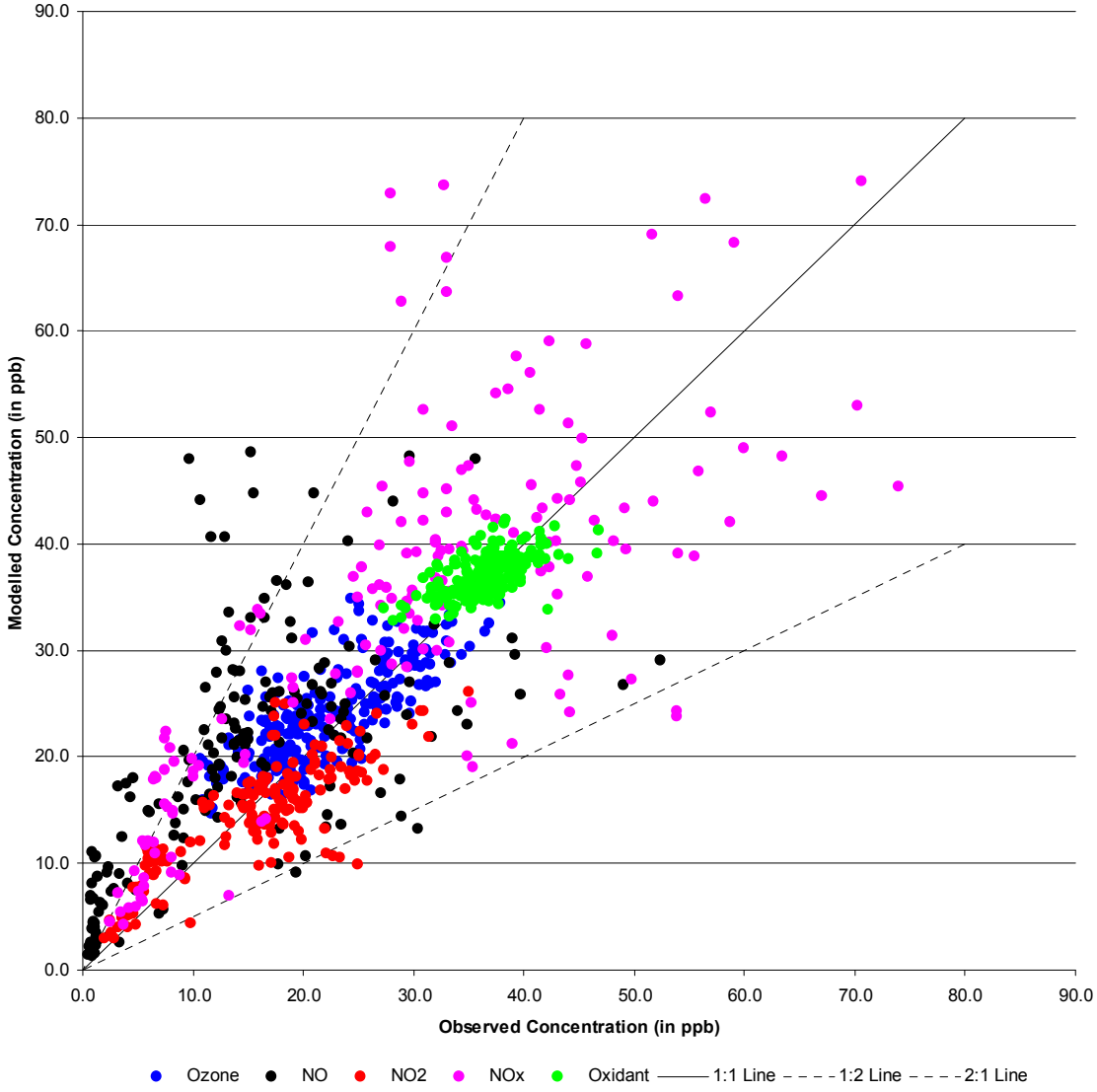

Figure 3: Scatter Plot of the Modelled vs. Observed Annual Mean Concentrations (in ppb) of Ozone (Blue), Nitric Oxide (Black), Nitrogen Dioxide (Red), Oxides of Nitrogen (Purple) and Oxidant (Green) for 41 UK Ozone Monitoring Sites for the Years 1999 to 2005.

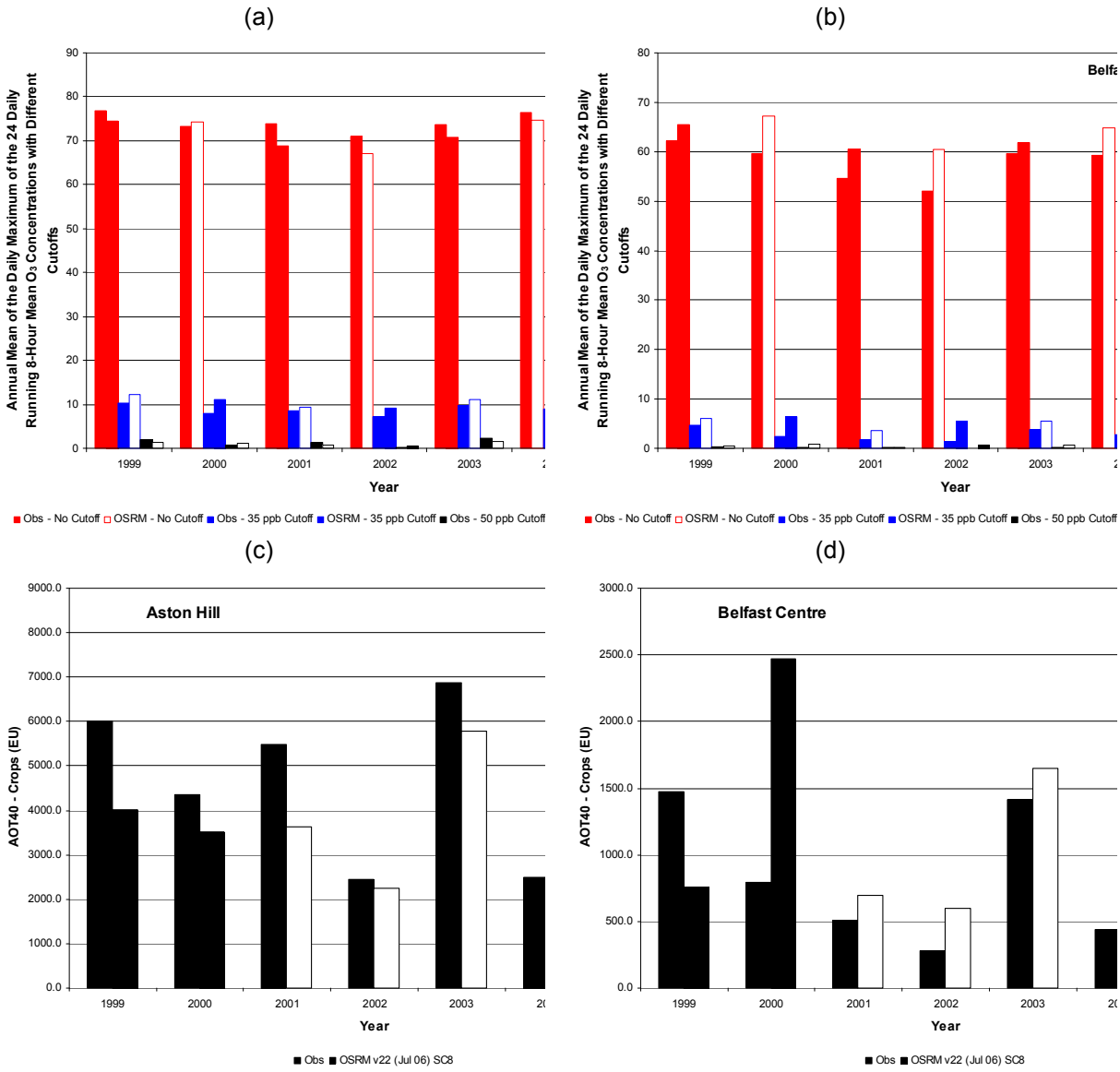

Figure 4: Comparison of Modelled and Measured Ozone Metrics for Aston Hill (Panels a and c) and Belfast Centre (Panels b and d) for the Years 1999 to 2005 Related to the Impacts of Ozone on Human Health (Upper Panels) and Vegetation (Lower Panels).

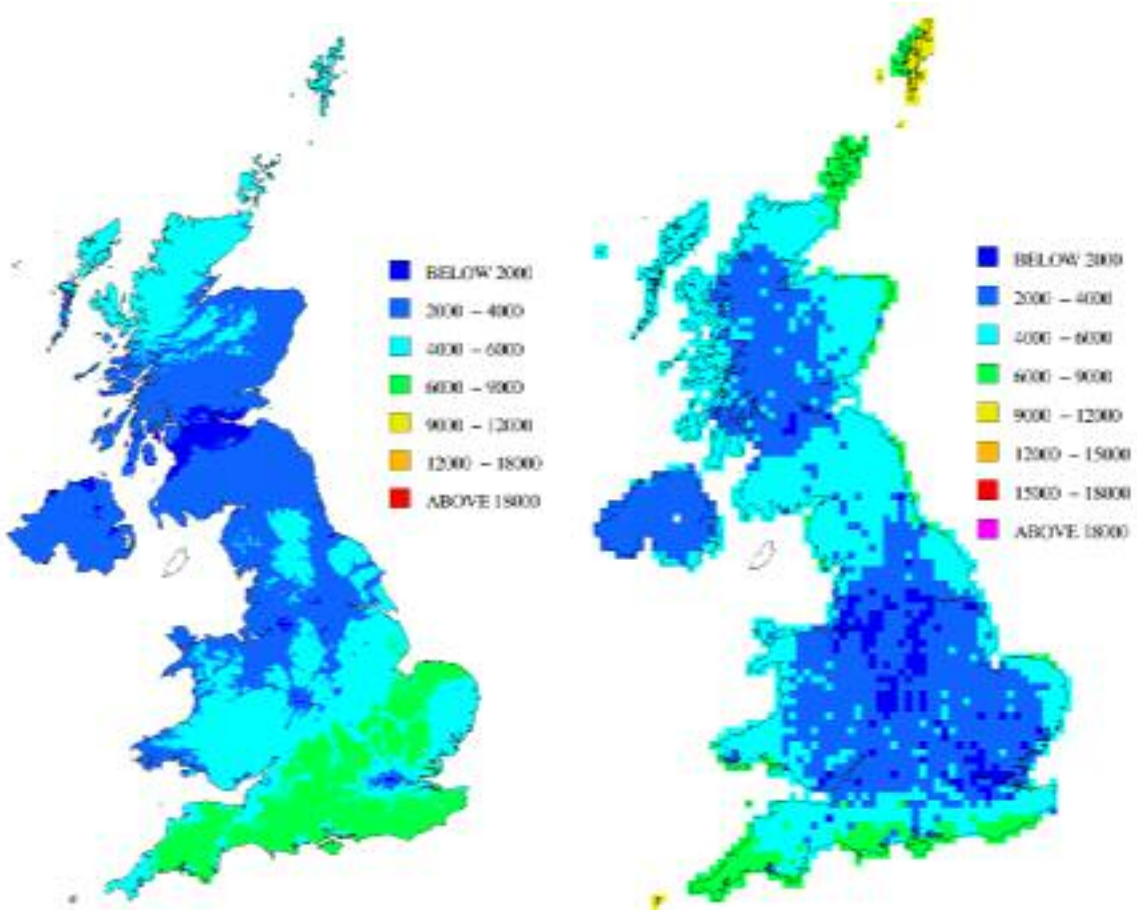

Figure 5: Maps of the AOT40 Crops Metric (Averaged over the 5 Years, 2000-2004), as derived from measurements (Left-hand Map) and calculated using the Ozone Source-Receptor Model.

