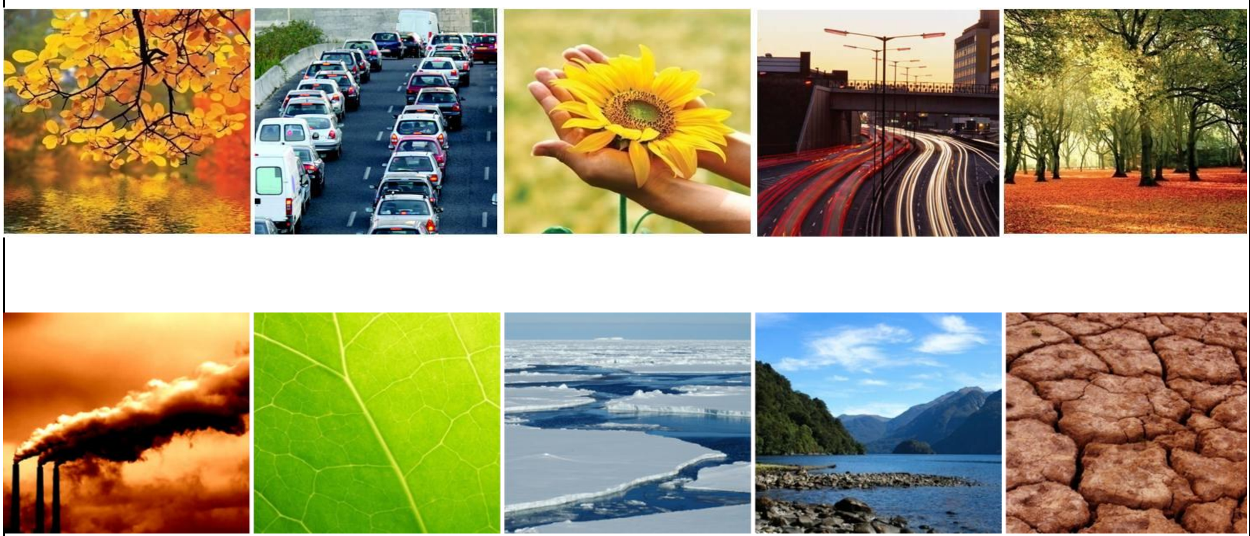
CMAQ Development for UK National Modelling

Phase 1 Project Summary Report



Report for Department for Environment, Food and Rural Affairs

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Approved By:

Tim Murrells

Date:

23 October 2012

Signed:

Executive summary

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

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

The project involves the development and evaluation of the CMAQ model optimised in a way that will best meet Defra's future modelling and assessment needs. The overall work programme is being delivered in two phases. The first phase which started in October 2011 has consisted of 4 main objectives to meet the overall aims of the project:

- **Demonstration of CMAQ for Defra's Evidence Needs**
- **Development and evaluation of a provisional CMAQ-UK Configuration**
- **Collaboration with the CMAQ community**
- **Recommendations for further optimisation and development**

This report brings together the main conclusions from the first phase of the project. It summarises the work described in two additional, more detailed technical reports from the project covering an assessment of CMAQ as a model for meeting Defra's different evidence needs and the development of an initial optimised CMAQ-UK configuration.

The report summarises feedback from a stakeholder review of the work in Phase 1. This included feedback from model developers at the USEPA and the wider air quality modelling community in the UK and stems from stakeholder workshops held in June/July 2012.

A summary of the choices made for the key parameters and set-ups in the initial proposed CMAQ-UK configuration is provided. This version will serve as a benchmark for further developments of the model.

The report sets out recommendations for further development and demonstration of CMAQ-UK under Phase 2 of the project to be carried out between September 2012 and August 2014.

We recommend a targeted improvement programme centred around optimising the meteorology, emissions and boundary condition input data.

We also recommend a programme to demonstrate the policy application of CMAQ-UK to assess compliance with regulatory obligations for $PM_{2.5}$ in 2020, but including gas species and deposition to demonstrate the strengths of using a "one atmosphere" model.

