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REVIEW OF AIR QUALITY MODELLING IN DEFRA

A report by the

Air Quality Modelling Review Steering Group

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Executive Summary

This report of the *Air Quality Modelling Steering Group* provides an assessment of the current use of air quality models by Defra in informing and evaluating policy, and in discharging obligations under various EU Directives. The report identifies specific policy needs for the use of models and evaluates each model in turn in terms of the scientific content and credibility of the models, their ease of use and transparency and their fitness for purpose in delivering Defra's needs. The assessment has been informed by the extensive analysis of the first phase of a model intercomparison exercise. Recommendations have been made in terms of a longer-term strategic direction for air quality model use in Defra, and for short- and medium-term actions for moving to this longer-term goal. Specific recommendations for the use by Defra of each model have also been made.

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1. Introduction

Modelling of air quality plays a central role in the development and evaluation of air quality policy in Defra. It also provides significant savings for the Department in reducing the requirement for expensive monitoring for compliance with EU Directives, it provides a wider assessment of the state of air quality across the UK both in terms of airborne concentrations and potential human exposures, and in terms of deposition of acidifying and eutrophying pollutants it can provide assessments of potential environmental damage. Modelling also provides an assessment of the effects of climate change policies on air quality and on the effects of climate change on air pollution. These various requirements demand modelling over a wide range of spatial and temporal scales and over the past years, unsurprisingly, a number of models have been developed and used in the Defra/ALE research programme. The Department has therefore decided that it would be appropriate to review the existing portfolio of models in use in the research programme to assess which models are or are not fit for purpose, whether there are redundancies or overlaps and generally to ensure that maximum value for money is being obtained. In September 2010 Defra therefore established an Air Quality Modelling Review Steering Group (AQMRSG) to undertake this task and to report in March 2011.

This review of the ALE air quality modelling capability is to be seen against the wider back-drop of a review of modelling across the whole of Defra being undertaken by the Science Advisory Council (SAC). In the course of this wider review, SAC set up a sub-group to assess the air quality modelling in Defra, providing input[1] to the final report of the full SAC review published on 13 December 2010. Amongst other findings, this report recommended that
"... Defra adopt regular departmental reviews of existing models by an independent expert panel that can advise on consequences or limitations of future development, or upon possible decommissioning." ALE had already commissioned the AQMRSG to undertake such a task and this report forms the first of these regular reviews.

In particular, the current Review will address the following questions:

- How does ALE currently meet evidence based policy needs through modelling and how should we meet these in the future?
- Are there any gaps or duplication in the evidence base to meet the policy needs and are any models not fit for purpose?
- How might ALE best optimise its current modelling capacity?
- What models ALE should be focusing on in the short, medium and long term for investigation and development?

In more detail the Review will:

- Review modelling capacity – models currently used, contractors undertaking work, outputs generated.
- Review extent to which current policy requirements are being met by these outputs.
- Highlight any gaps in policy requirements, any models being used which are not fit for purpose or any requirements not being generated by current capacity.

[1] Available at http://sac.defra.gov.uk/wp-content/uploads/2010/12/SAC-MOD_10_2009_Air_Quality.pdf

- Highlight likely future policy requirements and extent to which new tools might need to be developed or investigated.
- Investigate options available to ALE – other models which could be used now, other contractors, key areas for development and models which should be invested in and developed further.
- Summarise and provide prioritised short term and long term recommendations.

The Review builds on preceding work. Defra commissioned a review of ozone modelling undertaken by one of the present AQMRSG (Professor Paul Monks) and which reported in November 2007[2]. Subsequently, a protocol for model evaluation was drawn up and published by Defra in 2009[3].

In drawing conclusions and making recommendations, the AQMRSG was conscious that modelling use and capability within a particular contracting organisation must be seen within the wider context of an appreciation of the total system of air quality management tools – emission inventories and their development, air quality monitoring and the need to have regard to the strengths and deficiencies in these areas in obtaining the optimum performance of air quality models.

Ideally, this review would have undertaken a more detailed review of models and approaches in use in other European countries and in North America but the timing and scope of the current review did not allow this, although the earlier review of ozone models referred to above considered a wide range of models in use in Europe and in the US. Nonetheless some remarks are appropriate on the differing approaches adopted by the UK (via Defra) and others in relation to air quality modelling for policy and regulatory purposes.

Historically, the UK has avoided the formal architecture and structure associated with modelling development, in the way that, for example, the USA has done. As a consequence, models have been developed in an *ad hoc* way for each policy need as it arises. This also mirrors the deliberately non-prescriptive approach taken for dispersion models used in the regulation of industrial installations. Another consequence of this approach to model development and use is that the expertise and knowledge is dispersed and resides largely with model users.

In the USA, on the other hand, models are evaluated and then given formal approval by the US Environmental Protection Agency which maintains a central controlling role. This governance role also has a legal dimension in that regulatory models are cited for specific uses in Federal Registers, e.g. for demonstrating compliance with permits. This sharpens the need for development to be structured, transparent and fully documented. By the time models are formally approved for use, much knowledge has been acquired on their performance and validity. Often this knowledge is gained outside the USA, as users take advantage of the code being freely available. This can make the process of development for models seem long and drawn out, but it does at least ensure that the end result is the product of many separate inputs and a great deal of scrutiny.

The UK and other countries in Europe have not typically adopted the approach whereby one body has assumed formal responsibility for the strategic direction of model development and making recommendations of using particular models for particular purposes. At a European level, development of models for regional and trans-boundary modelling has been driven by the needs of

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[2] P.S.Monks, R.S.Blake and P.Borrell, Review of tools for modelling tropospheric ozone formation and assessing impacts on human health and ecosystems. University of Leicester report to Defra, 2007.

[3] Available at http://uk-air.defra.gov.uk/reports/cat05/1006241607_100608_MIP_Final_Version.pdf

CLRTAP and, to some extent, by the European Commission and the CAFE programme which have tended to use the same models for integrated assessment as CLRTAP (the atmospheric model being the EMEP model).There is no direction from the European Commission on which models should be used in the context of demonstrating compliance with air quality limit values (in contrast to the US EPA). Instead, the Air Quality Directive sets out performance criteria which models should satisfy, leaving the choice of which particular model to use to the particular operator or agency[4]. These performance criteria have been discussed in the FAIRMODE group under the auspices of the European Commission, and are discussed further in Section 3.

For dispersion over smaller scales, instances can be found where dispersion models have been developed by a national body. Obvious examples can be found in Germany and Belgium. In the former case, three German Länder funded the development costs in 2001 for the model now known as AUSTAL2000 ('Ausbreitungsrechnungen nach TA Luft', which translates as 'dispersion model for calculations according to TA Lüft'). This Lagrangian model is now the reference model for many regulatory applications in Germany, performing a similar role to ADMS and AERMOD in a UK context. Freely available via a web site, it was based on the LASAT modelling system. This perhaps illustrates a difference between the UK and other countries in Europe, where there is less separation between the responsibility for regulation of industrial sources and the wider management of air quality at the national level.

A full list of models in use across Europe can be found at the Model Documentation System provided by the European Environment Agency's Topic Centre[5]. One of these is CHIMERE, a French multi-scale, multi-pollutant model similar in concept to CMAQ and the code for which is also freely available. Its performance has been evaluated as part of the Europe wide City Delta project[6].
An interesting example in the UK where a single model was recommended – albeit in a tightly constrained circumstance-was the so-called 'Project for the Sustainable Development of Heathrow' led by the Department for Transport, where, after an evaluation exercise an independent expert panel recommended the use of the ADMS model to evaluate future scenarios for the development of Heathrow airport. This shows that the expertise is available in the UK, but is rarely convened to consider model performance and use in policy context and does not exist as a standing body for Defra's needs.

An important consideration looking to the longer term is the relationship between the modelling needs in ALE (and wider Defra) and the ability of the underpinning basic research in the science community in the UK to develop models further and to provide the necessary supply of skills and expertise. Detailed recommendations in this area are beyond the scope of this review but to ensure these long term needs are met, there will need to be close liaison between Defra, NERC and EPSRC. Complementary to this point is the desirability of supporting a thriving model user community, such that additional knowledge on model performance is retained and that capable contractors exist to perform model runs for Defra, as and when required.

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[4] See for example, Annex I of the 2008 EU Air Quality Directive (2008/50/EC) which specifies some uncertainty limits for model use. See Section 3 for further discussion.

[5] Available at: http://acm.eionet.europa.eu/databases/MDS/index_html

[6] Vautard *et al* (2007) Evaluation and Intercomparison of Ozone and PM_{10} simulations by several chemistry transport models over four European cities within the CityDelta project *Atmospheric Environment* **41** 173-188.

2. Policy needs for air quality models

2.1 Introduction

As with all science commissioned by Defra, policy and regulatory needs are the sole drivers. These have been specified by Defra and are shown in Appendix 1. The implications for models which aim to deliver these policy priorities are discussed below.

2.2 Compliance assessment and modelling as replacement for monitoring in EU Directives;

This requirement places considerable demands on models. They have to cover (i) a range of pollutants, (ii) a range of averaging times from an hour to a year, (iii) the whole territory of the UK at a spatial resolution of a few kilometres and (iv) hotspots, in particular roadsides[7].

This, (and the next) driver is probably the most important for Defra in the immediate future. The ability to satisfy this need adequately saves the Department almost £2 million per year in monitoring costs and provides compliance assessment relatively cheaply. Not only do models have to be able to calculate exceedences of Limit Values but also the metrics related to the exposure reduction obligations, and to the Critical Levels for vegetation specified in the Directive. It also worth noting here that for ozone, PAHs, arsenic, cadmium, mercury and nickel, Target Values rather than Limit Values are specified in the Directives.

2.3 Future compliance assessment (EU AQ Directive, AQ Strategy, critical loads/levels in EU Habitats Directive & CLRTAP);

The basic requirements for models here are as for 2.2 but with an extra dimension, namely the ability to handle the assessment of future policy scenarios in a manageably short timescale, ideally a matter of days or in extremis hours. Although not covered to any great extent in the current research programme, delivery of this item could in future also involve assessments of the robustness of emission forecasts and incorporate overall uncertainties in policy advice from models. The requirement for assessment of critical load exceedences is discussed in 2.5 below, and in section 5 the delivery of this item will be discussed separately from the rest of drivers 2.2 and 2.3.

2.4 Health impact assessment, public information;

The requirements here are similar to 2.2 and 2.3. At present, current epidemiological results which drive policy are based on fixed site monitors and relatively coarse 'static' exposure measures, so for these health impact assessments, models which satisfy 2.2 and 2.3 could be used. However, new research is addressing 'dynamic' exposure assessment involving spatio-temporal variations based to a greater extent on personal mobility and time-activity patterns. The ability of models to cope with such advances is an important consideration in delivering this requirement in the future. Similarly there may be new pollutant metrics emerging and models will need to be flexible enough to accommodate these.

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7 In this report, the term 'roadside' is used to mean any location close to a major road. No fine distinction is made in general here between the terms 'roadside' and 'kerbside'.

A component of Defra's public information activity is the daily air quality forecast. Models must be capable of being run quickly on a daily basis and should cover the whole UK, including traffic locations.

2.5 Ecosystem impacts

Although there are no explicit binding legal obligations to report exceedences of critical loads, or to ensure critical loads are not exceeded, implicit in the Habitats Directive (Council Directive 92/43/EEC of 21 May 1992 on the conservation of natural habitats and of wild fauna and flora) is the requirement to assess air quality impacts on vegetation and ecosystems, and assessment of critical load exceedences represents more generally a means both of gauging ecosystem health in the UK and of measuring progress toward the wider goals of the LRTAP Convention and the EU National Emission Ceilings Directive (2001/81/EC).