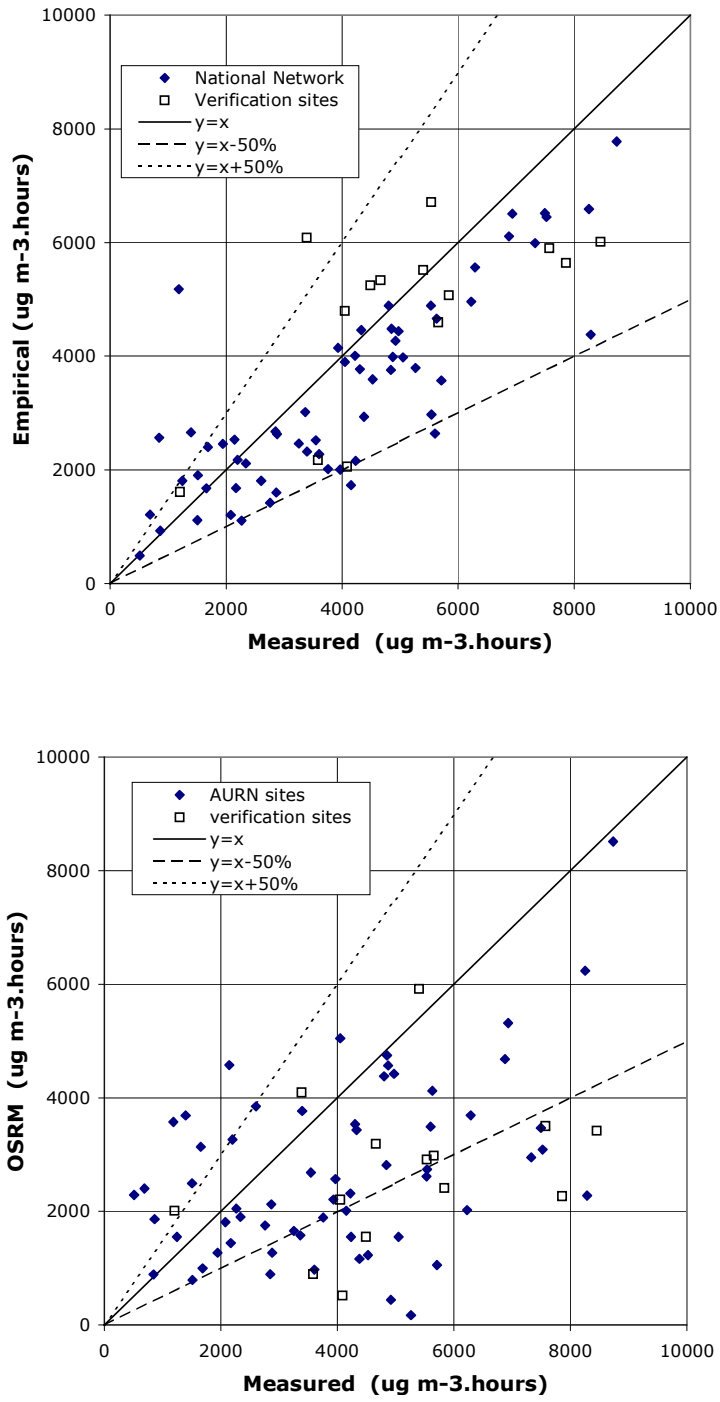

Figure 6: Scatter Plots of the Measured and Modelled Data for the Empirical Model [Upper Panel] and OSRM [Lower Panel] for the AOT40 Crops for the 5-Year Mean (2000-2004).

Model	***STOCHEM (UK)***
Institution/s	Met Office, rdscientific, U. of Edinburgh
Contact person/s Contact email address	bill.collins@metoffice.gov.uk dstevens@staffmail.ed.ac.uk
Type & scale Model Domain	Lagrangian parcel 1.875° x 1.25° Global
Chemistry	72 species including , SO_2, DMS, NH_3
Treatment of VOCs	<=C4 + isoprene, generic terpene
Meteorology	Met Office climate model
Emission inventories	IIASA + interactive biogenics
Chemical initialisation and model boundary ozone advection	Initialised from previous runs. Typically spun up for 1 year after initialisation.
Evaluation: (comparison with observations)	Multi annual comparisons against Mace Head, numerous papers by Derwent *et al.* Specific comparisons of particular species against observations in peer-reviewed papers according to the scientific questions being addressed. Comparisons with other models and with global datasets in model intercomparison papers.
Computer Resources (*super; mainframe; PC*) and typical run time	Super
Policy uses Is your model actually used for practical policy applications?	Transboundary pollution, climate change. Yes
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	AOT40, cumulative stomatal uptake, eight hourly max, SOMO35, monthly, seasonal
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	NO_2, SO_2, nitrate aerosol, sulfate aerosol, ammonium aerosol, biogenic aerosol. Nitrate, sulfate deposition.

Published Description *(Reports, Literature)*	Collins, W.J., Stevenson, D.S., Johnson, C.E.and Derwent, R.G.,(1997).Tropospheric ozone in a global-scale three-dimensional Lagrangian model and its response to NOx emission controls, J.Atmos. Chem., 26, 223-274. Collins, W.J., Stevenson, D.S., Johnson, C.E. and Derwent, R.G., (1999).The role of convection in determining the budget of odd hydrogen in the upper troposphere, J. Geophys. Res., 104, 26927-26940. Collins, W.J., Stevenson, D.S., Johnson, C.E. and Derwent, R.G., (2000).The European regional ozone distribution and its links with the global scale for the years 1992 and 2015, Atmos. Environ., 34, 255-267. Collins, W.J., Derwent, R.G, Johnson, C.E. and Stevenson, D.S., (2000).The impact of human activities on the photochemical production and destruction of tropospheric ozone, Q. J. R. Meteorol. Soc., 126, 1925-1951. Collins, W.J., Derwent, R.G., Johnson, C.E. and Stevenson, D.S., (2002). The oxidation of organic compounds in the troposphere and their global warming potentials, Clim. Change, 52, 453-479. Collins, W.J.,Derwent, R.G, Johnson, C.E. and Stevenson, D. S., (2002). A comparison of two schemes for the convective transport of chemical species in a Lagrangian global chemistry model, Q. J. R. Meteorol. Soc., 128, 991-1009. Collins, W.J., Derwent, R.G., Jenkin, M.E., Johnson, C.E., and Stevenson, D.S. (2003). The global distribution of secondary particulate matter in a 3-D Lagrangian chemistry transport model, J. Atmos. Chem., 44, 47-95. Collins, W.J., Derwent, R.G., Garnier, B., Johnson, C.E., Sanderson, M.G., and Stevenson, D.S. (2003). The effect of stratosphere-troposphere exchange on the future tropospheric ozone trend, J. Geophys. Res., 108, doi:10.1029/2002JD002617. F. Dentener, D. Stevenson, K. Ellingsen, T. van Noije, M. Schultz, M. Amann, C. Atherton, N. Bell, D. Bergmann, I. Bey, L. Bouwman, T. Butler, J. Cofala, B. Collins, J. Drevet, R. Doherty, B. Eickhout, H. Eskes, A. Fiore, M. Gauss, D. Hauglustaine, L. Horowitz, I. Isaksen, B. Josse, M. Lawrence, M. Krol, J.-F. Lamarque, V. Montanaro, J.-F. Muller, V. H. Peuch, G. Pitari, J. Pyle, S. Rast, J. Rodriguez, M. Sanderson, N. H. Savage, D. Shindell, S. Strahan, S. Szopa, K. Sudo, R. Van Dingenen,O. Wild, G. Zeng (2006). The global atmospheric environment for the next generation, Environmental Science and Technology, 40, 3586-3594 [doi:10.1021/ES0523845]. F. Dentener, J. Drevet, D. Stevenson, K. Ellingsen, T. Van Noije, M. Schultz, C. Atherton, N. Bell, I. Bey, T. Butler, B. Eickhout, A. Fiore, J. Galloway, C. Galy-Lacaux, U.C. Kulshrestha, J.F. Lamarque, V. Montanaro, J.-F. Muller, J. Rodriguez, M. Sanderson, N. Savage, S. Szopa, K. Sudo, O. Wild, G. Zeng (2006). Nitrogen and Sulphur Deposition on regional and global scales: a multi-model evaluation, Global Biogeochemical Cycles, 20, GB4003, do1:10.1029/2005GB002672. Derwent, R.G., Simmonds, P.G. and Collins, W.J., (1994). Ozone and carbon monoxide measurements at a remote maritime location, Mace Head, Ireland, from 1990 to 1992, Atmos. Environ., 28, 2623-2637. Derwent, R.G., Collins, W.J., Johnson, C.E., and Stevenson, D.S., (2001).Transient behaviour of tropospheric ozone precursors in a global 3-D CTM and their indirect greenhouse effects, Climatic Change, 49, 463-487.

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Comments	STOCHEM has been validated against observations and compared with other models in over 40 peer-reviewed publications.