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1 Introduction

The United States Environmental Protection Authority (USEPA) sponsored the development of the Community Multi-scale Air Quality (CMAQ) modelling system. CMAQ was designed to approach air quality as a whole by including state-of-the-science capabilities for modelling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation. Several groups of modellers have used CMAQ to model air quality in the UK.

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

There were three main tasks of Phase 1 of the project undertaken during 2011/2012. These were:

- Assessing the potential role to be played by CMAQ in addressing Defra's main evidence needs associated with different air quality policy drivers
- Developing an initial optimised configuration of CMAQ to meet Defra's evidence needs
- Collaboration with the wider CMAQ community

This report is a summary of the work carried out in Phase 1 and should be read in conjunction with two more detailed technical reports covering the main work areas (Beevers et al., 2012[1] and Abbott et al, 2012[2]). A further report was prepared on the testing of CMAQ v5.0[3].

This report brings together the main conclusions from Phase 1 of the project and summarises feedback from stakeholders with an interest in the project including other users of CMAQ in the UK and the model developers at the USEPA. The report sets out recommendations for further demonstration, optimisation and development under Phase 2 of the project to be carried out between September 2012 and August 2014.

[1] Beevers S, Kitwiroon N, Beddows A, Carslaw, D, Good N, Chemel C, Xavier Francis, Sokhi R, Derwent D, Fraser A, Murrells T, and Venfield H. (2012). CMAQ Development for UK National Modelling - Development of a provisional CMAQ-UK Configuration. Version: 23rd October 2012
[2] Abbott, J, Fraser A, Beevers S, Kitwiroon, N, Good, N, Chemel, C and Sokhi, R (2012). CMAQ Development for UK National Modelling – Demonstration of CMAQ for Defra's Evidence Needs
[3] University of Hertfordshire, report on CMAQ v5.0 testing, August 2012

2 Demonstration of CMAQ for Defra's evidence needs

2.1 Summary of Defra's evidence needs

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

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

CMAQ was designed to approach air quality as a whole by including state-of-the-science capabilities for modelling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.

Work in Phase 1 considered how CMAQ has been implemented by various UK modelling groups and the potential application of two developments of CMAQ: the Decoupled Direct Method (DDM) and the Adjoint Model. The work considered the potential application of CMAQ for each of the main policy drivers in turn. Further details are given in the main project report for this task by Abbott et al (2012)[4]. The report outlines the developments required to make the CMAQ model more useful for the purpose of meeting Defra's evidence needs.

The main limitations of CMAQ in the context of Defra's evidence needs were viewed as:

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

Considering each of these limitations, the developments required to make the CMAQ model more useful for the purpose of meeting Defra's evidence needs are outlined in the following recommendations.

2.2 Recommendations for Defra's evidence needs

Modelling uncertainty

Existing models are generally considered too uncertain for modelling regional and rural background concentrations for compliance assessment against the Air Quality Directives. Estimates of these rural and regional background concentrations are made by interpolation of measurement data. Recent model intercomparison studies have not shown that CMAQ

[4] Abbott, J, Fraser A, Beevers S, Kitwiroon, N, Good, N, Chemel, C and Sokhi, R (2012). CMAQ Development for UK National Modelling – Demonstration of CMAQ for Defra's Evidence Needs

performs significantly better than other models when compared with measurement data. The performance of CMAQ will be optimised during the course of this project and we expect that this will improve the performance of the model. Nevertheless, it remains to be seen whether CMAQ alone can provide adequate estimates of regional and rural background concentrations for compliance assessment.