In both the 5th EU Environmental Action Programme and in the National Emission Ceilings Directive (NECD) there is a long term aim of no exceedence of critical loads; in the NECD there is an interim objective which states that the ceilings shall have as their purpose "to meet broadly" the aim that "areas where critical loads are exceeded shall be reduced by at least 50% (in each grid cell) compared with the 1990 situation." There is also an obligation on the Commission to report periodically to the Parliament and to the Council on the exceedence of critical loads and levels. These various obligations mean that there is a requirement for the UK to assess critical load and level exceedence throughout the UK.

Models therefore need to be able to estimate both wet and dry deposition, including at higher altitudes, as well as airborne concentrations. They need to be flexible enough to accommodate advances in methods of calculating deposition (for example the flux-based approach recently adopted for calculating ozone deposition to vegetation and crops). The models need to be able to do this across the whole of the UK with sufficient spatial resolution to resolve adequately the important ecosystems, typically around ~5km.

2.6 Climate change impacts/Future proofing

Here models should be capable of handling future climate scenarios involving increased temperatures and other meteorological variations-circulation, stability frequencies etc. Should the input emission inventories not adequately account for temperature changes (e.g. in biogenic emissions in different temperature regimes), then the model operation will also need to incorporate these effects.

More generally the use of models in the ALE research programme needs to be 'future proofed', that is, decisions taken today need to have regard to future flexibilities insofar as they are known, or at least they should not knowingly lead the programme into blind alleys. One important aspect of this is the development of multi-pollutant/multi-effect models and the move to self-consistent modelling platforms. The relationship with the science base is important here and Defra will need to liaise with NERC and EPSRC to ensure there is an adequate supply of skilled scientists to continue research in atmospheric modelling within the basic science community and also to act as 'intelligent customers' within the policy environment in Defra. There is also merit in ensuring that links are established and maintained with model users external to the UK, so that awareness of useful developments elsewhere is embedded in the programme.

3. Scientific criteria for air quality models

Not only do models need to be structurally capable of delivering the policy drivers detailed in Section 2 in terms of their spatial and temporal coverage and their inherent physics and chemistry, they need also to be capable of performing acceptably in practice. Models need to be able to reproduce observations (*'operational evaluation'* in the terminology of recent studies of model evaluation carried out by the USEPA[8]) but their ability to calculate the responses to emission (and meteorology) changes with acceptable confidence also needs to be assessed, a process known as *'dynamic evaluation'*. The latter is crucially important in the policy context but is also the more difficult to assess. Future concentrations are not available obviously, so a comparison of observed and modelled weekday/weekend differences, modelled and observed trends over several years, or techniques such as 'back casting' are often used. It is worth noting here that these analyses are often strongly influenced by the quality of the emission inventory, errors in which can mask any deficiencies in the models themselves. The model intercomparison exercise organised by Defra provides an operational evaluation of the models taking part, and a degree of dynamical evaluation.

The only formal criteria of acceptability in the current exercise are set out in Annex I of the EU Air Quality Directive and these relate purely to comparison with measured values-unsurprisingly as the context is the use of models as a substitute for monitoring. The criteria are given in Table 1.

Table 1. Uncertainty criteria in the EU Air Quality Directive 2008/50/EC

Modelling Uncertainty	SO_2, NO_2, NO_x, CO	Benzene	PM_{10}, $PM_{2.5}$ and Pb	Ozone and related NO and NO_2
Hourly	50%	-	-	50%
Eight-hour averages	50%	-	-	50%
Daily averages	50%	-	Not yet defined	-
Annual	30%	50%	50%	-

In the Directive footnote to the Table in Annex I, the uncertainty is defined thus: *"The uncertainty for modelling is defined as the maximum deviation of the measured and calculated concentration levels for 90 % of individual monitoring points, over the period considered, by the limit value (or target value in the case of ozone), without taking into account the timing of the events. The uncertainty for modelling shall be interpreted as being applicable in the region of the appropriate limit value (or target value in the case of ozone). The fixed measurements that have to be selected for comparison with modelling results shall be representative of the scale covered by the model."*

Any model that is considered for use in delivering policy driver 2.3 should therefore satisfy the criteria in Table 1. The Directive criteria are missing from the Defra protocol for model intercomparison, which instead makes two recommendations for acceptable performance, firstly

8 Dennis et al, A framework for evaluating regional-scale numerical photochemical modelling systems, Environ. Fluid Mech (2010). 10:471-489.

that the fraction of modelled results that are within a factor of two of the observations[9] should be at least 50%, and that the Normalised Mean Bias[10] should lie between -0.2 and +0.2. These criteria are clearly different from the Directive requirements but could nonetheless provide useful yardsticks for evaluating model performance. Further work on model intercomparison should assess the relative stringency of these different criteria. However, the primary requirement is clearly to meet the Directive criteria. Guidance on the interpretation of the Directive criteria for model performance have been produced by the FAIRMODE group[11], and a preliminary assessment of UK models against these criteria has been provided by Carslaw[12], from the recent Defra model intercomparison exercise.

Two other forms of evaluation have been defined by the USEPA. The first, known as '*diagnostic evaluation*' relates to assessments of the physical and chemical modules/algorithms which attempt to simulate the processes taking place in the atmosphere. This is most relevant to regional scale models where chemistry and physics are important-modelling secondary aerosols and ozone for example. To carry out this form of evaluation fully places demands on measured quantities and chemical species (ideally in three dimensions) which a rarely if ever fulfilled. In practice *diagnostic evaluation* can be carried out through sensitivity tests on key parameters in the modules, 'off-line' comparisons of chemical mechanisms, or at a basic level, through peer scrutiny of the methods employed. The current Defra intercomparison exercise has not involved any formal diagnostic evaluation. This report will provide a basic peer review of the process descriptions in the various models used where this is relevant.

The final approach has been termed '*probabilistic evaluation'* by the USEPA and involves the use of statistical techniques to attempt to assess the uncertainty in model projections or forecasts.

As noted above, the first phase of the model intercomparison exercise provided an operational evaluation of model performance and a degree of dynamical evaluation. However, the main consideration in this review is the ability of models – either now or with some further development – to deliver the policy needs of Defra/ALE set out in section 2. This review has necessarily been at a strategic level. The role played by the intercomparison exercise in the current review has been twofold. Firstly it has screened out any obviously unacceptable models and secondly it has provided an initial, but not necessarily final, comparison of the performance of those models which could satisfy the policy needs. In formulating the Recommendations of this review discussed below, the Steering Group took these results into consideration, along with the two-day discussion meeting of the first phase of the intercomparison exercise.

9 Defined as $0.5 =< M_i/O_i =< 2.0$

10 Defined as $\Sigma(M_i - O_i)/\Sigma O_i$

11 http://fairmode.ew.eea.europa.eu/fol429189/forums-guidance/model_guidance_document_v6_2.pdf

12 Carslaw, D.C. (2011). Defra regional and transboundary model evaluation analysis. King's College London, version 14th March 2011, available at: http://uk-air.defra.gov.uk/library/reports?report_id=653
Carslaw, D.C. (2011). Defra urban model evaluation analysis. King's College London, version 24th March 2011, available at: http://uk-air.defra.gov.uk/library/reports?report_id=654
Carslaw, D.C. (2011). Defra deposition model evaluation analysis. King's College London, version 4th March 2011, available at: http://uk-air.defra.gov.uk/library/reports?report_id=652

4. Institutional framework for delivery of modelling

In considering the delivery of Defra's policy needs for modelling, it is important to consider institutional frameworks of organisations which can run candidate models, as well as the scientific and technical aspects of the models themselves. Defra needs organisations that are capable of meeting its full range of requirements, from the rapid production of model runs to address short-term needs, to detailed modelling to address a wide range of policy options. The organisation will need to respond in a timely and efficient manner with the appropriate level of scientific detail. Ideally these needs would be met by an organisation, or organisations, with the capability and flexibility to interact with the research community.

It is also noteworthy that the model intercomparison exercise showed that the same model implemented and run by different organisations could give different results. This, at least in the initial stages of further development of the Defra programme, could mean that there is a need for a plurality of capability and interaction between modelling groups. This will be elaborated on later in this report.

5. Assessment of individual models and packages

5.1 Introduction

This section gives an assessment of each model judged against its ability to meet the policy drivers in section 2, either as the model stands at present or with further development. Comments are also given on the performance of the models in the intercomparison exercise, where feasible against the criteria discussed in section 3, particularly the requirements of the EU Directive where a model is being used as a substitute for monitoring. We have not included detailed description of each of the models here but details are available in the published literature or from the organisations listed against each model in Appendix 3. In summarising the structure and content of the models, questionnaires submitted by the modellers have been used, as have relevant peer reviewed papers. These latter are not referenced explicitly here but are available on the modelling intercomparison exercise webpage on UK-AIR.

It is important to note here that messages or conclusions drawn from Phase 1 of the modelling intercomparison exercise need to take into account the fact that during the period of that exercise it became clear that the emission inventories for NO_x from road vehicles significantly underestimate the actual emissions. Any deterministic model, even if it were 'perfect', would therefore be expected to underestimate roadside/kerbside concentrations of NO_x and NO_2. This is not the case for PCM, where the results are calibrated to the measurements, which illustrates both the strength and weakness of PCM. Also to some extent one might expect the modelled PM_{10} values to be an underestimate, as resuspended material is not included in the inventories. Similar considerations apply to the accuracy of measured data of course and any systematic errors or biases in measured data could lead to spurious conclusions being drawn regarding the performance of models.

5.2 PCM

PCM (included in the 'Urban' section of the model intercomparison exercise[13]) is essentially a GIS based semi-empirical model, driven by the NAEI but consisting of modules which provide concentrations of different pollutants or in the case of PM, provide the different component parts of the PM mix. The basis of the model is the calculation of 'background' concentrations across the UK on a 1 km x 1 km grid using measured data to derive the regional background, with near sources (those within about 15 km) modelled as area sources using a kernel approach based on ADMS 4, and large point sources modelled explicitly using ADMS 4. Roadside concentrations are based on an empirical approach with concentrations defined for an effective distance of 4 m from the kerb. The model produces annual mean concentrations, relying on empirical relationships to derive shorter-period concentrations.

Pros

PCM is currently delivering the requirements of the EU Air Quality Directive. It provides concentrations for all relevant pollutants (apart from hourly NO_2 for which monitoring data are used

[13] In subsequent sub-paragraphs of Section 5 of this report, the terms 'Urban', 'Regional' or 'Deposition' will be used to denote the sections of Phase 1 of the model intercomparison exercise where the model in question was dealt with. This should not be taken to mean that models are restricted to one or two areas alone – with appropriate nesting and/or improvements in computer power in future, certain 'Regional' models could potentially operate at 'Urban' scales and also treat 'Deposition'.

in Directive reporting) at a resolution of 1 km x 1 km over all the relevant timescales. The modular form means it is capable of incorporating improved science as it develops, e.g. the relationship between changes in emissions of secondary inorganic aerosol precursors and the resulting PM_x components. It also provides estimates of roadside concentrations and lengths of road in non-compliance with Limit Values. It is capable of providing projections of future concentrations, including the $PM_{2.5}$ exposure reduction metrics, on an acceptable timescale, given a set of future emission projections. It is currently the only model used by Defra to provide annual compliance reports required by the Directive, and the only model used to provide assessments of future policy options with regard to future compliance with Directive obligations. In this task it is supplemented by ADMS to deal with urban scales. It is fast to run, which makes it suited to scenario testing, and it performed reasonably in the intercomparison.