Model	***UK PTM (UK)***
Institution/s	rdscientific; Imperial College, London: University of Birmingham
Possible contacts email	Dick Derwent *r.derwent@btopenworld.com* Michael Jenkin m.jenkin@imperial.ac.uk Helen Walker hlw245@bham.ac.uk
Type & scale Domain:	Lagrangian trajectory 10km x 10km -
Chemistry	Master Chemical Mechanism 4,414 species, 12,871 reactions Carbon Bond Mechanism version 4 36 species, 93 chemical reactions
Treatment of VOCs	175 man-made VOCs from NAEI + isoprene, α-pinene, β-pinene from natural biogenic sources
Meteorology	UK Met Office NAME archive 1000 x 96 hour 3-D trajectories per hour HYSPLIT/NCEP 6 x 96 hour back-track trajectories per day BADC/UK MO 6 x 96 hour back-track trajectories per day
Emission Inventories	UK NAEI emission inventories at 10 km x 10 km SO_2, NO_x, NH_3, VOCs, CO EMEP European emission inventories at 50 km x 50 km SO_2, NO_x, NH_3, VOCs, CO, methane EMEP natural biogenic isoprene emission inventory at 50 km x 50 km Global terpene emission inventory from GEIA Monthly at 1^o latitude x 1^o longitude
Chemical initialisation	O_3, CO, CH_4, H_2 based on observations for Mace Head, Ireland SO_2, NO_x, particulate sulphate, particulate nitrate and particulate ammonium based on observations for Valentia Observatory, Ireland HCHO from aircraft observations across North Atlantic

<table>
<tr><td>Evaluation</td><td>I use two criteria for judging model performance:
1. more than 50% of the model results should be within a factor of two of the observations
2. the mean fractional bias should be within the range -0.2 and +0.2
On this basis, the UK PTM scores between good and excellent.
I use the daily maximum 1-hour mean ozone concentrations as the evaluation metric of choice and the units are in ppb.
This below is the model evaluation for the rural ozone monitoring site at Harwell, Oxfordshire for each day in 2006.
<table>
<tr><th></th><th>Obs</th><th>Model</th><th>Mean Bias</th><th>Fractional</th><th>Number</th><th>RMSE</th></tr>
<tr><th></th><th>ppb</th><th>ppb</th><th>ppb</th><th>Bias ppb</th><th>factor 2</th><th>ppb</th></tr>
<tr><td>January</td><td>25.19</td><td>27.88</td><td>2.69</td><td>0.19</td><td>27</td><td>7.89</td></tr>
<tr><td>February</td><td>32.68</td><td>33.41</td><td>0.73</td><td>0.07</td><td>26</td><td>6.39</td></tr>
<tr><td>March</td><td>41.13</td><td>40.92</td><td>-0.21</td><td>0.00</td><td>31</td><td>6.02</td></tr>
<tr><td>April</td><td>42.63</td><td>45.73</td><td>3.10</td><td>0.09</td><td>29</td><td>7.82</td></tr>
<tr><td>May</td><td>47.87</td><td>42.63</td><td>-5.24</td><td>-0.09</td><td>23</td><td>13.13</td></tr>
<tr><td>June</td><td>53.25</td><td>43.65</td><td>-9.60</td><td>-0.15</td><td>12</td><td>18.19</td></tr>
<tr><td>July</td><td>52.23</td><td>40.65</td><td>-11.58</td><td>-0.19</td><td>30</td><td>20.12</td></tr>
<tr><td>August</td><td>43.68</td><td>37.34</td><td>-6.34</td><td>-0.11</td><td>29</td><td>17.00</td></tr>
<tr><td>September</td><td>36.77</td><td>36.74</td><td>-0.02</td><td>0.02</td><td>30</td><td>9.14</td></tr>
<tr><td>October</td><td>34.32</td><td>34.74</td><td>0.42</td><td>0.02</td><td>31</td><td>7.10</td></tr>
<tr><td>November</td><td>31.13</td><td>34.32</td><td>3.18</td><td>0.11</td><td>29</td><td>6.84</td></tr>
<tr><td>December</td><td>40.68</td><td>34.23</td><td>-6.45</td><td>-0.17</td><td>31</td><td>7.76</td></tr>
</table>
</td></tr>
<tr><td>Computer Resources (super; mainframe; PC) and typical run time</td><td>PC
MCM version 1800 seconds per trajectory
CBM version 4 version 5400 seconds per year</td></tr>
<tr><td>Policy relevance</td><td>UK policy application</td></tr>
<tr><td>To what other species can the model be reliably extended?</td><td>NO_2, HNO_3, PAN, organic nitrates, HCHO
NH_3, SO_2, particulate nitrate, particulate sulphate, particulate ammonium
Multi-functional carbonyls
Secondary carbonaceous PM</td></tr>
<tr><td>Producible ozone metrics (hourly, eight hourly, daily, seasonal, AOT40 etc.)</td><td>Maximum hourly mean ozone concentration
Annual mean of the daily maximum ozone concentrations</td></tr>
</table>

Comments	Comparison of model ozone results with observations is given in Johnson et al., 2003, Atmos. Chem. Phys. 6, 403-418.
	A partial publication list is attached in Annex A listing some of the publications that have used the Photochemical Trajectory Model.

Annex A. A partial list of publications that have used the Photochemical Trajectory Model PTM.

1. Reactivity-based strategies for photochemical ozone control in Europe. Environmental Science and Policy, doi:10.1016/j.envsci2007.01.005, (2007).
2. Photochemical ozone creation potentials POCPs for different emission sources of organic compounds under European conditions estimated with a Master Chemical Mechanism. Atmospheric Environment **41**, 2570-2579.
3. Particulate sulphate and nitrate in Southern England and Northern Ireland during 2002/3 and its formation in a photochemical trajectory model. Science of the Total Environment **368**, 769-780, (2006).
4. Simulating regional scale secondary organic aerosol formation during the TORCH 2003 campaign in the southern UK. Atmospheric Chemistry and Physics **6**, 403-418, (2006).
5. Simulating regional scale secondary organic aerosol formation during the TORCH 2003 campaign in the southern UK. Atmospheric Chemistry and Physics Discussions **5**, 7829-7874, (2005).
6. Modelling the ambient distribution of organic compounds during the August 2003 ozone episode in the southern UK. Faraday Discussions of the Royal Society of Chemistry **130**, 311-326, (2005).
7. Multi-day ozone formation for alkenes and carbonyls investigated with a Master Chemical Mechanism under European conditions. Atmospheric Environment **39**, 627-635, (2005).
8. Photochemical generation of particles in the United Kingdom. In: Ultrafine Particles in the Atmosphere. pp. 103-120. The Royal Society, Imperial College Press, (2003).
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Model	***EMEP4UK (UK)*** Application of the EMEP Unified
Institution/s	University of Edinburgh, Edinburgh, UK CEH, Edinburgh, UK Met.no, MSC-W, Oslo, Norway
Possible contacts email	Dr. Massimo Vieno, School of GeoSciences, University of Edinburgh mvieno@staffmail.ed.ac.uk
Type & scale	Eulerian grid 20 vetical layers in sigma coordinates. Horizontal; 50 km x 50 km EUROPE with nested 5 km x 5 km UK
Chemistry	EMEP Unified (www.emep.int). Extensively verified and validated for the 50 km x 50 km resolution over Europe. ~80 species (~140 reactions) also including: O_3, NO, NO_2, PAN, MPAN, NO_3, N_2O_5, $ISONO_3$, HNO_3, H_2O_2, H_2, CO, CH_4, SO_2, SO_4, pNO_3, NH_3, AMSU, AMNI, $PM_{2.5}$, PM_{10}, PM_{co}
Treatment of VOCs	Speciation of VOC emissions are specified separately for each snap source-sector. 9 man-made VOCs + isoprene C_2H_6, nC_4H_{10}, C_2H_4, C_3H_6, C_8H_{10}, HCHO, MEK, CH_3OH, C_2H_5OH
Meteorology	Weather Research Forecast model (WRF version 2.2), ECMWF ERA40 (interpolated). In principle any available meteorological driver.
Emission Inventories	NAEI over the UK, EMEP everywhere else
Computer Resources (*super; mainframe; PC*) and typical run time	CEH Linux Cluster, UoE EPCC IBM BlueGene EMEP4UK run time is 2 days for one simulated year, on the CEH cluster. The CEH cluster will be soon replaced; with a predicted EMEP4UK run time of less than one day
Policy relevance	Policy formulation for UN ECE LRTAP Input to RAINS, CAFÉ and NEC
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	In principle from hourly to yearly. AOT40
Comments	

<table>
<tr><td>Model</td><td colspan="5">MODELS-3/CMAQ (UK)</td></tr>
<tr><td>Institution/s</td><td colspan="5">ICL, Universities of: Manchester; Edinburgh; Hertfordshire; Eon</td></tr>
<tr><td>Possible contacts</td><td colspan="5">Ron Smith (CEH)
Bernard Fisher (EA)
Ranject Sokhi (Uni of Hert) [no contract with Defra]</td></tr>
<tr><td>Type & scale</td><td colspan="5">Inner grid: 240x170 cells, 5 km x 5 km resolution, Lambert Conformal Projection; Central Latitude and Longitude 55 and -3 degrees respectively

Outer grid: 45x45 cells, 45 Km x 45 Km resolution,
Lambert Conformal Projection; Central Latitude and Longitude 55 and -3 degrees respectively

A nesting process is used.</td></tr>
<tr><td>Chemistry</td><td>Name</td><td>Number of gas phase chemical species</td><td>Number of chemical reactions</td><td>Main species considered</td><td>Main task</td></tr>
<tr><td></td><td>RADM2 (Regional Acid Deposition Model)</td><td>57</td><td>157</td><td>O_3, HNO_3,HNO_4, NO_3,H_2O_2</td><td>Acidification processes</td></tr>
<tr><td></td><td>CB4 (Carbon Bond IV)</td><td>36</td><td>93</td><td>NO, NO_2,O_3</td><td>Photochemical processes</td></tr>
<tr><td></td><td>SAPRC99 (Statewide Air Pollution Research Center Chemical Mechanism)</td><td>400 (VOCs)</td><td>290</td><td>VOC, NO_X</td><td>Ozone impacts (reactivities) of VOCs emitted in atmosphere</td></tr>
<tr><td>Treatment of VOCs</td><td colspan="5">RADM2 is the chemical scheme used.</td></tr>
<tr><td></td><td colspan="5">1 OLN Higher organic peroxides
2 KET Ketones
3 ALD Aldehydes
4 OLT Terminal alkynes
5 OLI Alkenes and terpenes
6 CSL Cresols and phenols
7 TOL Aromatics
8 XYL Naphthalenes</td></tr>
</table>

Meteorology	9 ORA2 Higher organic acids 10 ORA1 Formic acid *"Lumped" groups of VOCs in RADM2* 3D meteorological fields from the 5th Generation Mesoscale Model MM5
Emission Inventories	EMEP database and National Emission Inventory for the UK (NAEI)
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	CMAQ is installed at the Centre for Ecology and Hydrology of Edinburgh on Nemesis, a 60 node dual-processor system running a derivative of Red Hat 7.2 Linux. Typical run time: a 5 days simulation takes about 3 hours. A 1 month simulation takes about 1 day.
Policy relevance	Most heavily used research and policy model in USA.
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Monthly runs of CMAQ provide 6-hourly pollutant concentrations and deposition fluxes
To what other species can the model be reliably extended?	
Comments	

Model	***CMAQ (UK)***
Institution/s	Imperial College
Contact person/s Contact email address	Prof. Helen ApSimon (h.apsimon@imperial.ac.uk) Andrea Fraser (a.fraser@imperial.ac.uk)
Type & scale Model Domain	The simulation is 3 one-way nested grids, all grids have 24 layers 8 below 500m, all grids are Lambert Conical Conformal projections centred on latitude and longitude 49 and -2 degrees respectively. European grid - 48x48 km, 70x60 cells England and N. Europe – 12x12 km 90x60 cells South East England – 4x4 km 64x48 cells
Chemistry	RADM2 is only available until V4.5 From V4.6 CB05 (Carbon Bond 05) is available with51 species and 155 reactions. All mechanisms can be used with/without modules for aqueous and aerosol chemistry.
Treatment of VOCs	The CB4 chemical scheme uses ALD2 – Aldehydes ETH - Ethene FORM - Formaldehyde OLE - Alkene PAR - Alkane XYL – Xylene TOL -Toluene Natural VOC's ISOP - Isoprene TERPB - Terpenes
Meteorology	Use UKMO UM data stored on BADC, processed into CMAQ ready files using an interface (UM-MCIP)
Emission inventories	EMEP, NAEI inventories and a Biogenic potential inventory. The VOC emissions pre-processing is related to CB4, the chemical mechanism used
Chemical initialisation and model boundary ozone advection *how is it done? - with observations, another model (specify) or another method?*	Monthly data from STOCHEM is used to create initial and boundary conditions for the outer (European) grid, all inner grids are nested from the previous grid