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

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

Low spatial resolution

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

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

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

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

The empirical model currently used for compliance assessment modelling in the *UK Ambient Air Quality Assessment* programme (the Pollution Climate Mapping model, PCM) uses a kernel approach to modelling area sources in which the contribution to concentrations in each 1 km square is calculated as the sum of the product of the emission from each surrounding square and a kernel dispersion factor. The calculation is carried out for the whole country within a Geographical Information System. Some alterations would be required to the GIS algorithms in order to ensure that the kernel of dispersion factors matched the boundaries imposed by the CMAQ grid. The PCM uses a dispersion model to determine the contribution from point sources: some changes will be required to ensure that the dispersion model domain corresponds to the boundaries imposed by the CMAQ grid.

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

Multiple scenarios

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

2.2.1 Phase 2 work programme

Table 2.1 lists the main elements of work required to develop CMAQ applications in the UK to meet Defra’s main evidence needs. The table lists the main tasks and subtasks and suggests the earliest start and end dates that these could be achieved given sufficient resources.

Table 2.1: List of tasks to develop CMAQ to meet Defra's evidence needs

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

3 Development of an initial provisional CMAQ-UK Configuration

3.1 CMAQ-UK Configuration

A key aspect of Phase 1 of the project involved investigating and producing recommendations for ***a provisional*** CMAQ model configuration specifically for Defra's UK modelling needs. This was achieved by sharing knowledge and experiences and input data and assumptions across the project partners.

The aim was to develop an initial, and provisional, optimised configuration of CMAQ to meet Defra's evidence needs. The approach taken was to understand the different configurations used by each group underlying the 2006 simulations submitted as part of the second phase of the Defra Regional Model Intercomparison Exercise (MIE 2) and to understand how a particular set-up leads to different results, particularly for simulations of ground-level ozone (O_3) and nitrogen dioxide (NO_2) which were the focus of the Regional MIE.

All chemical transport models like CMAQ should be capable of predicting ozone concentrations reasonably accurately. Modelling Particulate Matter (PM) concentrations and PM species is a lot more complex as it has many more primary sources and formation through several secondary processes. PM was looked at briefly but the results were 'highly variable' and unsuitable to be used when comparing three existing model simulations using different meteorology, emissions and grid resolutions. By focusing on O_3 and NO_2 the knowledge gained related to meteorology and emission sensitivity and the set-ups used by the three groups was more revealing. PM will be studied more in the second phase of the project (Phase 2) when the sensitivity studies will be based on the optimised configuration (CMAQ-UK) developed here in Phase 1. Deposition modelling was not considered on Phase 1 for similar reasons but will be included in Phase 2.

The seven different work areas investigated were:

- The operational evaluation of Weather Research Forecasting (WRF) model
- Air Quality Sensitivity
- Emissions Sources and Processing
- Chemical boundary conditions and an integrated modelling approach
- Chemical schemes
- CMAQ Operational details
- Model benchmarking protocol

Full details of this work are given in the main project report for this task by Beevers et al (2012)[5]. This report considers the findings from these work areas, recommends a provisional configuration for CMAQ-UK and conclusions of the work and suggested work areas for Phase 2 of the project.

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

3.1.1 Choice of WRF-setup

A dashboard approach has been developed to enable quick and easy comparison of model performance against observations. The dashboard fits onto a single A4 page and provides hourly scatter plots, hour of day, day of week and seasonal averages. They also include conditional quantile plots, model evaluation statistics and a summary of WRF and CMAQ set-up details. Using the dashboard approach, comparison has been made between model vs. model and models vs. observations using results from Defra's Model Intercomparison Exercise (MIE2). The observations have been based upon both surface Meteorological Office (MO) stations throughout the UK and observations vertically from the MO - global radiosonde data.

All three of the WRF model variants tested agreed well with measurements of wind speed, temperature, relative humidity and wind direction from up to 165 surface measurement stations in the UK. With the exception of wind direction the performance of the models was ranked using the Index of agreement (IOA) statistic, with the assumption that this statistics is best able to capture the overall model performance. Whilst predicting wind direction is important it is difficult to summarise into IOA and has only been presented graphically.