Cons

The major weakness of PCM is that it is calibrated annually to the current year's measured concentrations. This means that there is uncertainty over future projections of compliance provided by PCM. Steps have been taken to assess this uncertainty by for example using different base years for the projections. Furthermore, since the outputs of PCM are determined primarily by the NAEI, the results-in terms of past and future trends - are only as good as the emission estimates. This of course is true of any model in general but a key feature of PCM is that the roadside concentrations are obtained from an empirical relationship between measured levels and emission estimates on the relevant road link. There has not to date been any assessment of the uncertainty in the roadside calculations based on the scatter in this empirical relationship. Roadside concentrations are for a nominal 4 m from the kerb and there is no spatial detail provided. To meet EU assessment criteria for the limit values, concentrations are not modelled at road junctions (although this could be added as an option if required). Another problem with PCM is that daily PM_{10} concentrations are not modelled explicitly but estimates are based on empirical relationships between historical measured relationships with annual means. Future projections of compliance based on this technique must be considered uncertain as they rely on the empirical relationships holding in the future, which may not be the case.

5.3 ADMS

ADMS (included in the 'Urban' evaluation exercise) is a three-dimensional, steady state quasi-Gaussian dispersion model developed in the UK by CERC, following an initial collaboration and funding in 1990, involving a number of Government agencies and others (including the Met Office, power generators, HMIP-the forerunner of the Environment Agency - and the University of Surrey). It covers dispersion from point, area, volume and line sources with a straight-line plume trajectory from source to receptor or grid point. Concentrations are modelled on an hour by hour basis using an appropriate (usually) regional meteorological data set. The model is commercially available in a number of permutations: ADMS Urban, which essentially nests the point, area and volume model AMDS 4 and the line source model ADMS Roads into one package, while ADMS Airports is suitable for multiple sources on an airport. The point source component of the model takes account of plume rise and building downwash. The line source component is used to model open roads, with a separate module for dispersion within street canyons, based on the Danish OSPM model. There are options to apply diurnal, weekly and monthly profiles to the emissions or detailed hour-by-hour profiles for a full year. Concentrations are calculated for individual receptors and are thus geographically specific (to better than the nearest 0.1m), allowing detailed concentration patterns near sources to be shown.

The model is best suited to near field dispersion, i.e. within a few hundred metres or a few kilometres. Over these distances, straight-line assumptions on plume trajectory are reasonable and it is appropriate to ignore chemistry, apart from the NO_x:NO_2:O_3 cycle and deposition. There is no requirement for boundary conditions to be defined. The model is usually run in a mode where the concentrations due to the modelled near-field sources are added to background concentrations across the model domain. These background concentrations are either derived from monitoring data or from regional models. It is thus possible to nest ADMS within a regional model such as CMAQ. A variant of this was tested during the model intercomparison, with King's College ERG using CMAQ to provide both the regional and the urban background, while ADMS was used to add the road component. In the intercomparison this performed less well than the ERG Toolkit package, which used ADMS to model the roadside and urban background, with measurements used to provide the regional background.

While the use of ADMS Urban in the UK has been relatively limited, the ADMS 4 and ADMS Roads models are widely used and there is a strong user community with experience of using ADMS models. There are options to include dry deposition of particles and gases and the chemistry of NO_x:NO_2:O_3. Over the short distance scales for which the model is normally used the dry deposition is rarely applied. The chemistry module is relatively basic, and users often apply semi-empirical means of transforming NO_x emissions into NO_2 concentrations.

Pros

ADMS Roads is probably the most frequently used model in the UK for assessing concentrations due to road traffic. AMDS 4 is also widely used, although the USEPA model AERMOD is equally widely used for point, area and volume source modelling. ADMS Roads and ADMS 4 together form ADMS Urban. All ADMS models are commercially available and as such their use is not restricted to any one user group. They have also been developed with a Windows based user-friendly front-end, which makes them easy to use. It would also be possible to use ADMS Roads, together with AERMOD for area and volume sources, as an alternative approach. The use of monitoring data to define the regional background is likely to improve the accuracy of the modelled current-day total concentrations, but a regional model, such as CMAQ, could be used to define the regional background.

The ADMS urban model performed generally better than the other models in the intercomparison, but like the other models tended to under predict at the kerbside, especially for NOx and NO_2, which is undoubtedly due to the problems with the NOx emission factors for motor vehicles.

Cons

The inherent limitations of the model in the far field are such that it does not have the capability for modelling the contribution of distant sources, i.e. the use of ADMS Urban to model regional concentrations is not viable. This though can be overcome by using monitoring data to determine regional background or by nesting ADMS within a regional model. The run time can be long (days) when used to model a large area in detail. The ADMS Urban version, which is suitable for larger urban areas, is relatively expensive to maintain a licence for and represents a continuing cost (in contrast to the open source models where the code is free and the costs are associated with assembling a working version on the user's computing system). For roadside locations where complex building configurations influence dispersion at street level, the model has some difficulty in simulating dispersion, especially in low wind speed conditions. This is a characteristic of all models for this situation where airflows are complex and turbulent diffusion processes can dominate.

5.4 ERG Toolkit

This is a semi-empirical model developed by King's College ERG for application in London and was included in the 'Urban' part of the evaluation exercise. It is used to predict annual mean concentrations of NO_2, NO_x, PM_{10} and $PM_{2.5}$, with a high spatial resolution, especially near to roads. All sources more than 500 m from a receptor are modelled as shallow volume sources using ADMS 4, apart from point sources, which are modelled specifically. The road component is based on a kernel approach, involving splitting the road network into 10 m lengths and using ADMS roads to model the concentration. The OSPM module is used for modelling concentrations within street canyons. Hourly emission profiles are applied to weekdays, Saturdays and Sundays. The conversion of NO_x to NO_2 is based on an empirical relationship. The ADMS urban background and roadside concentrations are added to a regional background, which is derived from monitoring at rural locations.

Pros

The model is relatively quick (hours) to run, due to the use of a kernel approach. It can thus be envisaged as falling between the PCM model and the full application of ADMS. The use of monitoring data to define the regional background is likely to improve the accuracy of the modelled current day total concentrations.

Cons

The model does not predict hourly concentrations although the other roadside modelling system used by King's College, 'CMAQ-Urban', nests ADMS within CMAQ to provide hourly concentrations. The empirical relationship to derive NO_2 from the NO_x does not allow readily for varying primary NO_2 proportions in the emissions (fNO_2). The model does not deal with varying speeds near to junctions. It is not available to outside users. It has only been applied to London. The reliance on monitoring data to define regional background is a disadvantage for modelling of future scenarios, as there is no deterministic basis for projecting forwards the measured regional background.

5.5 BRUTAL

This model provides the urban component of the integrated assessment model, UKIAM. It uses an annual average wind rose for the UK and requires the running of ASAM to model the imported (regional) contribution. The focus has been on PM_{10}, although NO_2 is also modelled. Currently $PM_{2.5}$ is not modelled. Background concentrations are modelled on a 1x1 km grid with a kerbside enhancement determined for a nominal road in the grid square, based on population density. Primary NO_2 is incorporated but not in a detailed way.

Pros

The model is quick to run with run times of around 30 minutes making it ideally suited for use in the IAM system. It is also capable of delivering outputs for the urban background locations for the whole of the UK. It is also capable of modelling roadside concentrations across the whole of the UK (although this is based on ADMS methodology).

Cons

The model does not predict hourly concentrations. It also does not model concentrations along specific roads and for this reason performed poorly in the model intercomparison study. It is currently configured to produce concentrations of PM_{10}, NO_x and NO_2.

5.6 UK EMEP Unified Model and EMEP4UK

EMEP4UK is an Eulerian grid model, developed relatively recently at CEH from 2006 onwards. Its purpose is to develop source-receptor relationships, but it could easily be adapted for many purposes. It was included in the 'Regional' and 'Deposition' parts of the evaluation exercise. The meteorological module used as input is provided by WRF, with the chemistry and deposition by the EMEP unified model. In essence, it is an adaptation of the EMEP unified model, with an ability to make use of the NAEI for UK emissions and an ability to present outputs for the UK at a finely resolved scale (5 km by 5 km), with further sub domains, if required.

The chemistry scheme is relatively sophisticated and the model can provide outputs for a large number of pollutant and intermediate species, for a number of different averaging periods.

Computationally, the WRF model takes most of the run time (about 5 days at CEH for a 5 km^2) resolution, with the chemistry then taking a further 8 hours.

Pros

The model is sophisticated, making use of up to date models and algorithms for the meteorological and chemistry components, with adoption of UK and European emission data. It performed as well as any model in the intercomparison exercise, with only the nitrate in precipitation being noticeably underestimated and with some underestimation of nitric acid.

The EMEP Unified model is open source and has good documentation and supporting infrastructure. It has been subject to continuous evaluation of its performance, all of which is public domain material.

Cons

As a model for the regional and transboundary transport of pollutants associated with acidification and eutrophication (along with ozone), EMEP4UK has no obvious drawbacks, other than the amount of human and computing resources required to run WRF. It might be argued that the model system is not as well developed as some alternatives and it is not, of course, designed as a multi-scale model.

5.7 NAME

This model has a long history, having been developed by the Met Office originally in response to the Chernobyl nuclear accident as a means of simulating the long range transport and deposition of radionuclides. Since then, it has improved considerably in its sophistication and performance, through its treatment of plume chemistry, for example. The current version is 5_4 and it was included in the 'Regional' and 'Deposition' parts of the evaluation exercise.

The Numerical Atmospheric dispersion Modelling Environment model is a Lagrangian particle trajectory model, with pollutants represented by very large numbers of particles released from sources into the 3 dimensional wind field generated by the Met Office's Unified Model. Individual particles are tracked and concentrations calculated by summing particles in individual grid cells.

Deposition processes are simulated by conventional means, with a resistance analogy for dry deposition and a scavenging coefficient for wet deposition by washout and rainout. Plume chemistry in NAME was developed initially for sulphate, but has since been extended and now includes 100 reactions. Chemistry modelling in a Lagrangian framework has some complexity, given that the particles (or air parcels) are primary releases and any transformation of these particles has to be reconciled in terms of the primary particles at each model step (i.e. every 15 minutes). Background species outside of the plumes are modelled on a static Eulerian grid.

NAME has been used in a number of studies designed to investigate the long range transport of pollutants on a continental and hemispheric scale and is the mainstay model for emergency response modelling, as in the case of the volcanic ash, animal disease outbreaks and the Buncefield explosion.

Pros

The NAME model is sophisticated with regard to the long range transport and dispersion of pollutants, especially from point sources (for which it was originally designed). Its long history of continuous development ensures that it has a robustness and pedigree that provide assurance of its performance and integrity. The linkages with the Met Office numerical weather prediction models provide a good basis for the advection of pollutants and its chemistry scheme (based on STOCHEM) is sound and well understood. It has a capability for estimating concentrations of secondary PM_{10} species including Secondary Inorganic Aerosol (largely ammonium sulphate and nitrate) and Secondary Organic Aerosol (a complex mixture of organic compounds formed by reactions in the atmosphere) .

The model produced a convincing performance for most of the gaseous pollutant concentrations in the intercomparison exercise, whilst noting that its overprediction of the SO_2 concentrations was the most pronounced of all the models. Underprediction was observed for both nitrate and Non Sea-Salt sulphate in precipitation.

Cons

The model is very much the property of the Met Office and requires linkage with the Met Office weather prediction models, as well as running on the Met Office computing system. Run times are strongly dependent on the resolution sought, i.e. the number of particles released, but for a run giving annual outputs for the whole of the UK would be measured in weeks.