Evaluation: (comparison with observations)	For ozone in the 4km grid, 70.9 % of modelled concentrations fall within a factor of 2 of the observed value (38 sites, 39 days, 30480 observations) 85 % for Rural sites and 58 % for Roadside sites. During this period 9 days (2 episodes) were classed as high ozone levels as measured by the AURN. Over the diurnal cycle there is a tendency to over predict at night and under predict at midday but there is a much larger variation between different days, particularly when weather conditions change. NO_2 has only 59.6 % of modelled concentrations within a factor of 2.
Computer Resources (*super; mainframe; PC*) and typical run time	Using a (dual processor) desktop PC, a typical month run for all 3 grids takes about 7 days.
Policy uses Is your model actually used for practical policy applications?	In the UK CMAQ has been used in the power industry to study power station footprints.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Standard model output is hourly ppm (at end of timestep), additionally average hourly ppm is available. These can be further analysed to produce a range of metrics. Using process analysis ozone production and loss from chemistry, advection, diffusion, deposition, and aqueous cloud processes are available. The chemical processes involved with ozone production and loss can be further understood by analysing the hourly flux through all chemical reactions.
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	O_3, NO_2, NO_x, SO_2, Aerosol (speciated), $PM_{2.5}$, Additional files include hourly cumulative dry and wet deposition, visability metrics
Published Description *(Reports, Literature)*	Web link to science document for v4.6 www.cmaq-model.org/op_guidance_4.6/html/index.html

Model	***AQUM (UK)***
Institution/s	Met Office
Contact person/s & email address	Paul Agnew Paul.agnew@metoffice.gov.uk
Type & scale	Eulerian, on-line, global/regional
Chemistry	to be decided
Treatment of VOCs	to be decided
Meteorology	Unified Model
Emission Inventories	GEMS 2003, 5 km resolution
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	Mainframe, runtime tbd
Policy uses	Could be used for case studies
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	to be decided
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	None
Comments	Model is in early development phase. Expected to be available 2009

Model	***UKCA (UK)*** (UK Chemistry and Aerosols Model)
Institution/s	Met Office and NERC National Centre for Atmospheric Science (Universities of Cambridge and Leeds)
Contact person/s Contact email address	Colin Johnson (Met Office), Paul Agnew (Met Office), John Pyle (NCAS) paul.agnew@metoffice.gov.uk colin.johnson@metoffice.gov.uk john.pyle@atm.ch.cam.ac.uk
Type & scale Model Domain –	Eulerian Met Office's Global or Operational North Atlantic and Climate Model (HadGEM) European NWP Model 1.875° x 1.25° x L38 (12 km x 12 km x L38) Operational Global NWP Model (50 km x 50 km x L38) (UK 4 km Model planned)
Chemistry	UKCA currently supports 3 tropospheric chemistry schemes: a) TOMCAT b) TOMCAT + Mainz Isoprene Mechanism c) TOMCAT + Sulphur Chemistry Two additional mechanisms are in the process of being implemented: d) STOCHEM chemistry scheme e) Common Representative Intermediate (CRI) mechanism
Treatment of VOCs	The treatment of VOCs varies according to chemistry scheme. Schemes a) and c) above only treat ethane and propane. Scheme b) treats ethane, propane, and isoprene. Scheme d) will handle <= C4 species, isoprene, and a generic terpene. Scheme e) considers over 20 emitted VOCs.
Meteorology	Climate Model or operational models (with data assimilation). Can also be nudged with ECMWF analyses.
Emission inventories	IPCC (2001) OxCOMP or GEMS 2003, 5km resolution IIASA
Chemical initialisation and model boundary ozone advection	Previous runs or Previous runs with LBCs from GEMS or from nesting within the global model
Evaluation: (comparison with observations)	Multi-annual comparisons against CMDL surface sites, including Mace Head Comparison with EMEP sites Multi-annual comparisons against a climatology of vertical ozone profiles from ~40 worldwide sites

	Comparison with STOCHEM model
Computer Resources (*super; mainframe; PC*) and typical run time	Supercomputer
Policy uses Is your model actually used for practical policy applications?	Climate Change, Air quality The UKCA model will be used by the Met Office in their contract (Scientific Support for National and International Policy) with Defra AEQ.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Potentially: AOT40, cumulative stomatal uptake, eight hourly max, SOMO35, monthly, seasonal, annual
To what other species can the model be reliably extended?	NO_2, SO_2, Sulfate Aerosol A more comprehensive aerosol scheme is planned
Published Description *(Reports, Literature)*	1. Report to Defra on the combined chemistry and aerosols module in UKCA (MS-RAND-CPP-PROG0407; deliverable number 10.01.05). 2. Report to Defra on the evaluation of the UKCA chemistry-aerosols model (MS-RAND-CPP-PROG0407; deliverable number 10.01.06).
Comments	UKCA is a joint initiative between the Met Office and NCAS for the development of a community model for stratospheric and tropospheric chemistry and aerosols. It is expected to be released through the Met Office's Unified Model to the research community for development and use. The UKCA model has been coupled to the Met Office's climate model. AQUM has been used to refer to the implementation of UKCA in the Met Office's global and regional NWP models.

Model	***ADMS-Urban (UK)***
Institution/s	Cambridge Environmental Research Consultants (CERC)
Contact person/s Contact email address	David Carruthers David.Carruthers@cerc.co.uk
Type & scale Model Domain	Gaussian model nested in trajectory model. Variable resolution down to 10m local to large urban areas (*e.g* London area) and small regional
Chemistry	CB4 95 reactions and 36 species Or GRS 6 reactions
Treatment of VOCs	CB4 7 man-made VOCs +isoprene GRS – 1 surrogate VOC
Meteorology	Standard met data from one measurement site or mesoscale model
Emission inventories	Flexible. Gridded emissions or explicit source information for indiividual sources (eg point or road sources)
Chemical initialisation and model boundary ozone advection	Flexible. Able to make use of monitored data and/or regional model output. For example for London assessments, model uses rural background monitored data; for air quality forecasts model uses regional model input (EURAD and CHIMERE).
Evaluation:	Evaluation performed as part of Urban modelling study for DEFRA using all the ozone monitoring sites in London for both 2001 and 2003. Typically model calculates annual means, percentiles and predictions of number of exceedences of different thresholds which are compared with measured data. Means predicted well, highest peaks tend to show some underestimation greatest for the highest percentiles. Ongoing assessment of model used in forecast mode. Accuracy of forecasts consistent with the above with most predicted 'moderates' and 'highs' occurring but some of those occurring not predicted by the model.
Computer Resources (*super; mainframe; PC*) and typical run time	PC. Run time highly dependent on output required and domain size. Times range from a few minutes for receptor point output for episode to days for full contour plot for annual average and percentile run.
Policy uses Is your model actually used for practical policy applications?	Influences policy development in London especially the impact of future NOx concentrations on urban ozone. The impact of VOCs is small at urban scale so this aspect has not fed into policy.
Producible ozone metrics	Full range of ozone metrics may be calculated.

To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	The full range of air quality pollutants: NO_2,PM_{10},$PM_{2.5}$,SO_2,CO,VOCs,heavy metals *etc*.
Published Description *(Reports, Literature)*	Modelling of current and future concentrations of PM, NOx and O3 in London using ADMS-Urban. Wiiliams M, Carruthers D.J. and Johnson K. 2006 Report to DEFRA www.airquality.co.uk/qrchive/aqsreview2006.php Sensitivity studies of NO_2 and O_3 for London for 2010 and 2020 using ADMS-Urban, Carruthers D.J. , Wiiliams M and Johnson K. 2006 Report to DEFRA www.airquality.co.uk/archive/reports/reports.php
Comments	

Model	***EMEP (UN-ECE)***
Institution/s	MSC-W
Possible contacts email	EMEP (Leonor Tarrason, David Simpson) leonor.tarrason@met.no, david.simpson@met.no
Type & scale	Eulerian grid (Polar stereorgraphic) 50km x 50km (at 60N), European scale (Local, ca. 4km grid, and global scale versions in testing.)
Chemistry	EMEP (see Simpson *et al.*, 1993, 2003, Simpson, 1995, Andersson-Sköld and Simpson, 1999, Kuhn *et al.* 1998) 80 species, 140 reactions alpha-pinene chemistry in research SOA version from Andersson-Sköld and Simpson (2001). Also, aerosol dynamics in research version (Tsyro et al., 2001, 2002)
Treatment of VOCs	9 man-made VOCs +isoprene (+terpenes in SOA version). Surrogates used for man-made VOC are: C_2H_6, nC_4H_{10}, C_2H_4, C_3H_6, o-xylene, HCHO, MEK, CH_3OH, C_2H_5OH
Meteorology	HIRLAM-PS, see Sandnes-Lenschow and Tsyro, 2000.
Emission Inventories anthropogenic & biogenic	Anthropogenic emissions from official data supplied to EMEP where possible, otherwise estimated. See *e.g* Vestreng *et al.*, 2007, and http://webdab.emep.int Biogenic emissions calculated from landuse and model temperature & radiation, see Simpson *et al*. (1995, 1999)
Computer Resources (*super; mainframe; PC*) and typical run time	Typically cluster, e.g. Itanian 1 year requires ca. 4-5 hours with 32 processors.
Policy relevance	Policy formulation for UN ECE LRTAP Input to RAINS, CAFÉ and NEC
Producible metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly to yearly outputs (user-specified) of any gas or particle concentration. Seasonal outputs of SOMO35, AOT40, flux indices (*e.g.* Simpson *et al.*, 2007), and of S and N deposition. Deposition outputs available for each landuse within grid.
Suitability Peak ozone levels only Background ozone only both peak and background	Hourly to seasonal outputs, typically at 50km scale (but other scales being tested).
Comparison with ozone observations. No. of stations overall performance scale 1 (poorest) to 5 (best)	See e.g. van Loon et al. (2007), and all recent EMEP "Status" Reports, *e.g.* Status Report 1/2007, 1/2006, ... (available at http://www.emep.int)