Using 2006 annual average hourly comparisons at the MIE2 sites: for wind speed, KCL's WRF configuration showed the best overall performance (KCL (0.70), UH (0.60), AEA (0.56)), similarly for temperature (KCL (0.85), UH (0.84), AEA (0.81)) and for relative humidity (KCL (0.67), UH (0.63), AEA (0.6)). Spatially across the UK, for wind speed and relative humidity, the KCL WRF configuration also displayed the largest number of sites with an IOA statistic of >=0.71 (41%), with all models performing similarly for temperature.

The model predictions of vertical wind speed and temperature were in good agreement with observations across a range of seasonal, annual and hour of day statistics. The models also performed reasonably well during the O_3 event of 19th July 2006, where there was a recorded temperature of 36.5 ^{o}C. Model vs. model comparisons were very similar overall, although KCL's WRF configuration provided the closest agreement with observations. As a consequence the KCL WRF set-up has been provisionally recommended for CMAQ-UK, details of which include:

- The NOAH land surface and MYNN pbl schemes have proven to capture the diurnal variations of temperature and wind speed when compared with surface meteorological observations and are recommended in the WRF-UK model. Land use details taken from MODIS are also recommended ;
- Nudging plays an important role in to the accuracy of the WRF meteorological fields. Hence, the option of grid nudging is recommended as it performs consistently well for wind speed, wind direction, temperature and relative humidity;
- Both ECMWF and GFS provide equally good initial/boundary conditions. However, ECMWF is recommended if there is no restrictions on its use;
- Using horizontal grid downscaling ratios of either 1:3 or 1:5 produce similar results and therefore a horizontal grid resolution of 10km (UK) downscaled from 50km (Europe) is recommended. 2-way nesting produced better results for 50km grid predictions and its use is also recommended.;
- Using 23 vertical layers produces comparable results to those of UH (34 layers) as well as with observations and this is recommended.
- The most recent version of WRF should be used (v3.4);

- Other physics settings within WRF remain untested, however the Dudhia/RRTM radiation scheme, Kain-Fritsch cumulus scheme, and WSM6 microphysics scheme are recommended through published literature (OTC, 2010)[6];

3.1.2 Choice of chemical mechanism within CMAQ

An examination has been completed of four candidate chemical mechanisms (CBM-4, CB-05, SAPRC-99 and SAPRC-07) as to their suitability for use in the proposed CMAQ set-up for the evaluation and assessment of policy options by Defra. In each case, the mechanisms have been ranked in terms of the closeness they achieve to the results for O_3 generated with the 'gold standard' CRI mechanism linked to the Master Chemical Mechanism (MCM), an internationally-recognised mechanism, describing the detailed processes involved in the formation of ozone from the degradation of a large number of emitted precursor VOCs.

With respect to ozone predictions there was little to choose between any of the four candidate mechanisms and any of them would likely give satisfactory performance in CMAQ. Over a range of eight criteria selected for their relevance to ozone air quality policy formulation, the ranking of the four candidate mechanisms placed the CB-05 mechanism as being the closest to the CRI mechanism, followed by the SAPRC-99, CBM-4 and SAPRC-07 mechanisms.

The mechanism performance was only tested for O_3 to reflect the performance of the gas phase photochemical reactions involved in the breakdown of precursor VOCs and NO_x. This testing is a necessary precursor to further testing of mechanism performance for the photochemical production of secondary organic aerosols involved in PM formation.

3.1.3 Choice of emissions inventory within CMAQ

An examination of the alternative emissions sources used by the project partners was a difficult task in that, despite advances in emissions inventory analysis in recent years, a method by which emissions inventories can be compared directly and the 'correct' inventory identified does not exist. As a consequence, our analysis limited itself to model *vs.* model comparisons and to decisions based upon expert judgement, best practise and availability of data.