5.8 CMAQ

The Community Multi-scale Air Quality model has been in existence for some time, with the first version being released by the US EPA in 1998, after six years of investment. It was developed in specific recognition of the need to adopt a more strategic approach to modelling in which the dispersion and transformation of multiple pollutants across could be modelled. Previous regional models had tended to be focused on specific issues, such as regional acid deposition (e.g. RADM) or attainment of ozone air quality standards (e.g. UAM). CMAQ is part of the Models 3 framework or system, which also includes emissions and meteorological modelling. The system was developed by the USEPA with the intention of providing a unified 'single airshed' modelling system as an open-source community model. The framework was always intended to be flexible, such that CMAQ can be used with alternative meteorological models or emissions inventories. Reflecting this, CMAQ was used by three groups in the 'Regional' and 'Deposition' parts of the evaluation exercise and also by one group (with a nested roadside module) in the 'Urban' part.

CMAQ was conceived and developed with the clear intention of creating a 'one atmosphere', high quality model capable of simulating air quality over a wide range of length and time scales. It was also deliberately structured in a modular form, such that new formulations for specific atmospheric processes could be inserted and tested without requiring a whole new model formulation. Its open source nature and wide user group encourages development and improvement that is not necessarily led by any single 'owner' of the model. A co-ordination centre exists to provide a central repository for knowledge on CMAQ use and performance and to assist in its development. This is the US EPA funded Community Modelling and Analysis System (CMAS), based at the University of North Carolina. The centre provides a resource for model users in terms of assistance and knowledge sharing, as well as fostering a sense of community and collaboration amongst model users.

The model itself is an Eulerian grid model and can be run on multiple computer platforms, but which are typically high performance computer clusters. The modules used for describing chemistry and deposition are largely based on US schemes, often taken originally from previous models. Some of these have been adapted and improved over time.

The modular nature of CMAQ means that individual users will choose different options for inputs, such as emissions and meteorological models and, in some cases, the more integral schemes for deposition and plume chemistry. The Table in Appendix 4 summarises the choices made by the different model users for the intercomparison runs.

Pros

CMAQ offers a number of advantages, most notably its flexibility and multiple uses, along with the extensive body of development work that has accumulated knowledge on its performance over successive versions since 1998. Its ability to accept inputs from a variety of meteorological models and emission models means that it can be relatively easily adapted for use in a UK context, despite not being designed for UK policy needs.   CMAQ is an 'open source' model and is therefore fully transparent.

The performance of the two versions of CMAQ in the intercomparison exercise, with regard to the deposition element, was good, but with some differences between the two. Both versions tended to overpredict concentrations of SO_2 and underpredict NO_2 and NH_4. The model versions performed similarly in terms of nitrate in precipitation, ammonium in precipitation and annual mean nitric acid concentrations. The differences occurred for NH_4^+ and NO_3^- concentrations, for which the University of Hertfordshire version gave significant underprediction. The source of these differences could lie in the choice of wet deposition module, for which the version used in the Joint Environmental Programme of the electricity generators uses more recently developed algorithms. The recently developed dry deposition methodology for ozone based on stomatal flux, known as DO_3SE has been implemented in CMAQ in use in the UK.

The modelling of ozone across the urban and regional scale shows the flexibility and power of the CMAQ system. It is of note that different model configurations will give varying answers and demonstrate the need for benchmarking of performance.

Cons

CMAQ is a relatively complex model that requires a meteorological model such as WRF to provide an input. Like other models requiring the use of meteorological models, it is computationally intensive and has total run times measured in days or weeks, depending on the available computing set up. This means that successive runs, to explore policy options that might be an outcome of the previous run, could take up considerable time and resources.

5.9 OSRM

OSRM (Ozone Source Receptor Model) is a Lagrangian trajectory model. The OSRM was developed to model the range of ozone metrics for which there are policy targets and it has been used to model UK ground-level ozone concentrations at 10 km x 10 km resolution (at 3,000 specified receptors) on an annual basis. Maps of various annual concentration metrics can be produced. It has also been used for forecasting ozone under future UK and European-wide emission scenarios for Defra ozone policy and assessing future compliance with EU target values. It can also model NO and NO_2 at ground-level and is currently being adapted for modelling of secondary organic aerosols. It was used in the 'Regional' part of the evaluation exercise.OSRM is driven by meteorological data from the NAME model and uses the STOCHEM chemical mechanism and it can also be configured to use the CRI (Common Reactive Intermediate) mechanism related to the MCM (Master Chemical Mechanism).

Pros

At the present time it is the only operational model in the Defra portfolio which has delivered modelled results for the whole UK for ozone on every day of the year (as opposed to ozone episodes).It can be run for a large number of sites in a relatively short time. OSRM has a pedigree in delivery of policy relevant outputs. It can cover urban and rural scales and has been used to assess the effect of precursor reduction scenarios in the UK and Europe on ozone concentrations across the UK, including, uniquely, in urban areas.

Cons

Unlike the 'community models' it is a stand-alone model and development pathway. It is a relatively simple model in that it is essentially a Lagrangian moving box albeit with comprehensive chemistry.The vertical layering requires an empirical boundary post-processor scheme to deal with surface interactions. It is not designed to be able to distinguish between different source categories, and it has not taken part in the EU regional model comparisons such as EuroDelta comparison[14].

[14]van Loon, M., R. Vautard, M. Schaap, R. Bergström, B. Bessagnet, J. Brandt, P.J.H. Builtjes, J.H. Christensen, K. Cuvelier, A. Graf, J.E. Jonson, M. Krol, J. Langner, P. Roberts, L. Rouil, R. Stern, L. Tarrasón, P. Thunis, E. Vignati, L. White, and P. Wind, *Evaluation of long-term ozone*

There is limited peer reviewed output on performance, and the model includesa number of simple treatments driven by expediency against full models e.g. wet deposition (missing), dry deposition and biogenic emissions, single boundary layer box.

5.10 FRAME

FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange) is a straight line Lagrangian trajectory model, developed and used at the Centre for Ecology and Hydrology and funded by Defra from the mid-1990s onwards. Originally a model that treats atmospheric processes in a vertical column of air along 24 wind directions (i.e. 15° resolution), the model has since been improved to a resolution of 1°. The columns are well resolved vertically, with 33 layers of variable depth incorporating the vertical mixing of emissions. The frequency of wind in each direction is taken from a wind rose homogenised for the UK and Ireland. FRAME was used in both 'Regional' and 'Deposition' parts of the evaluation exercise.

FRAME has been a mainstay long range transport model for UK policy on acidification for the last decade and has contributed to an understanding of the effects of emissions reduction on deposition of all the important pollutants, including ammonia. It features strongly, for example, in the NEGTAP report of 2001, which remains a definitive statement on the atmospheric processes that influence deposition of sulphur and nitrogen compounds and their effect on ecosystems. In addition, outputs from FRAME are used to estimate current and future deposition rates of acid and nitrogen on the UK's Natura 2000 sites and thereby define where critical loads are exceeded. This information forms the basis of the information found on the Air Pollution Information System (APIS[15]), the principal source of information on this subject for individual habitat sites.

Pros

The Lagrangian approach is well suited for the purpose of long range transport modelling and evaluating the effects of emission control policies, because of its simplicity and low computational costs, which are particularly important in an Integrated Assessment Modelling regime. Arguably, it has provided very cost effective policy guidance over its lifetime. Not surprisingly, given its primary purpose, it includes some good physics on dry deposition processes and the relevant algorithms have been successively improved. Wet deposition is represented by a simple scavenging process, although it should be noted that orographic enhancement process is simulated for high latitude and high rainfall locations. FRAME is able to provide a reasonable simulation of annual average concentrations of the key pollutants across the country and consequently wet and dry deposition rates. In comparison with estimated national budgets, FRAME has performed well for oxidised nitrogen and sulphur deposition, but nitric acid is known to be strongly underestimated. This latter point was also shown in the intercomparison exercise, which illustrated a good performance from FRAME in respect of annual average concentrations of SO_2, NO_x and NH_3.

The model provides good spatial resolution in outputs, with results available on a 5km x 5km grid, or alternatively at 1km x 1km. Run times are short on the CEH computing system, with 20 minutes cited for the lower resolution output.

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simulations from seven regional air quality models and their ensemble average. Atmos. Environ., 2007. **41**: p. 2083-2097.

[15] http://www.apis.ac.uk/

Evaluation of the merits of FRAME for policy making is not simply a matter of the model's performance, but it must also be recognised that the model developers (and users) represent a considerable body of expertise and knowledge relating to long range transport of pollution and the effects of acidification and eutrophication.

Cons

The virtues of simplicity and relatively low computational costs can also be seen as a disadvantage at a time when the available computing power is increasing and are considerably greater than when FRAME was developed initially. The straight line trajectory approach can only be taken so far and the angular resolution within FRAME has been improved to its logical limit. After a period of 15 years or more, the scope for significant improvement in the performance of FRAME is probably limited.

FRAME has some known characteristics where performance is not as good as desired. Specifically, these are the treatment of plume rise for large point sources of SO_2 (where the plume is assumed to remain always in the boundary layer), the underestimation of concentrations and deposition rates in remote areas and, conversely, the overestimation in source areas. The spatial variation in accuracy is partly the result of how imported pollution is represented in the model , as this affects northern and western areas of the UK, relative to south east England. The simple, uniform wind rose also represents a limitation, as does the constant drizzle assumption for rainfall. However, some of these shortcomings (e.g. the plume rise problem) have been corrected following a 'peer review' by the Joint Environmental Programme of the electricity generating industry.

5.11 HARM

The Hull Acid Rain Model (HARM) has, like FRAME, been developed with funding from Defra and is also a Lagrangian trajectory model. Its origins lie in the Harwell Trajectory Model, developed in the 1980s with first version of HARM (HARM 7) being used in 1993. The current version of HARM (HARM 12.2) and the model has been relatively little changed since 2004.

The model uses straight line trajectories, based on a single wind rose and produces outputs on a 10 km x 10 km grid for annual average concentrations of acidic species of gases and aerosols and also calculates wet and dry deposition rates. HARM has also been adapted to model the dispersion of primary PM_{10}. Vertical resolution in the 800 m mixing layer is provided by three layers. It was used in the 'Deposition' part of the evaluation exercise.

Pros

HARM shares many of the virtues of FRAME, in that it provides a very cost effective basis for emission reduction policy formulation. Run times are short and the model can be run on a PC.

Cons

The model was shown not to perform as well as some of the other models in the intercomparison exercise for many of the pollutant species considered. In particular, it was conspicuously less successful for annual average concentrations of NO_2, NH_3, HNO_3, $NH_4^+$and NSS SO_4, where it consistently underpredicted concentrations, relative to observations. SO_2 concentrations appeared to be overpredicted, but this could be an artefact of some of the measurements, as noted elsewhere. Nitrate concentrations are simulated reasonably well. All these characteristics are broadly consistent with the model's previously reported performance against measurements, (e.g. Metcalfe *et al* 2005), allowing for some differences in the magnitudes of deviation.

The model has less resolution than FRAME, both in the spatial representation of the outputs and in the vertical representation of the mixing layer.

5.12 AQUM

AQUM (Air Quality Unified Model) is a limited area implementation of the full UK Meteorological Office(MO) Unified Model (MetUM) which uses the UKCA (UK Chemistry and Aerosol) chemistry scheme. The MetUM is a system capable of modelling regions from limited areas to global scales and with timescales from less than hourly to decadal climate scales. AQUM used MO meteorological data and a regional air quality mechanism enhanced from STOCHEM. It seems to be a well set-up model with modern chemistry and physics, and was used in the 'Regional' part of the evaluation exercise.

Pros

AQUM has the potential for seamless modelling of air quality from relatively short time scales – up to the few decades characteristic of air quality policy problems, to many-decade climatic timescales with high quality meteorological input. It produces hourly and daily (and 15-minute concentrations for SO_2) values. It is able to deal with the multiple spatial scales for linking long-range transport and regional impact, including intercontinental transport. AQUM is capable of being run in 'climate mode' either globally (150km resolution) or regionally (50km) to provide advice on the impact of climate change.