References to literature or reports, describing the model and its performance	Extensive comparisons of modelled versus ozone, sulphur and nitrogen compounds are published each year as part of standard EMEP reporting, reports available at www.emep.int. The main documentation of the current model is contained in Simpson et al. (2003) with updates in Fagerli *et al.* (2004). Published articles on comparisons include: van Loon et al. (2007) and Jonson *et al*. (2006) for O_3 (and NO_2), Simpson et al. (2006a,b) for N-compounds over forests, Simpson *et al*. (2007) for OC+BC, Tsyro *et al.* (2007) for BC, Tsyro *et al*. (2005) for PM, Fagerli *et al*. (2007) for inorganics and EC in ice-cores.
Comments	References given are: Andersson-Skold, Y. and Simpson, D., (2001), Secondary organic aerosol formation in Northern Europe: a model study, J. Geophys. Res., 106(D7), 7357-7374. Andersson-Skold, Y. and Simpson, D., (1999), Comparison of the chemical schemes of the EMEP MSC-W and the IVL photochemical trajectory models, Atmos. Environ., 33, 1111-1129. Fagerli, H., Legrand, M. R., Preunkert, S., Vestreng, V., Simpson, D., and M. Cerqueira (2007), Modeling historical long-term trends of sulfate, ammonium and elemental carbon over Europe: A comparison with ice core records in the Alps, J. Geophys. Res., doi:10.1029/2006JD008044, in press. Fagerli, H., D. Simpson and S. Tsyro, 2004, Unified EMEP model: Updates, Transboundary acidification, eutrophication and ground level ozone in Europe. EMEP Status Report 1/2004, 11—18. Jonson, J.E., L. Tarrason, P. Wind, M. Gauss, S. Valiyaveetil S., S. Tsyro, H. Klein, I.S.A. Isaksen and A. Benedictow. First evaluation of the global EMEP model and comparison with the global OsloCTM2 model. EMEP MSC-W Report 2/2007. Jonson, J.E., Simpson, D., Fagerli, H. and Solberg, S., (2006), Can we explain the trends in European ozone levels?, Atmos. Chem. Phys., 6, 51-66, SRef-ID: 1680-7324/acp/2006-6-51. Sandnes Lenschow, H. and Tsyro, S., (2000), Meteorological input data for EMEP/MSC-W air pollution models, EMEP/MSC-W Note 2/00. Simpson, D., (1995), Biogenic emissions in Europe 2: Implications for ozone control strategies, J. Geophys. Res., 100(D11), 22891-22906. Simpson, D., K. Yttri, Z. Klimont, A. Caseiro, A. Gelencser, C. Pio, H. Puxbaum, and M. R. Legrand, (2007) Modelling carbonaceous aerosol over Europe: Analysis of the CARBOSOL and EMEP EC/OC campaigns, J. Geophys. Res., D23S14, doi:10.1029/2006JD008158. Simpson, D, M. Ashmore, L. Emberson and J.-P. Tuovinen (2007), A comparison of two different approaches for mapping potential ozone damage to vegetation. A model study. Environ. Poll., 46, 715-725

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Model	***CAMx (Czech Republic)*** (ENVIRON, USA)
Institution/s	Inst. of Computer Science, Academy of Sciences of the Czech Republic, Prague, Czech Rep.
Contact person/s & email address	Krystof Eben eben@cs.cas.cz
Type & scale	Eulerian, 2 domains Europe, Czech Rep. horizontal. res. 27 km resp. 9 km
Chemistry	SAPRC 99 – for ozone, 56 species CBM-aero – for aerosols (2 separate runs)
Treatment of VOCs	
Meteorology	MM5
Emission Inventories	
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	linux PC cluster (meteorology), a single 2-processor PC (CAMx), run time about two hours
Policy uses	outputs (images) free for noncommercial use
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	hourly
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	CAMx – ENVIRON website: www.camx.com our website: www.medard-online.cz

	some more details Eben,K., Jurus, P., Resler, J., Belda, M., Pelikan, E., Krueer, B.C., Keder, J.: An Ensemble Kalman Filter for Short-Term Forecasting of Tropospheric Ozone Concentrations. QJRMS 131 (2005), 3313-3322.
Comments	operational forecast for the current day and the following one issued daily in the early morning ground-level concentrations of ozone, NO_2, PM_{10} presented on the web

Model	***DEHM (Denmark)*** Danish Eulerian Hemispheric Model
Institution/s	National Environmental Research Institute, Aarhus University
Contact person/s & email address	Jesper H. Christensen & Jørgen Brandt jc@dmu.dk & jbr@dmu.dk
Type & scale	Eulerian 3-D model with two way nesting: 150 km x 150 km (hemisphere), 50 km x 50 km (Europe), 16.67 km x 16.67 km (Northern Europe)
Chemistry	Modified EMEP scheme, presently with 63 species, 130 reactions.
Treatment of VOCs	10 Man-made VOCs + isoprene
Meteorology	Eta/NCEP MM5v3/ECMWF MM5v3/NCEP
Emission Inventories	Geia/EMEP/DK
To what other species can the model be reliably extended?	
To what other species can the model be reliably extended?	
Computer Resources (*super; mainframe; PC*) and typical run time	PC and PC Clusters with Linux
Policy uses	DK and EU policy applications, part of DK monitoring programme, forecasting. AMAP policy application, UNECE HTAP policy application,
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Everything – eg. hourly, eight hourly, daily, seasonal, AOT40 etc.
To what other species can the model be reliably extended?	
Comments	

Model	***DEOM (Denmark)*** Danish Eulerian Operational Model ()
Institution/s	National Environmental Research Institute, Aarhus University
Contact person/s & email address	Jørgen Brandt & Jesper H. Christensen jbr@dmu.dk & jc@dmu.dk
Type & scale	Eulerian model covering Europe with 50 km x 50 km resolution, 3 vertical layers (mixed layer, reservoir layer and free troposphere).
Chemistry	CBM-IV with 35 species.
Treatment of VOCs	CBM-IV
Meteorology	Eta/NCEP
Emission Inventories	EMEP/DK
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	PC and PC Clusters with Linux
Policy uses	Air quality forecasting
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Everything – eg. hourly, eight hourly, daily, seasonal, AOT40 etc.
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	Brandt, J., J. H. Christensen, L. M. Frohn, F. Palmgren, R. Berkowicz and Z. Zlatev, 2001: "Operational air pollution forecasts from European to local scale". *Atmospheric Environment*, Vol. 35, Sup. No. 1, pp. S91-S98, 2001 Brandt, J., J. H. Christensen, L. M. Frohn and R Berkowicz, 2003: "Air pollution forecasting from regional to urban street scale – implementation and validation for two cities in Denmark". *Physics and Chemistry of the Earth,* Vol. 28, pp. 335-344, 2003.
Comments	

Model	***CAC (Denmark)***
Institution/s	Danish Meteorological Institute (DMI)
Contact person/s & email address	Allan Gross agr@dmi.dk
Type & scale	Eulerian 0.2º×0.2º 40 vertical levels
Chemistry	Extended Carbon Bound-IV (CBM-IV) + aerosol species. 49 gas-phase + 11 aerosol species, 105 reactions.
Treatment of VOCs	67 man-made VOCs + isoprene, αpinene, βpinene.
Meteorology	HIRLAM / ECMWF
Emission Inventories	TNO
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	NEC-sx6 75 min.
Policy uses	Public Information.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly.
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	Ref. 1, 2, 3
Comments	

Model	***MOON (Denmark)***
Institution/s	Danish Meteorological Institute (DMI)
Contact person/s & email address	Allan Gross agr@dmi.dk
Type & scale	Lagrangian trajectory 5km×5km
Chemistry	Regional Acid Deposition Model (RACM) 77 gas-phase species, 237 reactions.
Treatment of VOCs	67 man-made VOCs + isoprene, αpinene, βpinene.
Meteorology	HIRLAM / ECMWF
Emission Inventories	EMEP
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	NEC-sx6 60 min.
Policy uses	Public information.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly.
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	Ref. 4
Comments	

Model	***CHIMERE (France)***
Institution/s	IPSL/INERIS/LISA, Paris
Contact person/s Contact email address	Laurent MENUT [menut@lmd.polytechnique.fr] Robert VAUTARD [robert.vautard@cea.fr] Bertrand BESSAGNET [bertrand.bessagnet@ineris.fr] Developers contact: chimere@lmd.polytechnique.fr
Type & scale Model Domain – *National, Europe, Global?*	Eulerian grid From 2 km x 2 km to 0.5° x 0.5° From local (Paris, Marseille) to regional (Europe, China)
Chemistry	MELCHIOR (Lattuati, PhD thesis, Vautard *et al*., 2001, Atmospheric Environment) 80 species, 300 reactions, or reduced mechanism, 44 species 110 reactions 6 aerosol chemical species, bins, POPs
Treatment of VOCs	12 man-made VOCs +isoprene
Meteorology	MM5, WRF, ECMWF/IFS, ARPEGE
Emission inventories	EMEP, local inventories
Chemical initialisation and model boundary ozone advection *how is it done? - with observations, another model (specify) or another method?*	
Evaluation: (comparison with observations)	The model evaluation was recently done in the framework of the PREVAIR forecast system (among other projects such as CITY-DELTA, ESCOMPTE etc.). Scores are done for 'peak' values i.e maximum ozone values recorded each day, during several months (not only surface concentrations exceeding 200 µg/m^3). Results are splitted into three parts, corresponding to surface stations representativities: urban, suburban and rural types. Number of days: 540 days Number of stations for ozone: 149 rural, 84 suburban, 75 urban. Bias: 0.9 µg/m^3 rural, 2.6 µg/m^3 suburban, 4.8 µg/m^3 urban RMSE: 17.3 µg/m^3 rural, 18.2µg/m^3 suburban , 17.7 correlation: 0.81 rural, 0.82 suburban , 0.82 urban

	These results are published in [*Honore et al., 2007, Predictability of European air quality: The assessment of three years of operational forecasts and analyses by the PREV'AIR system, JGR-Atm*]
Computer Resources (*super; mainframe; PC*) and typical run time	Personal computer or cluster of PC
Policy uses Is your model actually used for practical policy applications?	Most accurate ozone daily maxima forecast model in Europe, and among most accurate models for daily average PMs The model is daily used for French national forecast with PREVAIR, air quality networks in France (such as Paris area, Marseille area) in Italy, Portugal, Spain, The Netherlands. CHIMERE is used by INERIS to provide technical support to the french ministry for ecology, sustainable development and spatial planning. Such topics as transboundary air pollution controls, efficiency of emissions abatement strategies are addressed.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	All possible
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	NO, NO_2, SO_2, $PM_{2.5}$, PM_{10} among others
Published Description *(Reports, Literature)*	More than 40 papers in peer-reviewed journals, and scientific and numeric documentation on the CHIMERE web site.
Comments	Free software with a GNU license, available on http://euler.lmd.polytechnique.fr/chimere *Forecast products available in real time on* http://www.prevair.org*, or at finer scale over Paris http://www.airparif.asso.fr*

Model	***EURAD (Germany)***
Institution/s	Rhenish Insitute for Environmental Research at the University of Cologne
Contact person/s & email address	Adolf Ebel eb@riu.uni-koeln.de Hermann Jakobs hj@riu.uni-koeln.de Hendrik Elbern he@riu.uni-koeln.de Michael Memmesheimer mm@riu.uni-koeln.de
Type Scale Domain: National, Europe, Global	Hemispheric to regional/urban background, troposphere (and partially stratosphere) Horizontal grid sizes: 1 – 250 km Hemispheric, Europe, urban as Berlin, Rhein-Ruhr (1 km grid)
Chemistry	RADM2, RACM-MIM 60 -70 species, 200 reactions
Treatment of VOCs	15 lumped species, isoprene, α-pinene, β-pinene
Meteorology	MM5, driven by ECMWF, NCEP
Emission Inventories	EDGAR, EMEP, TNO, IER-Stuttgart, local inventories
Computer Resources (*super; mainframe; PC*) and typical run time	PC-Pool, 1 year standard real time Calculation with 125 - 25 - 5 km Nested grid (included particles) needs about two months computing time
Policy uses Is your model actually used for practical policy applications?	Daily chemical weather forecast (www.riu.uni-koeln.de) used by several local environmental agencies (including data assimilation, daily evaluation) Yes: Emission scenarios
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly, 180 µg/m^3 threshhold, 240 µg/m^3 threshhold; AOT40, SOMO35, 8h-running average (120 µg/m^3 threshhold) according to EC/2002/3 all based on annual long-term runs with hourly output for the years 2002, 2003, 2005, scenarios for 2010
To what other species can the model be reliably extended? ***E.g.* NO_2, SO_2, aerosol *etc.***	NO, NO_2, CO, benzene, SO_2, PM_{10}, $PM_{2.5}$, PM_1, … (concentrations near sources can only partially be resolved even with a 1 km resolution (e.g. NO_2 in street canyons)