- At a UK scale the National Atmospheric Emissions Inventory (NAEI) and at European scale, the EMEP emissions inventories were chosen.
- The decisions regarding horizontal grid resolution for CMAQ followed these choices, with the European domain specified at a 50km x 50 km resolution and downscaling to 10km x 10km in the UK.
- Publically available and supported emissions processing methods were favoured over in-house emissions processing, which lead to the choice of SMOKE (v 3.4) as the preferred method for CMAQ, combined with MEGAN as the choice for biogenic emissions.
- The European database EPRTR, which provides a comprehensive list of point sources, was chosen to supplement those data held in the UK by the NAEI.
- Incorporation of plume rise (calculated by SMOKE) should also be undertaken for all future CMAQ-UK runs.
- Use of emissions based temporal profiles produced by University of Stuttgart and TNO and used in the AQMEII model evaluation project were chosen, as well as, London based road traffic emissions profiles.

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[6] OTC, 2010. Sensitivity Testing of WRF Physics Parameterizations for Meteorological Modeling and Protocol in Support of Regional SIP Air Quality Modeling in the OTR

- Whilst Biomass burning is a potentially important emissions source of both NO_X and PM, a decision regarding its use through MACC or through FMI (or other) emissions estimates is still a point of debate.
- The speciation of VOC emissions for use with CMAQ-UK was chosen to be that of the model developed as part of the UK Environment Agency CREMO project to be run with different chemical schemes.

3.1.4 Choice of boundary conditions within CMAQ

Three modelling systems have been used by the project partners to generate chemical boundary conditions: the UK Met Office's STOCHEM model, ECMWF's GEMS system and the GEOS-Chem global model. These were assessed in terms of:

- the accuracy of the concentrations produced
- the number of species they represent
- their suitability specifically for Defra's envisaged CMAQ applications
- the practicality of applying the different approaches.

Both the GEMS/MACC and Geos-Chem boundary conditions have strengths and weaknesses, GEMS does not perform as well for high percentile boundary conditions for O_3 as GEOS-Chem but GEOS-Chem boundary conditions are produced through additional model runs, with associated time and expertise overheads. In contrast STOCHEM has the weakness of only providing gas phase species and has not been considered further. At the time of writing the relative merits of both GEMS and GEOS-Chem have not been fully resolved and hence both are recommended for use as boundary conditions for the CMAQ-UK model.

3.1.5 Proposed CMAQ-UK Configuration

The following Table 3.1 summarises the proposed CMAQ-UK configuration emerging from the study.

3.2 CMAQ-UK Recommendations

Within the scope of Phase 1 it was impossible to resolve all of the associated issues surrounding WRF-CMAQ model use. Consequently there are numerous other avenues of research that could/should be undertaken. As part of our work a number of notable issues arose which merit further investigation:

- The use of Geos-Chem boundary conditions has improved CMAQ predictive capabilities for high O_3 concentrations although the benefits are less apparent for average O_3, NO_X and NO_2. Hence further analysis of the benefits of the predictive capability of boundary conditions from Geos-Chem, MACCII and other sources such as EMEP should be considered.

- The comparisons between WRF outputs and meteorological measurements were limited to those that were readily available in the UK. However, it is recognised that there are a number of additional and important comparisons that could be undertaken using WRF. In Phase 2 of the project it is hoped that further comparison can be made between WRF and UK Met. Office models, and with parameters that are important to dispersion but are not routinely measured. These include boundary layer height (h), atmospheric stability (h/ Monin Obukhov length), Turbulent Kinetic Energy, ustar and wstar. Further