Cons

Unlike the other large Eulerian models under consideration, AQUM is not a community model but is run internally in the UK Meteorological Office. At this stage it seems very much like a development model and this is reflected in some of the data coming out of the model comparison. There are no peer reviewed publications of the AQUM itself, nor is there a significant user-base. The model needs more evaluation in terms of checking agreement with observations and development to enable air quality outcomes and scenarios to be assessed.

5.13 PTM

The Photochemical Trajectory model is a Lagrangian trajectory model that has been extensively used to assess regional ozone formation in short term (days) ozone episodes. The PTM model is used to quantify the contribution made by each VOC species and each VOC source category to the long-range transboundary formation and transport of ozone across North West Europe. The PTM model can also be used to characterise the ability of each VOC species to form secondary organic aerosol under transboundary conditions.It is configured to be give output at 15:00hrseach day for Harwell for most years and Aston Hill, Auchencorth Moss, Glazebury, High Muffles and Rochester for 2008 from a large number of 4-day back trajectories (up to 1000) from the MetUM. It can run with a range of detailed chemical mechanisms. PTM is essentially used as a scenario chemistry model. In the 'Regional' part of the intercomparison exercise it was output for Harwell at 15.00 hrs.

Pros

PTM has an extensive track-record in policy and science evaluation of VOCs and particles/regional ozone formation in episode conditions. It contains several very detailed chemical schemes and is the only European model able to evaluate the role of a wide range of VOCs and their sources in ozone formation.

Cons

PTM is designed to investigate the performance of chemical schemes; in this sense it is a specialist model. It is limited in terms of spatial and temporal coverage, currently being configured to produce ozone concentrations at 1500hrs at Harwell. It delivers no direct policy needs in terms of reporting against Directive/Protocol requirements; the policy role is focussed on the response of peak ozone concentrations to precursor emission controls.

6. Synthesis and evaluation of models and policy needs

6.1 Introduction

This section will discuss the models which are potentially capable of delivering the policy needs described in Section 2. It will comment on the fitness for purpose of all the models for delivering Defra's policy needs and, where changes to the present deployment of models are recommended, it will outline a methodology for managing that change.

6.2 Policy drivers 2.1 and 2.2-assessing compliance with the Air Quality Directive now and in the future.

6.2.1 Discussion

At present only one model is being used to provide this service (PCM) although in principle there is no reason why other models (EMEP, CMAQ, NAME, AQUM) could not also be used, given sufficient preparation. Apart from the empirical treatment of roadsides in PCM, only ADMS (and the ERG/King's Toolkit in London) at present offers a credible alternative for the crucial calculation of roadside/kerbside concentrations where Defra's major policy issues currently arise, although at present no attempt has been made to model these locations across the whole UK as PCM does. If EMEP, CMAQ, NAME and AQUM were considered as alternatives to PCM, then at present they could only deliver urban background concentrations so that a separate roadside calculation would be necessary. One could envisage nesting ADMS within the models to potentially provide the requirements of the Directive.

It is worth exploring reasons why Defra might seek alternatives to PCM to deliver these requirements. One characteristic of PCM as noted above is the fact that it is calibrated each year to measured data. This is helpful in the task of 'filling in' the gaps between monitoring sites to provide estimates of current concentrations over the UK. Indeed, some form of adjustment or 'assimilation' of the results of a deterministic model would probably be needed to align modelled results to measurements for reporting of the 'current' situation. However, for the important process of assessing policy options to achieve future compliance or to attain other policy targets, reliance on a calibrated model must be considered scientifically questionable and open to criticism, as it introduces potentially significant uncertainties into future projections. The use of deterministic models with full (or as full as practicable) descriptions of physics and chemistry would add confidence to the future projections. Moreover, the structure of PCM is modular in the sense that it seeks to adopt results from other (usually deterministic) models to obtain the 'rules' by which emission changes affect concentration changes. In future as the understanding of different processes improves, potentially more such modules or external sources of information would have to be added to PCM (the treatment of secondary inorganic and organic aerosols is an example). This approach was appropriate some years ago when PCM was developed as the larger deterministic models required large amounts of computer time. However this is no longer the case. These external sources of information are now models which are potentially usable in their own right, and it therefore seems sensible to use these deterministic models directly, not least because they could provide all the required information in single runs rather than conflating a series of calculations from different sources. Not only would this remove unnecessary complexity-which will only increase with time-but will also provide significantly greater confidence in the outputs and projections. There is therefore an overwhelming argument in the view of the AQMRSG for taking steps to move to the use of deterministic models for delivering these, and the other, policy drivers.

We would recommend the use of a deterministic model to supplement PCM in the short term (over the next 3 years say). In the longer term, should the performance of such a model prove acceptable, moving to sole use of this model would put the scientific basis of policy assessment on a firmer footing, give more confidence in the outputs and make the Defra research more robust against possible criticism .

There are several models capable in principle of fulfilling this task. Of those which participated in the first phase of the model intercomparison programme, there were four which could be potential candidates, namely EMEP4UK, CMAQ, NAME and the AQUM. Of these, all but NAME are Eulerian models and it is relevant here to note that the earlier review of ozone models carried out by Monks, Blake and Borrell weighed carefully the pros and cons of an Eulerian versus a Lagrangian approach and that, while both had their merits, they concluded that Eulerian models were, on balance, to be favoured. Moreover, they recommended that Defra should consider moving its ozone modelling capability to an Eulerian basis. (At that time the main ozone model for policy use was the Lagrangian model OSRM with some input from PTM). The reasons for this choice were that Eulerian models provide a better representation of 3-dimensional meteorological fields. Wind speeds and directions at the surface are often quite different from values at higher levels. Moreover, Eulerian models are easier to 'nest' and hence can cover a wide range of spatial scales, and they are more appropriate for a 'multi-pollutant' approach. Apart from the foregoing, Lagrangian models have an inherent difficulty in representing pollutants that are not directly released and assigning values to the 'background' pollutants. Earlier developments of chemical models in the UK used a Lagrangian approach largely because such models allowed the use of large chemical schemes. However, with the advances in computer power and the more rigorous testing of reduced schemes, this difference is now much less marked.

Although the earlier review focussed only on ozone models, the reasons for preferring Eulerian to Lagrangian models apply equally well to other pollutants and hence the present review endorses the earlier conclusion and recommends moving to an Eulerian framework for future modelling in Defra.

The Monks et al review also noted that the USEPA concluded that their future modelling should be based on an Eulerian approach, and that the EMEP model used in the CLRTAP process was changed from an earlier Lagrangian model to an Eulerian model over ten years ago. This argues against further use of the NAME model in the Defra research portfolio.

Of the other three models, the AQUM (section 5.11 above) is to some extent a model which is still under development and evaluation and as such is not as operationally advanced as the other two models, although this might change in the future. AQUM is a scientifically credible and powerful model and it performed similarly to the other Eulerian models in the intercomparison exercise. What sets the other models apart however is their open source code and their extensive user community and development resources. In assessing what could be our suggested direction for Defra, we are therefore persuaded more by the advantages of other models as discussed below, than through having any specific criticisms of AQUM. However, AQUM has the potential to be a powerful model (albeit still requiring a roadside module to be nested within it).

There are therefore two other models which are credible supplements or alternatives to PCM, namely the EMEP and CMAQ model systems. Both are large Eulerian models which treat atmospheric transport, dispersion and chemistry explicitly in a relatively sophisticated way. Both too are 'open source' models, freely available, with continuing scientific development by expert teams. Both also have extensive user communities although the size of the community for the CMAQ system probably far outweighs that for the EMEP model. By joining such communities Defra would be joining a pool of expertise and development, a large part of which operates in a policy/regulatory context.

The EMEP 'suite' of models – the unified EMEP model and EMEP4UK – are capable of providing a UK coverage at a resolution of a few kilometres (EMEP4UK in particular) and performed credibly well in the intercomparison exercises carried out so far. In terms of value for money however, using this/these models to the exclusion of all others may not be the most effective way forward. Along with all the other 42 Parties to the UNECE CLRTAP EMEP Protocol, the UK through Defra already contributes financially to the development and operation of the EMEP models and to European scale emission inventories, a mandatory requirement which cost the UK £201.5k in a total EMEP budget of some £1.468 million in 2010[16]. There is thus a considerable amount of gearing in this expenditure and it therefore seems sensible to 'bank' this and allow the development and use of the EMEP model to continue, with a relatively small expenditure on the EMEP4UK version funded from the ALE research programme, separate from the contribution to the EMEP budget.

The other credible model is CMAQ, which is broadly similar in concept to the EMEP model in that it is an Eulerian model incorporating relatively sophisticated descriptions of atmospheric physics and chemistry. CMAQ also performed overall relatively well in the evaluation exercises to date, although there were differences largely due to the different meteorological processing and the different boundary conditions employed. Indeed, overall it was difficult to separate the quality of the performance of the EMEP and CMAQ models in that exercise.

As well as the models already discussed there are others which are possible candidates, one example being the French model CHIMERE. While this is an open source model and has many of the same features as CMAQ and EMEP, it does not at present have the same user community or resources for development. Accordingly we considered that use of this model should not be pursued further at this stage. However, it will be important to engage in intercomparison exercises with users of CHIMERE in future as Defra's work progresses. Another open source model used by a number of groups in Europe is FLEXPART. This is a Lagrangian model similar in concept to NAME (it too has its origins in the Chernobyl accident). While this is fairly widely used and is freely available, it suffers at present at least by not including anything beyond very simple chemistry and loss processes. We therefore suggest that future activities in Defra's research portfolio concentrate on CMAQ and the EMEP models in the short to medium term.

The recent model intercomparison exercise has been useful in evaluating aspects of the performance of various models in reproducing observed concentrations. There is more that can be done to evaluate model performance, and at the present time Defra is considering a second phase of this intercomparison/evaluation, involving for example comparisons of model performance for emission reduction scenarios. Moreover, if models are being considered to run in parallel with PCM, or even ultimately to replace it, then it is essential that some initial trials of candidate models are carried out in the near future to assess the prospects for delivering this capability, in particular the

[16] The EMEP budget is used for activities other than the modelling of acidification, eutrophication, ozone and PM and the development of emission inventories. It also covers monitoring and QA/QC activities, modelling of Persistent Organic Pollutants and Heavy Metals, and Integrated Assessment Modelling.

Directive requirements – estimating concentrations across the UK at an appropriate spatial resolution, estimating roadside concentrations, identifying exceedences of Limit and Target Values etc. ***We would therefore recommend a programme of evaluation be carried out by Defra, firstly developing and configuring these models (EMEP4UK and CMAQ) to facilitate delivery of Directive requirements, and secondly running alongside PCM over a period of, say, up to three years in order to evaluate performance. This would include the appropriate nesting of a roadside model within the larger scale models. At the end of such a programme, Defra would be in a position to make firm choices over future model deployment based on a much firmer evidence base. Given the potential of AQUM to deliver these requirements, it would be prudent to invite the Meteorological Office to contribute AQUM runs to this evaluation programme.***

In considering organisations which might be involved in this exercise, Defra should consider some wider aspects than simply the models themselves. The modelling capacity of potential contractors will need to be considered, along with other desirable attributes of contractors. Along with the aforementioned capacity, other attributes to be considered should be those of an organisations competence, capability and continuity, an appreciation of the whole air quality management process involving monitoring, modelling and emission inventories, as well as an appreciation of Defra's policy needs and priorities. All of these criteria are important in securing a continuing delivery of modelling for long-term policy needs. We suggest that Defra should be looking to cultivate a UK modelling capability that has the resources to deliver, as required, which has sufficient expertise to understand what the models are doing and which is engaged with the subject enough to participate in wider model development. The AQMRSG feels that it is important that Defra provides real support for this activity as the main customer for studies involving these models and modelling groups, and hence with a strong interest in preserving a capable community.