Published Description *(Reports, Literature)*	Jakobs *et al*., 2002, JAC Memmesheimer *et al.*, 2005, IJEP Elbern *et al.*, 2007, ACP
Comments	

Model	***REM-CALGRID (RCG) (Germany)***
Institution/s	Free University Berlin, Institute for Meteorology, Carl-Heinrich-Becker Weg 6-10, 12165 Berlin, Germany
Contact person/s Contact email address	Dr. Rainer Stern rstern@zedat.fu-berlin.de
Type & scale Model Domain –	Eulerian grid model that can be used on the regional- through urban-scales Europe in a resolution of 0.5° Lon, 0.25°Lat Germany, in a resolution of 0.25° Lon, 0.125°Lat urban areas in a resolution up to approx. 1 km x 1 km
Chemistry	CBM-IV including a 1-Product Isoprene scheme
Treatment of VOCs	Individual VOCs are assigned to 6 Carbon Bond classes
Meteorology	Diagnostic meteorological analysis system based on an optimum interpolation procedure on isentropic surfaces utilizing all available observed synoptic surface and upper air data
Emission inventories	International, national, local inventories
Chemical initialisation and model boundary ozone advection	European scale: monthly varying climatological background values derived from observations National, local scale: Boundary conditions are taken from RCG runs for the next larger grid (one-way nesting)
Evaluation: (comparison with observations)	Comparison against available observations in all scales for several years; ozone evaluation is described in: Van Loon *et al.*, 2007: Evaluation of long-term ozone simulations from seven regional air quality models and their ensemble average. Atmos. Environ. 41, 2083-2097 Vautard, R. *et al.*, 2007. Evaluation and intercomparison of Ozone and PM_{10} simulations by several chemistry-transport models over 4 european cities within the City-Delta project. Atmos. Environ. 41, 173-188.
Computer Resources (*super; mainframe; PC*) and typical run time	PC, one year calculation for a 80 x 120 x 5 grid in a resolution of 0.5° Lon, 0.25° Lat: approx. 80 hours
Policy uses Is your model actually used for practical policy applications?	Yes National and local applications (Germany) to predict the impact of air quality action plans International applications within the framework of the EURODELTA and CITYDELTA exercises
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	hourly, eight-hourly, daily, seasonal, AOT40, AOT60, SOMO35

To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	RCG treats all relevant gas-phase species including NO2, SO_2, NH_3 and primary and secondary aerosols (SIA, SOA)
Published Description *(Reports, Literature)*	Stern, R., Yamartino, R., Graff, A., 2006. Analyzing the response of a chemical transport model to emissions reductions utilizing various grid resolutions. 28th ITM on Air Pollution Modelling and its Application. May 15-19, 2006, Leipzig, Germany. Beekmann, M., Kerschbaumer, A., Reimer, E., Stern, R., Möller, D., 2007. PM Measurement Campaign HOVERT in the Greater Berlin area: model evaluation with chemically specified observations for a one year period. Atmos. Chem. Phys. 7, 55-68. Stern, R. , 2004. Weitere Entwicklung und Anwendung des chemischen Transportmodells REM-CALGRID für die bundeseinheitliche Umsetzung der EU-Rahmenrichtlinie Luftqualität und ihrer Tochterrichtlinien. Abschlussbericht im Rahmen des Forschungs- und Entwicklungsvorhaben 201 43 250 auf dem Gebiet des Umweltschutzes „Anwendung modellgestützter Beurteilungssyteme für die bundeseinheitliche Umsetzung der EU-Rahmenrichtlinie Luftqualität und ihrer Tochterrichtlinien“.
Comments	provided in original reply

Model	***CAMx (Greece)***
Institution/s	Laboratory of Atmospheric Physics, Aristotle University of Thessaloniki
Contact person/s & email address	Dr. Dimitris Melas, melas@auth.gr
Type & scale	Eulerian photochemical dispersion model combined with meteorological prognostic Mesoscale, Urban
Chemistry	CB-IV
Treatment of VOCs	
Meteorology	MM5
Emission Inventories	anthropogenic NOx, NMVOCs and CO emission variations for every month of the year derived from an emission inventory with spatial resolution of 10km by the Laboratory of Atmospheric Physics
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	
Policy uses	regulatory assessments in the U.S.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	hourly average concentration output files
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	
Comments	

Model	***EPA-UAM-IV (Greece)***
Institution/s	N.C.S.R. Demokritos, Athens
Contact person/s & email address	Dr. John Bartzis, bartzis@ipta.demokritos.gr
Type & scale	3D, Eulerian photochemical Mesoscale, urban scale
Chemistry	Carbon-Bond IV, 81 reactions, 33 species
Treatment of VOCs	Anthropogenic and biogenic
Meteorology	
Emission Inventories	
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	
Policy uses	
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	
Comments	

Model	***MAP (Greece)*** **Modelling of Atmospheric Pollution**
Institution/s	National Technical University of Athens
Contact person/s & email address	Prof. George Bergeles, bergeles@fluid.mech.ntua.gr
Type & scale	3D, prognostic, Lagrangian Urban, local scale
Chemistry	Carbon-Bond IV, QSSA with 81 reactions, 93 species
Treatment of VOCs	
Meteorology	
Emission Inventories	
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	
Policy uses	
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Pollutants concentrations for each grid-cell location and after each integration time period
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	
Comments	

Model	***MARS Greece)*** **(Model for the Atmospheric Dispersion of Reactive Species)**
Institution/s	Aristotle University of Thessaloniki, LHTEE
Contact person/s Contact email address	Prof. Nicolas Moussiopoulos moussio@eng.auth.gr
Type & scale	3-D Eulerian dispersion model for reactive species. Local-to-Regional scale.
Model Domain	Horizontal resolution Domain size: 50-500 km Grid cell size: 500-10000 m Vertical resolution Domain height: up to 10 km Grid cell height: 20-500 m (varying with height)
Chemistry	Pollutants transformation can be treated using any suitable chemical reaction mechanism. Therefore, for that purpose various schemes may be used: KOREM, 20 species, 39 reactions EMEP, 66 species, 139 reactions RADM2, 56 species, 156 reactions RACM, 72 species, 234 reactions
Treatment of VOCs	VOCs are split into CH_4 and other 42 NMVOCs
Meteorology	3-D wind fields contain wind speed in x- and y-direction as well as TKE, surface roughness, Monin-Obukhov length and friction velocity are coming from the 3-D, nonhydrostatic, prognostic mesoscale model MEMO.
Emission Inventories	3-D gridded emission inventory of 47 species. Emission values are provided in kg/h/cell area for each grid cell.
Chemical initialisation and model boundary ozone advection *how is it done? - with observations, another model (specify) or another method?*	Regional background concentrations of NO, NO_2, O_3, PM_{10}, $PM_{2.5}$ and all other species included in the chemical reaction mechanism either from measurements of from large scale model application.
Evaluation: (comparison with observations)	Extensive model evaluation has been performed, but uncertainties still exist because of major uncertainties and limitations in the input and measured data. Individual modules have been validated against other modules, e.g. chemistry module, advection module, diffusion module - cf. Graf J. and Moussiopoulos N. (1991), Kessler Ch. (1995) *etc.* The model also took part in the "CITY-DELTA European Modelling Exercise".

Computer Resources (*super; mainframe; PC*) and typical run time	Can be run on Linux/Unix and windows machines.
Policy uses	• Summer smog • Winter smog • Air toxics • Urban air quality • Industrial pollutants
Is your model actually used for practical policy applications?	Yes
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Concentrations of chemically reacting pollutants for each grid location.
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	.
Published Description *(Reports, Literature)*	Yes
Comments	The model calculates concentrations in the unit ppb.

Model	***OFIS (Greece)***
Institution/s	Aristotle University of Thessaloniki, LHTEE
Contact person/s & email address	Prof. Nicolas Moussiopoulos, moussio@eng.auth.gr
Type & scale	Two-layer two-dimensional Eulerian photochemical dispersion model Urban scale
Chemistry	EMEP MSC-W, 66 species, 139 reactions
Treatment of VOCs	
Meteorology	MEMO mesoscale Eulerian model
Emission Inventories	
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	
Policy uses	
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Concentrations of chemically reacting pollutants for each grid location. Annual average concentrations; percentiles; exceedance probabilities of threshold values
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	
Comments	

Model	***MUSE (Greece)*** **(Multilayer Dispersion Model)**
Institution/s	Aristotle University of Thessaloniki, LHTEE
Contact person/s Contact email address	Prof. Nicolas Moussiopoulos moussio@eng.auth.gr
Type & scale	Multilayer (with 5, time-dependent layers) eulerian dispersion model for reactive species Local-to-Regional scale
Model Domain	Horizontal resolution Domain size: 50-500 km Grid cell size: 500-10000 m Vertical resolution Domain height: up to 10 km Grid cell height: 20-500 m (varying with height)
Chemistry	Pollutants transformation can be treated using any suitable chemical reaction mechanism. Therefore, for that purpose various schemes may be used: KOREM, 20 species, 39 reactions EMEP, 66 species, 139 reactions RADM2, 56 species, 156 reactions RACM, 72 species, 234 reactions SORGAM, 8 organic aerosol species, 16 oxidation reactions (ammended to RACM model)
Treatment of VOCs	VOCs are split into CH_4 and other 42 NMVOCs
Meteorology	3-D wind fields containg wind speed in x- and y-direction as well as TKE, surface roughness, Monin-Obukhov length and friction velocity are coming from the 3-D, nonhydrostatic, prognostic mesoscale model MEMO.
Emission Inventories	3-D gridded emission inventory of 50 species. Emission values are provided in kg/h/cell area for each grid cell.
Chemical initialisation and model boundary ozone advection *how is it done? - with observations, another model (specify) or another method?*	Regional background concentrations of NO, NO_2, O_3 and all other species included in the chemical reaction mechanism either from measurements of from large scale model application.

Evaluation: (comparison with observations)	Extensive model evaluation has been performed, but still uncertainties exist because of major uncertainties and limitations in the input and measured data. Model participated successfully at model intercomparison activities such as "Athens 2004 Air Quality Study" (Moussiopoulos N. and Papagrigoriou S., eds. 1997, Athens 2004 Air Quality, Proceedings of the International Scientific Workshop Athens 2004 Air Quality Study, Athens, 18-19 February 1997, 183 pp.available also as a CD-ROM from http://www.envirocomp.org/).
Computer Resources (*super; mainframe; PC*) and typical run time	Can be run on Linux/Unix and windows machines.
Policy uses	• Summer smog • Winter smog • Air toxics • Urban air quality • Industrial pollutants
Is your model actually used for practical policy applications?	Yes
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Concentrations of chemically reacting pollutants for each grid location.
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	
Published Description *(Reports, Literature)*	Yes
Comments	

Model	***LOTOS-EUROS (Netherlands)***
Institution/s	TNO and RIVM/MNP
Contact person/s & email address	Peter Builtjes; peter.builtjes@tno.nl Martijn Schaap; martijn.schaap@tno.nl
Type & scale	Eulerian grid model Scale: European lowest 3.5 km of atmosphere Resolution: 0.5x0.25 longitude-latitude; zoom versions available
Chemistry	CBM-IV: 28 species and 66 reactions CB99: 42 species and 95 reactions
Treatment of VOCs	8 (CBM-IV) or 10 (CB99) species, plus isoprene and terpene (α,β)
Meteorology	Choice between FUB (Freie Universität Berlin) or ECMWF
Emission Inventories	TNO or EMEP
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	Linux Runtime full chemistry, highest resolution, one year simulation: 6 days
Policy uses	EU and NL policy application
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly concentrations and deposition fluxes AOT40f, AOT40, AOT60, SOMO35, SOMO0, *etc*
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	Schaap *et al.,* (2005) LOTOS-EUROS documentation TNO report B&O-A R2005/297, Apeldoorn, NL Schaap, M., Timmermans, R.M.A., Sauter, F.J., Roemer, M., Velders, G.J.M., Boersen, G.A.C., Beck, J.P., and Builtjes, P.J.H. (2007). The LOTOS-EUROS model: description, validation and latest developments. International Journal of Environment and Pollution, in press.
Comments	

Model	***CAO-HMC (Russia)*** statistical model for forecasting maximal 1-hour ozone concentration in Moscow
Institution/s	*CAO, Dolgoprudny, and HMC, Moscow*
Contact person/s & email address	*Anatoly Zvyagintsev,* *azvyagintsev@cao-rhms.ru;* *Irina Kuznetsova,* *muza@mecom.ru*
Type & scale	Statistical; for Moscow city and its suburbs (to 100 km)
Chemistry	Uses current O_3 and NO_2 measurements
Treatment of VOCs	Absent
Meteorology	Russian HydroMetCentre
Emission Inventories	Absent
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	*PC*
Policy uses	Moscow policy application
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Maximal daily 1-hour mean
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	Zvyagintsev *et al.,* submitted to Izvestiya, Atmospheric and oceanic physics, in 2006; submitted to Meteorology and Hydrology (Russia) in 2007
Comments	

Model	***CHIMERE (Russia)*** (an extended version)
Institution/s	Institute of Applied Physics of Russian Academy of Sciences (Nizhny Novgorod, Russia)
Contact person/s & email address	Konovalov I.B. konov@appl.sci-nnov.ru
Type & scale	Eulerian 3D model, Continental scale (Europe) 0.5^0x0.5^0 or 1^0x1^0 plus a nested domain (Central Russia, including the Moscow megacity region) 0.25^0x0.125^0
Chemistry	MELCHIOR2 (a reduced chemical scheme) 44 species 120 reactions MELCHIOR1 (optional) 80 species >300 reactions
Treatment of VOCs	Man-made VOCs are aggregated into 9 classes represented by model species + isoprene and α-pinene representing biogenic VOCs
Meteorology	Output from MM5 initialised with NCEP data
Emission Inventories	EMEP
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	PC or PC cluster several hours
Policy uses	
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly ozone mixing ratios (standard output), other metrics are also easily available
To what other species can the model be reliably extended?	
Comments	Currently, the model is used in Russia as a tool in scientific studies (*e.g.* inverse modelling of emissions). So far there has been no demand for practical air quality applications of the model in Russia

Model	***CAMx (Spain, Iberinco)*** Comprehensive Air Model with eXtensions
Institution/s	Iberdrola Ingenieria y Construccion, S.A.U. (Iberinco)
Contact person/s & email address	Eloy Piernagorda epa@iberinco.com
Type & scale	Eulerian Many scales ranking from sub-urban to continental
Chemistry	3 versions of CB-IV, SAPRC99 and user defined 38-47 species, 96-110 reactions (CB-IV) 76 species, 217 reactions (SAPRC99)
Treatment of VOCs	Specific properties of VOC species: average carbon numbers, kOH values ($ppm^{-1}min^{-1}$) and maximum incremental reactivity values (mole O_3/mole VOC).
Meteorology	Prognostic meteorological models: MM5, RAMS, WRF
Emission Inventories	Emission inputs from any emissions processor (SMOKE, CONCEPT, EPS, EMS)
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	Two main approaches to parallel processing: OpenMP (OMP) for “sharedmemory”or “symmetric multi-processing” machines or Message Passing Interface (MPI) for distributed-memory computers Example: On a dualprocessor Athlon 2800+ (2.1Ghz) PC, 2 grids VISTAS domain (148x112x19) and (170x179x19)~ 608,000 grid cells. Mechanism 4 CMU (4 sections, 86 total species), 1 CPU, 1GB: run time 8 h/episode day, disk usage 2,3 gB/episode day Current applications at Iberinco: 48 Intel-Xeon based platforms with MPI
Policy uses	Regulatory assessments and general research throughout the U.S.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly

To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	http://www.camx.com/publ/
Comments	

Model	***CAMx (Spain, CEAM)*** Comprehensive air quality model with extensions.
Institution/s	Fundacion CEAM.
Contact person/s & email address	Nuria Castell nuria@ceam.es
Type & scale	Eulerian photochemical dispersion model.
Chemistry	Multiple photochemical and gas phase chemistry mechanism options. 3 versions CB4, SAPRD 3 chemical kinetics solver options Aerosol Chemistry
Treatment of VOCs	
Meteorology	MM5, RAMS and WRF
Emission Inventories	
Computer Resources (*super; mainframe; PC*) and typical run time	PC/cluster GNU-Linux
Policy uses	Impact assessment, prognostic
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly, eight hourly, daily, seasonal, AOT, source-receptor, etc.
Published Description *(Reports, Literature)*	http://www.camx.com Reports and user's guide
Comments	

Model	***CAMx (Spain, Compostella)***
Institution/s	University of Santiago de Compostela. Spain
Contact person/s & email address	Jose Antonio Souto Gonzalez. jasouto@usc.es
Type & scale	Eulerian model, regional to mesoscale (horizontal resolutions: 27kmx27km, 9kmx9km)
Chemistry	Carbon Bound 4 with aerosol chemistry (CF)
Treatment of VOCs	CAMx default
Meteorology	PSU-NCAR MM5
Emission Inventories	EMEP & Galician Industrial emissions inventory
Computer Resources (*super; mainframe; PC*) and typical run time	Supercomputers (scalar processors, share memory) & PC
Policy uses	Research
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly
Published Description *(Reports, Literature)*	CAMx User's Guide. Environ Inc. CA, USA.
Comments	

Model	***CALGRID (Spain)***
Institution/s	Iberdrola Ingenieria y Construccion, S.A.U. (Iberinco)
Contact person/s & email address	Eloy Piernagorda epa@iberinco.com
Type & scale	Eulerian grid-based model Mesoscale and regional scale Grid size: 500 - 20,000 m, domain dimension: 20-1000 km
Chemistry	CB-IV and 1990 SAPRC chemical mechanism 54 species, 129 reactions
Treatment of VOCs	
Meteorology	Gridded fields of CALMET model
Emission Inventories	Point, mobile and area source emissions
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	
Computer Resources (*super; mainframe; PC*) and typical run time	Runs on PCs, NT-Alpha, and UNIX workstations Example: CALGRID required approximately 2 Mbytes of memory for a test application with a 20 by 20 horizontal grid, 10 vertical layers, and 36 advected species
Policy uses	General research
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly
To what other species can the model be reliably extended?	
Published Description *(Reports, Literature)*	http://www.arb.ca.gov/eos/soft.htm
Comments	

Model	***CMAQ and CHIMERE (Spain)*** Chemistry Transport Models
Institution/s	*Applications:* Barcelona Supercomputing Center-Centro Nacional de Supercomputación, Spain. *CMAQ Developers:* Community Modeling and Analysis System (CMAS) Center at the University of North Carolina at Chapel Hill, USA. *CHIMERE Developers:* Institut Pierre-Simon Laplace, INERIS, LISA, C.N.R.S., France
Contact person/s & email address	*Applications of the models in the Iberian Peninsula and Europe:* José Baldasano and Pedro Jiménez-Guerrero (jose.baldasano@bsc.es; pedro.jimenez@bsc.es) *CMAQ Developers:* *CHIMERE Developers:* Zac Adelman Laurent Menut (cmas@unc.edu) (chimere@lmd.polytechnique.fr)
Type & scale	Eulerian 1km x 1km, 2km x 2km (local applications in Madrid, Catalonia, Valencia, Basque Country); 4 km x 4 km (Iberian Peninsula). 12 km x 12 km, 20 km x 20 km, 50 km x 50 km (Europe).
Chemistry	CMAQ: Carbon Bond-IV Chemical Mechanism with aerosols and heterogeneous chemistry, 36 species, 96 reactions CHIMERE: MELCHIOR2 Chemical Mechanism with aerosols and heterogeneous chemistry, 44 species, 120 reactions
Treatment of VOCs	CMAQ: 10 man-made VOCs from emission inventories + biogenic isoprene and terpenes CHIMERE: 10 man-made VOCs from emission inventories + biogenic isoprene and α-pinene
Meteorology	MM5, WRF-ARW and WRF-NMM meteorological inputs both with CMAQ and CHIMERE
Emission Inventories	HERMES, EMICAT and EMIVAL at BSC-CNS (developed specifically for the Iberian Peninsula) and EMEP emission inventory coupled with CMAQ and CHIMERE
Chemical initialisation and model boundary ozone advection	
Evaluation: (comparison with observations)	

Computer Resources (*super; mainframe; PC*) and typical run time	MareNostrum Supercomputer (94.21 TFlops peak): run time of 7 hours using 192 processors for 2-days forecast of both Europe (12x12 km) and the Iberian Peninsula (4 x 4 km). Run time of 4 hours for 2-days forecasts of air quality in the cities of Barcelona and Madrid (domain of 300 x 300 km^2, resolution of 1x1 km) using 200 processors.
Policy uses	Scientific, regulatory, policy, environmental impact assessment, air quality forecasting
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly, 8-hr, daily, seasonal, annual, AOT40, statistical and categorical evaluation (skill scores such as accuracy, probability of detection, critical success index, false alarm ratio, etc).
To what other species can the model be reliably extended?	
Comments	CMAQ and CHIMERE models are the chemistry transport models used ***AQForescast system*** of BSC-CNS and in the ***CALIOPE project*** funded by the Spanish Ministry of the Environment for providing and operational service for air quality forecasting in the Iberian Peninsula. The consortium of CALIOPE is formed by research groups in Spain as BSC-CNS, CIEMAT, CSIC-IJA and CEAM.