In setting up such a programme, Defra should consider the field of potential contractors – noting that this could potentially extend beyond those groups who participated in the recent intercomparison exercise.

Experience with the model intercomparison exercise carried out recently has shown that such activities generate a large amount of complex information and also raise issues that need considerable discussion among practitioners and evaluation by disinterested independent experts. An important and fundamental aspect of these evaluation exercises as the recent one has already shown, is that they can potentially provide an excellent forum for the peer-review of models, quantification of their performance - a means of benchmarking their performance - and providing a quality assurance function through open and inclusive debate. ***We recommend that in order to obtain the maximum benefit from such a programme, the work be carried out in the framework of a continuing discussion forum of the modelling practitioners, overseen by a small group of independent experts who could act as arbiters as necessary.***

Such a programme would not only provide much more information than is currently available to allow Defra to take important strategic decisions over its modelling capability, at a more detailed level it would also allow an investigation of the relative merits of the various options for implementation of CMAQ, which were shown to be very important in the recent evaluation exercise. Through such an exercise in a discussion forum of the kind recommended, by developing such benchmarks and performance information, Defra would be in a much better position to evaluate potential new contractors and to ensure longer-term continuity in modelling performance. Such a forum would also help to cultivate and sustain a modelling community in the UK which was tuned and sensitive to Defra's continuing needs for air quality modelling.

It should also be noted that the organisations which participated in the model intercomparison exercise are not necessarily the only ones capable of running CMAQ and delivering Defra's needs and this should be taken into account if Defra pursue the option of exploring further the performance of the CMAQ modelling system.

The Directives deal with a range of pollutants including those like PM_{10}, $PM_{2.5}$ and ozone which are formed wholly or partly from processes occurring on regional scales. Using models such as EMEP/EMEP4UK and CMAQ would have the benefit of treating virtually all[17] of the relevant pollutants, time- and space-scales consistently in one model, without the need for a series of separate modules from different sources. This would also to some extent 'future proof' the modelling capability in that these models already embody physical and chemical processes which could in the future potentially provide estimates of species or metrics not currently regulated. Implementing either EMEP/EMEP4UK or CMAQ would allow nesting of the UK within a larger European and potentially global grid – a key feature for assessing the future behaviour of PM_{10} and $PM_{2.5}$ against the Limit Values and exposure-reduction criteria, and also for assessing future ozone concentrations, as discussed further in Section 6.4 below.

Given the argument discussed above regarding the non-discretionary nature of the funding for the EMEP model through the CRLTAP EMEP Protocol, it is worth addressing the need for anything more within the Defra/ALE programme, or whether one could envisage simply running the EMEP4UK model alongside PCM to assess delivery of the Directive requirements. There are two main reasons why another model should also be considered in this context. Firstly, there are inherent uncertainties in modelling and in the first phase of evaluating the performance of a model like EMEP against PCM and the Directive requirements, as recommended above, it is essential that as much information as practicable is obtained on model performance. The best way of doing this in this timeframe would be to run two alternative models. Secondly, the development of both EMEP and CMAQ models is outside the direct control of Defra and its research programme. Some influence over the future development of the EMEP modelling suite is possible but this is relatively weak. A three year programme (or thereabouts) running both models would allow time to assess the prospects for the continued future development of both models to allow a more informed choice at the end of the evaluation period.

The other component of this policy driver is the assessment of future air quality and legal compliance given prescribed or potential policies and emission scenarios. Assessing the future compliance with Directive requirements could also be carried out with the models described above and part of the parallel running of PCM, EMEP and CMAQ should address their relative performance in this task. Concluding which model is 'best' in predictive mode in this context is difficult of course, but at the very least measures of the spread of projections, and responses to emission changes can be evaluated and compared across models.

6.2.2 Uncertainty

[17] Modelling of roadsides would need a separate nested model such as ADMS, and the modelling of heavy metals, and possibly PAHs in some situations, would probably need single-source modelling of 'hot-spots' which could also potentially be carried out with ADMS.

The treatment of uncertainty is important in making projections of future compliance and policy evaluation. The air quality sub-group of the Science Advisory Council recommended that more needed to be done to address uncertainty more explicitly, and that protocols should be drawn up to evaluate and quantify uncertainty. The FAIRMODE group in the EU is also producing guidance on uncertainty, largely within the context of the EU Air Quality Directive. It will be important for Defra to ensure that this group produces guidance and interpretation of modelling uncertainty that is robust. Defra should have regard to developments more generally on modelling within FAIRMODE as this will influence the view the Commission takes on the UK's air quality modelling with regard to the Directive. ***The Air Quality Modelling Review Steering Group fully endorses this recommendation of the SAC and recommends that evaluation and quantification of modelling uncertainty be put into effect in the comparison/evaluation exercise with PCM, EMEP and CMAQ. Even before this exercise were to start, uncertainties in PCM should be quantified and built into policy assessments (examples would be the inclusion of the uncertainty in the empirical relationship between road-link emissions and concentrations in the roadside module of PCM and assessments of uncertainties in emissions obtained from 'backcasting' PCM).The Group recommends that Defra ensure that work on uncertainty within the FAIRMODE group is sound and robust, and that the Department takes into account wider developments of modelling guidance in its future work.***

The SAC sub-group, however, did not distinguish between the uncertainties inherent in models and those inherent in the input data (for example, it referred to the inability of PCM to predict the effects of the economic downturn as emission reductions could not be predicted in advance – this is not an uncertainty in the models but in the input data). Such uncertainties in inputs – particularly in emission forecasts – are crucially important and need to be addressed separately from evaluating uncertainties in the models themselves. It is outside the scope of this review to explore this point in detail.

6.2.3 Roadside concentrations

Concentrations of some pollutants at roadside/kerbside/street canyon locations currently pose the biggest problem for policy in ALE. These are the main areas of non-compliance now and in the medium-term future. Pollutant concentrations in these locations are dominated by fine spatial and temporal scales of turbulence, by building effects and by the influence of rapid turbulent diffusion on chemistry, so that they are also the most difficult locations to model with confidence. In contrast with other areas of lower importance for the assessment of compliance, roadsides and canyons have received a relatively small share of scientific attention in the UK in recent years. Current approaches are either empirical/statistical as in PCM (with consequent uncertainties over future projections) or they approximate the physics and chemistry in relatively simple ways as in ADMS. While any one individual location could be studied in great detail, using Computational Fluid Dynamics or Large Eddy Simulations and including simple chemistry, a workable modelling approach to roadsides that fulfilled Defra's needs would need to be relatively simple given the large number of such locations in the UK. Consequently, it may not be possible to avoid a degree of empiricism or approximation in such models but an objective evaluation of possible approaches has not to date been carried out. Apart from the models already mentioned above, the OSPM model developed in Denmark is in use in Europe in large area policy contexts. ***We therefore recommend that an evaluation of roadside/kerbside models be carried out over the next year with the aim of choosing a preferred deterministic model for use in conjunction with larger scale Eulerian models. This should include other models such as OSPM in use in Europe.***

6.3 Policy driver 2.3 – Health impacts and public information

The models discussed in the previous section should all be capable of providing estimates of the impacts on health across the UK, given the inherent assumption that exposure can be represented by concentration fields fixed in space. At the present time the most important pollutants from a health perspective are $PM_{2.5}$, PM_{10} and ozone as these are the pollutants for which credible relationships exist between concentrations and mortality and morbidity health outcomes. For PM, the current assumption is that the concentration-response relationships are linear and go through the origin so that the annual total health outcome is simply proportional to the annual mean concentration. This simplifies matters so that a simple model such as PCM is capable of estimating health effects on this basis. So too of course would the more complex deterministic models discussed in Section 6.1, but the averaging times needed for estimating health impacts will potentially vary from pollutant to pollutant. Indeed, for ozone other metrics such as the daily maximum 8-hourly average are currently used so that the flexibility afforded by the deterministic models discussed above would be an important consideration for performing health assessments for pollutants other than PM, and particularly when looking to the future in order to be able to handle other pollutants and different averaging times.

One important development relevant to air quality modelling in the assessment of health impacts is the likely improvement in exposure assessment methods, beyond the straightforward assumption that exposures can be represented by a concentration field fixed in space but variable in time. Developments in the research community in the UK and in the US are already under way to move closer to the ideal representation of exposure as a 'Lagrangian' time series of concentrations that moves with the individual through a temporally varying concentration field. These developments place more of a burden on the collection of time-activity data rather than requiring significant developments in air quality modelling per se, and the models identified for further evaluation are capable of being used in improved exposure assessments such as these.

6.4 Policy driver 2.4 - Ecosystem impacts

Currently, the assessment of critical loads is done using the FRAME model run at CEH Edinburgh. This as noted in section 5 is a relatively simple model and as such might be considered to be open to criticism. This has indeed occurred in the recent past where comparisons with results from CMAQ run by the electricity generating industry revealed flaws in FRAME. However, these have now been rectified and, as a consequence, FRAME is considerably more robust than originally. The question therefore arises as to whether or not there is any reason to stop using FRAME for the assessment of ecosystem impacts. The alternative would be to use either CMAQ or EMEP4UK, which was originally commissioned because of the perceived inability of the full EMEP model, as it then existed, to account adequately for orographically enhanced wet deposition in upland UK.

Given the strategy recommended in section 6.1 above for delivery of the Air Quality Directive requirements, which involves running EMEP4UK alongside CMAQ in an extended evaluation exercise, ***we would recommend the retention of FRAME pending further evaluation of the ability of EMEP4UK and/or CMAQ to assess ecosystem impacts and the exceedence of critical loads and levels.***

6.5 Policy driver 2.5 - Climate change impacts and 'Future proofing'

6.5.1 Discussion

In order to assess adequately the impacts of climate change on air quality – due to the changes in temperature and other parameters as well as the effects of policies to address climate change – models which explicitly incorporate physical and chemical processes have a clear advantage in terms of engendering confidence in the results compared with empirical or statistical models. Changes in the temperature regime for example will affect wind fields via tracks of mid-latitude depressions, thermally induced turbulence and boundary layer height, atmospheric stability frequencies including the frequency of inversions, and the rates of chemical reactions, all of which would be difficult to handle with confidence in overly simplified models.

Moreover, an important component of 'future proofing' is the increasingly global nature of air pollution. This is now clear, particularly in the case of ozone where recent assessments from the Royal Society, from the CLRTAP Task Force on Hemispheric Transport (HTAP) and UNEP have all shown that 'local' ozone levels in a given country can be very strongly influenced by emissions on a global scale. Indeed, the report of the Convention on Long Range Transboundary Air Pollution Task Force on the Hemispheric Transport of Air Pollution[18]went further, noting that intercontinental transport of ozone and its precursors could lead to exceedences of health and ecosystem damage thresholds and standards in North America and Europe.

The ability to nest a 'UK' model in a wider global model, or at least to use a global model to provide boundary conditions, is therefore essential for an adequate description of atmospheric physics and chemistry processes operating at a global scale as they affect the UK. The deterministic models recommended for further investigation above would meet this requirement, and at present STOCHEM, a global model, is used to provide boundary conditions and also to explore global scale air quality issues. Ideally a review of global models would be helpful here – there are a number of such models in use around the world, including some which incorporate climate impacts – but such a review is outside the scope of this report. Nonetheless, STOCHEM is in use already and has participated in multiple model comparisons and performed reasonably well. In the interim therefore, we would recommend that the use of STOCHEM continues, and that the performance of STOCHEM continue to be evaluated against other global/intercontinental models such as those used at the UK Meteorological Office and via fora such as the CLRTAP Task Force on Hemispheric Transport of Air Pollution. This continuing comparison could be carried out under the overview of the modelling discussion forum referred to in section 6.1 above, which could also continue to explore other models and methods for providing boundary conditions to UK scale models.

When assessing impacts of climate changes on pollutant levels in the UK, there are other factors as important, and possibly more so, as the choice of model. As global temperatures change, the balance between biogenic and manmade, or man-influenced emissions will change, and this could have significant implications for the estimation of concentrations of ozone and of secondary organic aerosols. It was clear from the evaluation exercise that different biogenic emission inventories were in use by different groups, and as a first step ***we recommend an evaluation of biogenic emission inventories. This could be done separately from the modelling evaluation programme described above.***

[18] Available at http://www.htap.org/

Furthermore, it has recently become clear that for some pollutants such as NO_x, current emission inventories are inaccurate[19] and this has been reflected in the model intercomparison exercise where the normalised mean bias (NMB) at kerbside sites for all models was negative (implying the models underpredict the observed concentrations) for both NO_x and NO_2 and all values of the NMB were outside the range considered 'acceptable' by the Defra Model Intercomparison Protocol. The NMB (and the absolute mean bias) decreased in the sequence kerbside-roadside-urban-suburban. Future improvements in Defra's modelling expertise will be wasted unless action is taken to ensure that emission estimates are as accurate as possible. This would require a combination of modelling and analysis of monitoring data along with scrutiny of the emission inventories to probe both the trends in emissions but also the accuracy of their absolute values. This latter test is a further argument for a deterministic as opposed to statistical/calibrated model. ***We recommend that a programme be established to investigate on a regular basis the accuracy of the National Atmospheric Emission Inventory in terms of absolute values and trends over time. This activity is fundamentally important to modelling and should continue for as long as modelling is needed in the ALE/Defra research programme.***

In terms of assessing the impacts of policies to address climate change the models recommended for further investigation could all be used. Again the international/global dimension is important as policies to address climate change will be at the least regional (EU-wide) and potentially global.

There is another dimension to 'future proofing' and that concerns the possibility of Defra/ALE needing to address pollutants or metrics which are not currently regulated. Possible candidates include some measure of primary particles emitted by combustion – either elemental carbon (EC)/black carbon (BC) or some measure of ultrafine particles. The requirements for modelling will be determined to a great extent by the form which legislation takes. Regulating EC/BC on a mass basis should not prove difficult for models of the form considered here. The more difficult aspect will be to generate adequate emission inventories. If ultrafine particles are regulated on a number basis, then a quite new approach to modelling will be required whereby the dynamics of particle behaviour will need to be simulated along with normal turbulent dispersion. Such considerations are already embodied in recent versions of CMAQ, although the performance of these modules would need to be evaluated rigorously before being used in assessments of legal compliance, were policy and regulation to evolve in this direction. Nonetheless, these features of CMAQ illustrate one of the benefits of an open source model which is supported by a considerable amount of resource for development.

The future direction of air quality regulation will be determined to a large extent by the review of the Air Quality Directive in 2013 and the anticipated revision of the NECD in the same year. In the short term it is likely that Defra will be best placed to assess the prospects for new pollutants, or new metrics entering legislation, depending on how open and inclusive are the discussions around the review of the Directives. Therefore, ***we recommend that Defra consider as early as practicable the implications for modelling in future regulation and policy as discussions evolve between now and the Directive reviews in 2013, referring back to expert opinion as appropriate.***

[19] Carslaw, D., Beevers S., Westmoreland E., Williams M.L., Tate J., Murrels, T., Stedman J., Li Y., Grice S., Kent, A., and Tsagatakis, I. (2011). Trends in NO_x and NO_2 emissions and ambient measurements in the UK. Version: 3rd March 2011. Draft for Comment. Available at http://uk-air.defra.gov.uk/reports/cat05/1103041401_110303_Draft_NOx_NO2_trends_report.pdf

A more general consideration regarding 'future proofing' of the modelling capability concerns the continuing improvement in computer power, particularly in relation to the use of the sophisticated Eulerian models such as EMEP and CMAQ. In some implementations of these at the present time, runs can take of the order of weeks (in fairness some implementations are faster) and may argue against the use of such models in a rapid response context. This need not be the case currently (note the use of CMAQ by AEA for daily forecasting) and is only likely to improve in the future. In practice, computer power will continue to improve and while the rate of improvement is difficult to quantify precisely, it is likely that run times will improve dramatically in the short to medium term. With this in mind, it could very well appear a grave mistake in a few years' time *not* to invest in the use of such models now, *purely on the grounds of run times*[20].

6.5.2 A UK capability in Integrated Assessment Modelling (IAM)

During the lead-up to the negotiations on the second Sulphur Protocol and the Gothenburg Protocols in the LRTAP Convention in the 1990s, Defra commissioned a UK-scale IAM capability to 'shadow' the work done at a European scale by IIASA who carried out the IAM and cost-benefit analysis for CLRTAP and also for the NECD. The process of IAM involves many runs of an atmospheric module(s) in a linear-programming system to generate optimal emission reduction strategies which in general are designed to achieve a given level of environmental benefit at the minimum cost. At present simple models are used in the UKIAM – FRAME and BRUTAL (which covers roadside and urban levels). The AQMRSG could find no problems with the use of these models in the IAM context. Moreover, with a review of the CLRTAP Gothenburg Protocol already under way, and the prospect of a revision to the NECD imminent, it would be prudent to retain this capability in the medium term, at least until these instruments are agreed. ***We therefore recommend continued use of BRUTAL and also of FRAME (in addition to possible further use in ecosystem impact assessment as discussed in Section 6.4 above) in the UK Integrated Assessment Model.***

6.6 Models for which no further evaluation is recommended.

The foregoing discussion has set out a strategy for future modelling of air quality in the Defra/ALE research programme, and has discussed which models are recommended for further evaluation. This leaves some models which fall outside these recommendations and for which therefore, the AQMRSG recommends no further evaluation or development. These models are all regional or mesoscale models and, while they are still to some degree credible and potentially useful models, they are largely being overtaken by more comprehensive and more sophisticated models which can –at least in principle – deliver the same and more in one model given the advances in computer power, which will only improve further with time. Examples are OSRM and PTM which have delivered useful-and unique-scenario assessments of ozone control policies. However, the larger models like EMEP, CMAQ and potentially AQUM are capable of doing the same and more in terms of other pollutants as well as ozone. NAME too has been useful in past applications, and is still in use in emergency response applications, but for wider air quality policy assessments it too is potentially overtaken by the other models, not least the Meteorological Office's own AQUM Eulerian model.

[20] The danger in the increasing improvement of computer power of course is that the atmospheric physics and chemistry processes in the models develop in complexity with the results that run times remain static. Were this to occur – and it may not as computer power increases - the improvements in the science would clearly need to be balanced against run times in future implementations.

Older models such as HARM and TRACK-ADMS are also now overly simplistic given the development of computer power and are no longer recommended for use in the research programme.

7. Conclusions and recommendations for model use and future development of models and techniques

A summary of the conclusions and recommendations of the review is given in this section, including recommendations for which models should be considered further for evaluation and which models are no longer required, or should not be considered for inclusion, in the research programme.

The overall strategy of this review has been to formulate a vision that will put the modelling programme on as firm a scientific basis as practicable while still delivering Defra's policy needs. This has been possible without requiring the use or evaluation of overly complex models which are impracticable to run in a policy assessment context. Increases in computer power – which will only improve with time – mean that models which embody quite sophisticated physics and chemistry can now be run relatively quickly – certainly quickly enough to satisfy policy needs. It is therefore an appropriate time to evaluate such models for use by Defra/ALE. The recent model evaluation exercise has been very helpful in demonstrating this capability, but it has not been extensive or detailed enough to allow firm, final choices to be made without more detailed evaluation of the models' performance in the specific policy-relevant roles which Defra need them to perform. The recommendations in this review are designed to address this problem.

The assessment of the structure of the models, supplemented by the evaluation exercise, and a consideration of the institutions which run them, has allowed the AQMSRG to draw up a short-list of candidate models which could potentially fulfil Defra's needs and also supplement or ultimately replace the simpler models which are currently used. These models – the EMEP/EMEP4UK model and the CMAQ modelling system - are both open source models, freely available and have continuing scientific development taking place to improve them as new knowledge becomes available. This is clearly attractive. As noted above, by adopting such a system Defra would be joining a large user community which contributes to model development. There is thus the prospect of a considerable amount of 'gearing' in any Defra spend by going down these routes.

It also however carries a degree of risk, not least in that were Defra to rely totally on such models, it could be at the mercy of funding cuts and the withdrawal of support from organisations over which it has little or no control. However, the likelihood of this happening is, in our judgement, small in the next 5-10 years, not least because too many organisations and legal processes (particularly in the case of CMAQ) are reliant on them. In the view of the AQMRSG the substantial benefits to be gained from the use of one or other, or both, of these models far outweighs the risks involved.

However, it would be prudent to take steps to plan for an eventuality such as the removal of developmental support for these models. Taking into account institutional capability when commissioning future deployment of these models is therefore important, and it would be prudent to involve at least one organisation with a strong research base to develop expertise in the basic structure of the models so that were support to be scaled down or even withdrawn, use of the models need not be compromised. Looking to the longer term, it is important that the UK maintains a body of expertise in atmospheric modelling, the needs for which go wider than the air quality research programme in Defra. This falls squarely within the remit of the research councils and ***we recommend that Defra begin discussion with NERC, and EPSRC if appropriate, to ensure the provision of atmospheric modelling skills in the UK in the future.***

It should also be noted here that the short-list of models for further consideration and evaluation excludes some models currently included in the ALE/Defra research programme, or models which have been used in the past, or which could potentially have been considered for use in the future. The consequence of this is that the AQMRSG considers that their use be discontinued in the ALE research programme. However, should work with these models continue through other sources of funding, as is very likely at least for some models, developments and findings from the use of these models could be reported to the discussion group/forum on modelling suggested in Recommendation 2 below. This would maintain contact with as wide a science base as feasible for Defra but would also provide one potential source of peer review for Defra's in-house modelling.

In summary, the recommendations of the AQMRSG are presented below, with an indication of the duration. (Short term means within approximately one year, medium within ~3 years, long term within ~3-10 years.)