Model	***KINMOD 7.0 (Spain)***
Institution/s	Fundacion CEAM
Contact person/s & email address	M. Vazquez (monica@ceam.es)
Type & scale	A suite for coupled modeling of ozone and secondary organic aerosols based on the Master Chemical Mechanism and standards
Chemistry	Master Chemical Mechanism, MCM
Treatment of VOCs	For any VOC to be modeled, the gas phase chemical mechanism is extracted from MCM. If not available in full, MCM is taken as a reference model, the needed mechanisms or part of them is built following MCM 3.1 protocol as long as possible. As soon as the oxidation reaction path converges to chemical species present in MCM 3.1 subsequent reactions are extracted from it.
Meteorology	
Emission Inventories	
Computer Resources (*super; mainframe; PC*) and typical run time	PC with FORTRAN 90, XML and industry standard MS EXCEL. Typical run time: 15-20 minutes
Policy uses	
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Every minute
Published Description *(Reports, Literature)*	L.G. Ruiz Suárez. Final report PSEBASO project (A Pseudo Binary Approach to Secondary Aerosols), Sixth Framework Programme Marie Curie International Incoming Fellowship. Contract: M1F1-CT-2004-002869
Comments	Model used to simulate SOA at the EUPHORE smog chambers.

Model	***MCM (Spain)*** **Master Chemical Mechanism –MCM v3.1**
Institution/s	Fundacion CEAM
Contact person/s & email address	M. Vazquez (monica@ceam.es)
Type & scale	Explicit chemical mechanism
Chemistry	This mechanism describes the tropospheric degradation in the gas phase of 135 volatile organic compounds that generate ozone and other secondary pollutants; it includes 12871 reactions of 4414 organic species and 46 associated inorganic reactions.
Treatment of VOCs	
Meteorology	
Emission Inventories	
Computer Resources (*super; mainframe; PC*) and typical run time	PC. The mechanism can be used in Facsimile, Fortran, KPP, HTML or XML Run time depends on the number of species considered.
Policy uses	Free
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Every second
Published Description *(Reports, Literature)*	M.E.Jenkin, S.M. Saunders and M.J.Pilling. *The tropospheric degradation of volatile organic compounds: a protocol for mechanism development.* Atmospheric Environment. Vol. 31, No. 1, pp. 81-104, 1997
Comments	Model used to simulate the gas phase reactions during the experiments carried out at the EUPHORE smog chambers.

Model	***MdPA (Spain)*** Modelo Diagnóstico por Análogos (Spain)
Institution/s	Meteológica S.A.
Contact person/s & email address	Manuel Blanco mbb@meteologica.es
Type & scale	It is an empirical model which uses observed (non-linear) relationships between today's O3 and: 4. Today's Wind Direction and Speed, 5. Today's Maximum Temperature 6. Today's Day of Week and calendar 7. Yesterday's Maximum O3 concentration
Chemistry	No
Treatment of VOCs	No
Meteorology	Uses forecasts of Wind and Temperature
Emission Inventories	No
Computer Resources (*super; mainframe; PC*) and typical run time	PC, seconds
Policy uses	No
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Daily Maximum Number of hour above threshold
Published Description *(Reports, Literature)*	No
Comments	Neuronal Networks model used in information protocols to population about exceedances of EC ozone threshold values. Environmental Regional Ministry of Andalusia (Spain).

Model	***SMOC (Spain)*** (System for Modelling tropospheric Ozone in Catalonia)
Institution/s	University of Barcelona, Department of Astronomy and Meteorology (Group of Micrometeorology)
Contact person/s & email address	Maria Rosa Soler: rosa@am.ub.es Raúl Arasa: rarasa@am.ub.es Eva Pérez: weperezg@gencat.net David Pagès: dpagesf@gencat.net
Type & scale	Eulerian and Lagrangian 20km x 20km (Eulerian column) , 3km x 3km (emissions)
Chemistry	OZIPR (Ozone Isopleth Plotting Program research)
Treatment of VOCs	SAPRC97 mechanism (Statewide Air Pollution Research Center), 12 hydrocarbons groups and 140 reactions
Meteorology	MASS: three-dimensional mesoscale meteorological Model Blackadar and Transilient: microescale boundary layer models
Emission Inventories	MECA (Emission Model for Catalonia)
Computer Resources (*super; mainframe; PC*) and typical run time	PC, thirty minutes
Policy uses	Directive 02/03/CE
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Hourly
Published Description *(Reports, Literature)*	Beneito, J., 2006: Desenvolupament, aplicació i validació d'un model numèric operacional per al pronòstic de l'ozó troposfèric a Catalunya. Ph. D. Thesis. University of Barcelona, 178 pp. www.am.ub.es/ozo
Comments	

Model	***MM5/CAMx (Switzerland)***
Institution/s	Paul Scherrer Institut (PSI), Laboratory of Atmospheric Chemistry (LAC), 5232 Villigen PSI Switzerland
Contact person/s & email address	Sebnem Andreani-Aksoyoglu (sebnem.andreani@psi.ch) Johannes Keller (johannes.keller@psi.ch)
Type & scale	Eulerian meso-scale model. Domains: from continental Europe down to parts of Switzerland. Europe as mother domain, nested domains national Grid cell size: 27, 9, 3 and 1 km
Chemistry	CBM-IV (gas-phase) RADM-AQ (aqueous) CF and CMU (aerosol chemistry)
Treatment of VOCs	Lumped according to CBM-IV, + Isoprene, biogenic olefins
Meteorology	MM5, driven by assimilated data of the Swiss forecast model (alpine Local Model, aLMo)
Emission Inventories	Europe: UBA/FUB/TNO inventory Lombardy: CityDelta Switzerland, various data sources on the basis of information from the Federal Office of Environment (FOEN)
Chemical initialisation and model boundary ozone advection	*Using global model MOZART output*
Evaluation: (comparison with observations)	**For the evaluation: choose two periods –** "peak" which should include an appreciable number of days with observed peak ozone above 200 µg m^{-3} (*ca*. 100ppb) "background" which should only include values less than 100 µg m^{-3} (*ca*. 50 ppb) **For each**, give the no. of days, the no. of observation stations simultaneously covered, and an overall rating of general goodness of fit on the scale: 1 (middling); 2 (good); 3 (excellent) ???? Peak period: No. of stations: 7 No. of days: 4

	Rating (1-5): 3 Background period: No. of stations: 6 No. of days: 15 Rating (1-5): 4 We haven't done yet any detailed statistical model evaluation. Hourly modelled ozone concentrations were compared by hourly ground level measurements and (if available during field campaigns) aircraft measurements. Evaluations were done so far with graphical tools. The time of the peaks and diurnal variations could be well modelled. In general, for moderate wind speed conditions in summer, model results match measurements well. Depending on the performance of meteorological model (not very good for very low wind speed and foggy situations especially during wintertime), the modelled peak concentrations can differ from measurements. The rating given above refer to a 30 day simulation in June 2006.
Computer Resources (*super; mainframe; PC*) and typical run time	Linux PC. Currently 1 processor. Migration to multi-processor PCs or super computer in progress.
Policy uses	Our results are used as scientific information by our authorities
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	hourly
To what other species can the model be reliably extended?	We are able to model gaseous as well as particulate pollutants such as particulate sulfate, nitrate, ammonium, primary and secondary organic aerosols. However, SOA formation is still being updated by new developments by ENVIRON and not yet fully reliable at the moment.
Published Description *(Reports, Literature)*	Keller J., Andreani-Aksoyoglu S., Tinguely M., Prevot A., 2005. Emission Scenarios 1985 – 2010: Their Influence on Ozone in Switzerland. PSI Bericht Nr. 05-07, Paul Scherrer Institut, Villigen PSI. Johannes Keller, Sebnem Andreani-Aksoyoglu, Michel Tinguely, Johannes Flemming, Juerg Heldstab, Mario Keller, Rene Zbinden and Andre S.H. Prevot, 2007. The impact of reducing the maximum speed limit on motorways in Switzerland to 80 km h-1 on emissions and peak ozone. Environmental Modelling & Software. In press. Andreani-Aksoyoglu et al., Modelling of formation and distribution of secondary aerosols in the Milan area (Italy), JGR, 109, D05306,doi:10.1029/2003JD004231, 2004

Model	***CMAQ (USA)***
Institution/s	Howard University
Contact person/s Contact email address	William Stockwell wstock@dri.edu William.R.Stockwell@gmail,com
Type & scale Model Domain	Adjustable, with multi-nesting available. 4 km is the typical lower limit Used for modelling the entire U.S.; Regional scales and Urban scales
Chemistry	RADM2 is only available until V4.5. CB05 (Carbon Bond 05) is available with 52 species and 156 reactions. SAPRC is available. RACM2 is being implemented in research version. All mechanisms can be used with/without modules for aqueous and aerosol chemistry.
Treatment of VOCs	The CB-V chemical scheme uses a highly lumped approach where chemical functional groups are treated regardless of the molecule to which they are attached. RADM2, SAPRC and RACM2 are all lumped molecule approaches where similar molecules are grouped into the same model species. RACM2 is the most detailed and explicit of the three available mechanisms.
Meteorology	MM5 or WRF provides the meteorology. WRF is now the standard for NOAA's air quality forcasting program.
Emission inventories	SMOKE
Chemical initialisation and model boundary ozone advection *how is it done? - with observations, another model (specify) or another method?*	Available climatological data and simulation of extra 'spin-up" days are most typically used. Formal data assimilation methods using satellite data and global scale models are under investigation at NOAA and NASA for the air quality forecasting program.
Evaluation: (comparison with observations)	For U.S. EPA regularity modelling applications the model is required to have a paired mean normalized gross error of less than 35% and a paired normalized bias ±15 %. Typically the model can meet these requirements.

Computer Resources (*super; mainframe; PC*) and typical run time	Using a (dual processor) desktop PC, a typical month run for all 3 grids takes about 7 days. With a super – multiprocessor system simulation of the entire U.S. can be performed within a few hours.
Policy uses Is your model actually used for practical policy applications?	It is the standard model used for determining state and U.S. EPA approved air pollution control stratagies and for NOAA's National Weather Service's air quality forecasting program.
Producible ozone metrics *(hourly, eight hourly, daily, seasonal, AOT40 etc.)*	Standard model output is hourly ppm (at end of timestep), additionally average hourly ppm is available. These can be further analysed to produce a range of metrics. Using process analysis ozone production and loss from chemistry, advection, diffusion, deposition, and aqueous cloud processes are available. The chemical processes involved with ozone production and loss can be further understood by analysing the hourly flux through all chemical reactions. Hourly 3-D gridded chemical concentrations of ozone, nitrogen oxides, CO, PM, mercury, VOC and most other air pollutants and 2-D fields of acid deposition.
To what other species can the model be reliably extended? *e.g.* NO_2, SO_2, aerosol *etc*.	O_3, NO_2, NO_x, SO_2, VOC, Hg, Aerosol (speciated), $PM_{2.5}$, Additional files include hourly cumulative dry and wet deposition, visibility metrics
Published Description *(Reports, Literature)*	Web link to science document for v4.6 www.cmaq-model.org/op_guidance_4.6/html/index.html