1. ***We would recommend the use of a deterministic model to supplement PCM in the medium term (over the next 3 years say). In the longer term, should the performance of such a model prove acceptable, moving to sole use of this model would put the scientific basis of policy assessment on a firmer footing. An earlier review of ozone modelling for Defra recommended that future modelling should move to an Eulerian framework. While both Eulerian and Lagrangian approaches have their merits, our overall judgement, as with the earlier review, is that an Eulerian framework would be a preferable way forward for Defra's modelling needs. (Medium to long term)***

2. ***We recommend a programme of evaluation, firstly developing and configuring candidate models (EMEP4UK and CMAQ) to facilitate delivery of Defra's policy needs including requirements of the Air Quality Directive, and secondly running alongside PCM over a period of, say, three years in order to assess performance. This would include the appropriate nesting of a roadside model within the larger scale models. We would also recommend the retention of FRAME pending further evaluation of the ability of EMEP4UK and/or CMAQ to assess ecosystem impacts and the exceedence of critical loads and levels. At the end of such a programme, Defra would be in a position to make firm choices over future model deployment based on a much firmer evidence base. Given the potential of AQUM to deliver these requirements it would be prudent to invite the Meteorological Office to contribute AQUM runs to this evaluation programme. (Medium to long term)***

3. ***We recommend that, in order to obtain the maximum benefit from such a programme, the work could be carried out in the framework of a continuing discussion forum of modelling practitioners, overseen by a small group of independent experts who could act as arbiters as necessary. Such a forum could in addition, if required, provide advice to Defra on broader modelling-related issues (Long term)***

4. ***The Air Quality Modelling Review Steering Group fully endorses the recommendation of the SAC regarding uncertainty and recommends that evaluation and quantification of modelling uncertainty be put into effect in the comparison/evaluation exercise with PCM, EMEP and CMAQ. Even before such an exercise, uncertainties in PCM should be quantified and built into policy assessments (examples would be the inclusion of the uncertainty in the empirical relationship between road-link emissions and concentrations in the roadside module of PCM***

and assessments of uncertainties in emissions obtained from 'backcasting' PCM).The discussion forum mentioned in Recommendation 3 could provide a source of expert advice on this issue. (Short to Medium term)

5. ***We recommend that Defra ensures that work on uncertainty in the FAIRMODE group within the EU is sound and robust, and that the Department takes into account wider developments of modelling guidance within FAIRMODE in its future work.***

6. ***We recommend that an evaluation of roadside/kerbside models be carried out over the next year with the aim of assessing the performance of deterministic models which might be nested within larger scale Eulerian models. This should include ADMS, the ERG 'Toolkit' and other models such as OSPM in use in Europe. (Short term)***

7. ***We recommend an evaluation of biogenic emission inventories. These largely relate to natural sources and are a source of large uncertainty in modelling of future ozone and the secondary organic component of PM. The balance between man-made and natural sources is already important and will become more so in the future and quantifying this balance is thus of great importance for policy. This evaluation could in principle be done separately from the modelling evaluation programme described above. (Short to medium term)***

8. ***Arguably the largest area of uncertainty in model results is the input emission inventory. Any evaluation of model performance and capability will be constrained by the quality of the emission data. We recommend that a programme be established to investigate on a regular basis the accuracy of the National Atmospheric Emission Inventory in terms of absolute values and trends over time. This activity is fundamentally important to modelling and should continue for as long as modelling is needed in the ALE/Defra research programme.***

9. ***We recommend that Defra consider as early as practicable the implications for modelling in future regulation and policy as discussions evolve between now and the Directive reviews in 2013, referring back to expert opinion as appropriate. (Short to medium term)***

10. ***Were Defra to continue with a UK IAM capability, then we recommend continued use of BRUTAL and also of FRAME (in addition to possible further use in ecosystem impact assessment as discussed in Section 6.4 above) in such a system.***

11. ***We recommend that Defra continue discussions with NERC, and EPSRC if appropriate, to ensure the provision of atmospheric modelling skills in the UK in the future.***

A summary of the recommendations for each model is shown in Table 2 below.

Table 2 Summary of recommendations for individual models

Name of Model	Full Model Name	Conclusions
ADMS	Atmospheric Dispersion Modelling Software	Suitable for further development/use by Defra
CMAQ[21]	Community Multiscale Air Quality	Suitable for further development/use by Defra
DO_3SE	Deposition of Ozone and Stomatal Exchange	Continue, nested in CMAQ
EMEP4UK	European Monitoring and Evaluation Programme UK Model	Suitable for further development/use by Defra
EMEP MSC-W	European Monitoring and Evaluation Programme MSC-W Model	Suitable for further development/use by Defra
ERG-Toolkit	Environmental Research Group-London Air Pollution Toolkit	Suitable for further development/use by Defra
FRAME	Fine Resolution Atmospheric Multi-pollutant Exchange	Suitable for further development/use by Defra
HARM	Hull Acid Rain Model	Not recommended for further development by Defra
NAME	Numerical Atmospheric-dispersion Modelling Environment	Not recommended for further development by Defra
OSRM	Ozone Source Receptor Model	Not recommended for further development by Defra
PCM	Pollution Climate Mapping Model	Suitable for further development/use by Defra
PTM	Photochemical Trajectory Model	Not recommended for further development by Defra
TRACK-ADMS	Lagrangian model + Atmospheric Dispersion Modelling Software	Not recommended for further development by Defra
AQUM	Air Quality Unified Model (Meteorological Office) Model	Suitable for further evaluation
STOCHEM	Global 3-D Lagrangian chemistry-transport model	Continue, with external evaluation
UKIAM	UK Integrated Assessment Model	Continue; includes BRUTAL and FRAME, which AQMRSG recommends retaining in UKIAM

[21] Note that there are several potential implementations of the CMAQ system in different institutions, some of which have nested different roadside models within CMAQ. At the time of writing, Defra are formulating a programme involving several organisations who run CMAQ.

8. Acknowledgement.

The Group would like to acknowledge the work carried out by the participants in the model intercomparison exercise and the comprehensive and clear analyses of the results of that exercise carried out by Dr. David Carslaw, King's College London. This analysis has informed much of this report. The Group is also grateful to Andrew Smith, on a work placement at Defra for preparing the descriptive information on the models.

Air Quality Modelling Review Steering Group

17 March 2011

APPENDIX 1. POLICY DRIVERS FOR AIR QUALITY MODELS

The following Table sets out the policy drivers for air quality models as stated by Defra in the initial terms of reference for the current review.

Policy Driver/evidence need		Requirements:
1. Directive Compliance (2008/50/EC, 2004/107/EC)	National scale modelling capacity – base case and projection s	Flexible approach, to national models - limited options, more than one would be preferable so that comparisons could be made and risks from being reliant on one source reduced. Others: Hourly NO_2, Daily PM instead of annual mean proxy. Natural sources on a daily basis.
	Site specific modelling of hotspots	
	Point source modelling	
	Urban scale modelling	
	Regional scale modelling	
	Ozone modelling capacity	
2. Assessment of Policy Options including revision of the Air Quality Strategy	Measures testing – screening and testing of local, regional and national measures.	Flexible inputs/outputs. Multi source – airports, shipping, vehicles, point sources etc., emissions inventories etc. Quantification of soft and hard measures. Multi pollutant –gases, particulates, deposition, heavy metals etc.
3. Health protection impact assessment	Population exposure	Multi pollutant, cumulative impacts, spatial flexibility, projections and baseline data.
4. Ecosystems impact assessment	Deposition modelling to estimate and forecast exceedences of critical loads	Base and projections, scenario testing.
	Concentration data	
	Screening and detailed modelling capacity	
	Ozone flux	
5. Modelling to account for impact of climate change and of climate change measures.	Measures testing, Scenario analysis, projections, application and links to urban, regional and national scale modelling.	Flexible to new input data, account for new meteorology, new chemical composition of atmosphere, new deposition values. Modelling of measures in place to mitigate climate change.
6. Negotiations for new Directives - potentially new metrics required.	Unknown yet. Need to be flexible.	

APPENDIX 2: GLOSSARY OF MODEL NAMES:

Model Acronym	Model Name
ADMS	Atmospheric Dispersion Modelling Software
AQUM	Air Quality Unified Model
CHIMERE	French chemistry-transport model
CMAQ	Community Multi-scale Air Quality
DO_3SE	Deposition of Ozone and Stomatal Exchange Model
ELMO model	Edinburgh-Lancaster Model for Ozone
EMEP4UK	European Monitoring and Evaluation Programme UK Model
ERG Toolkit	Environmental Research Group (King's College, London) tool kit for urban modelling
FRAME	Fine Resolution Atmospheric Multi-pollutant Exchange
FRAME- HM	Fine Resolution Atmospheric Multi-pollutant Exchange –HM
HARM model	Hull Acid Rain Model
NAME	The UK Meteorological Office (UKMO) atmospheric pollution dispersion model
OSPM	Operational street pollution model – developed originally in Denmark.
OSRM	Ozone Source Receptor Model
PCM	Pollution Climate Mapping
PTM	Photochemical Trajectory Model
STOCHEM	UK Meteorological Office Global Lagrangian Model
TRACK	Lagrangian Model
UKIAM	UK Integrated Assessment Model, incorporates FRAME and BRUTAL.

APPENDIX 3: LIST OF MODELS & ORGANISATIONS INCLUDED IN PHASE 1 OF THE MODEL INTERCOMPARISON EXERCISE:

Name of Model	Full Model Name	Name of Organisation Representing the Model
ADMS	Atmospheric Dispersion Modelling Software	CERC
AQUM	United Kingdom Chemistry and Aerosols Model	The Met Office
BRUTAL	Background Road and Urban Transport model of Air quality Limit values)	Imperial College London
CMAQ	Community Multi-Scale Air Quality Model	University of Hertfordshire
		AEA
		E-ON
		Kings College, London
		RWE npower
DO_3SE	Deposition of Ozone and Stomatal Exchange	University of York
EMEP4UK	European Monitoring and Evaluation Programme UK Model	CEH-Edinburgh/University of Edinburgh
EMEP MSC-W	European Monitoring and Evaluation Programme MSC-W Model	Norwegian Meteorological Inst.
ERG-Toolkit	Environmental Research Group-London Air Pollution Toolkit	Kings College, London
FRAME	Fine Resolution Atmospheric Multi-pollutant Exchange	CEH-Edinburgh
HARM	Hull Acid Rain Model	University of Nottingham
NAME	Nuclear Accident ModEl	The Met Office
OSRM	Ozone Source Receptor Model	AEA
PCM	Pollution Climate Mapping Model	AEA
PTM	Photochemical Trajectory Model	RdScientific
TRACK-ADMS	Lagrangian model + Atmospheric Dispersion Modelling Software	AEA
UKIAM	UK Integrated Assessment Model	Imperial College London

APPENDIX 4: Model implementation choices by users of the CMAQ system in Phase 1 of the model intercomparison exercise.

Model Option	JEP	UoH	AEA	KCL
CMAQ version	4.7.1	4.6 (deposition) 4.7.1 (regional)	4.7	4.6
Emissions module	SMOKE 2.5	Developed in house, incl. SMOKE 2.4 (deposition) Developed in house, incl. SMOKE 2.6 (regional)	Bespoke model	SMOKE 2.4
Source emissions (non UK)	EMEP (inc. shipping)	EMEP (deposition) TNO (regional)	EMEP 2006 (inc. shipping)	EMEP 2005
Source emissions (UK)	NAEI	NAEI (deposition) TNO (regional)	NAEI 2006	NAEI 2005, 2006
Source emissions (other)	Hourly power station from JEP	NA (deposition) Fires from FMI (regional)	-	Point source emissions from E-PRTR
Biogenic emissions	GEIA	Developed in house, using CLC2000 dataset for the land cover (deposition) Using MEGAN (regional)	Biogenic Potential Inventory	Estimated after Guenther *et al* (1995) and Sanderson (2002)
Horizontal grid (mesh size and cells)	45 km, 78 x 73 15 km, 96 x 75 5 km, 195 x 130	45 km, 76x76 15 km, 93x108 5 km, 177x219 (deposition) 18 km, 260x240 (regional)	48 km, 59 x 79 12 km, 78 x 98	81 km, 47 x 44 27 km, 39 x 39 9 km, 66 x 108 3 km, 72 x 72 1 km, 62 x 51
Vertical	15 layers, total depth = 15 km	15 levels (deposition) 34 levels (regional)	26 layers, with 12 below 800 m	23 layers
Meteorological model	WRF 3.0.1	WRF 3.0.1.1 (deposition) WRF 3.2.1 (regional) Using analysis nudging Initial and lateral boundary conditions from ECMWF	WRF 3.0, with initial and boundary conditions from ECWMF	WRF 3.1 with NCEP for initial and boundary conditions
Boundary	2003 STOCHEM (CREMO)	STOCHEM (deposition) GEMS (regional)	STOCHEM	
Dry deposition	Pleim-Xui scheme	'resistance analogue' concept	Pleim-Xiu scheme	'resistance' analogue, after Pleim *et al* (2001)
Wet deposition	Sub grid and resolved cloud model with scavenging and washout	Derived from RADM	Derived from RADM	Derived from RADM (Chang *et al* 1987)
Chemical mechanism	CB 05	CB 05	CB 05	CB 05