Table 3.1: Proposed initial CMAQ-UK configuration

WRF		CMAQ	
Parameter	**Assumption**	**Parameter**	**Assumption**
WRF version	3.4	CMAQ version	4.7.1
Grid resolution	50km (Europe) to 10km (UK)	Grid resolution	50km (Europe) to 10km (UK)
Spatial projection	ETRS89-LCC	Spatial projection	ETRS89-LCC
Vertical layers	23 (7 below 1km)	Vertical layers	23 (7 below 1km)
IC/BC	EMWF/GFS	IC/BC	GEOS-Chem, GEMS/MACC2
Nudging	Grid (T, WS, Q)	Chemical Scheme	CB 05
PBL	MYNN 2.5 level TKE	Temporal emissions profiles	FMI-TNO-KCL
Microphysics	WSM 3-class simple ice	Point source details	Include plume rise calculations
Cumulus	Kain-Fritsch	Emissions processor	Smoke (v3.X)
Radiation (SW/LW)	RRTM/Dudhia	Area anthropogenic emissions	EMEP/NAEI
Land surface	NOAH	Point anthropogenic emissions	NAEI/EPRTR
Land use	WPS IGPB MODIS 30s+20m	Natural emissions	MEGAN/Biomass burning
Surface layer	MYNN		

consideration is required in the use of the surface layer scheme ACM2 in WRF. Finally, whilst the number of layers within the preferred WRF model was 23, alternative configurations should also be considered in Phase 2 of the project.

- The comparisons between WRF outputs and meteorological measurements were limited to those that were readily available in the UK. However, it is recognised that there are a number of additional and important comparisons that could be undertaken using WRF. In Phase 2 of the project it is hoped that further comparison can be made between WRF and UK Met. Office models, and with parameters that are important to dispersion but are not routinely measured. These include boundary layer height (h), atmospheric stability (h/ Monin Obukhov length), Turbulent Kinetic Energy, ustar and wstar. Further consideration will also be given to the use of the surface layer scheme ACM2 in WRF. Finally, whilst the number of layers within the preferred WRF model was 23, alternative configurations should also be considered in Phase 2 of the project.

- Predicting high O_3 concentrations relies on correctly predicting O_3 dry deposition. The role that the UK DO3SE model can play in improving CMAQ's high O_3 predictions should be considered.

- Defra's evidence needs point towards the development of urban modelling for issues such as human exposure and to meet EU limit values. This is worthy of further investigation by consortium members as part of future work.

- Improvements in prediction of PM should be considered using the soon to be released version of the CMAQ v5.0.1.

- Interpretation of the CMAQ results is difficult, because of the potential for larger errors in the emissions inventories and WRF predictions, and so it is suggested that to improve our understanding of the causes of model differences, CMAQ-UK is used as the base for model sensitivity testing of the different methods developed by the group in Phase 2.

4 Stakeholder feedback

An important part of Phase 1 of the project involved interaction with stakeholders with an interest in the project including other users of CMAQ in the UK and the model developers at the USEPA. This interaction culminated in meetings held with representatives of the USEPA, Defra and Environment Agency on 11th June and with the wider UK modelling community on the 3rd July 2012.

The aims of both meetings were to present and discuss the findings of the work at the time and to solicit feedback from stakeholders.

4.1 UK-USEPA meeting

A meeting was held at Defra on 11th June 2012, including representatives from Defra, Environment Agency, USEPA and project partners. The structure and aims of the project were discussed and the main conclusions reached at the time including some preliminary ideas for Phase 2 were discussed. The meeting also gave a chance for the EPA to provide an update on the development and application of CMAQ to air quality policy in the U.S.

This meeting preceded a wider UK-US meeting on air quality research held at the University of Lancaster between 11th-14th June.

Items of interest

- ST Rao Director of the modelling division at EPA is retiring – Rohit Mathur is taking over as Acting Director until the appointment committee makes its decision on a replacement. ST will continue as Editor-in-Chief for the *Journal of the Air &Waste Management Association*.

- From the extensive evaluation they have done, the USEPA have confidences that CMAQ is a suitable tool for regional policy applications. It may not be replicating absolute concentration values but it is a robust tool for policy “what if” scenario studies. There is still the need to interpret uncertainty and reduce some variability.

- The USA accepts that the diagnostic evaluation of CMAQ in the USA is reliable and can be used with confidence for scenario analysis. Where the model is required to match measurements, e.g. for the daily forecast, bias correction is used.

- CMAQv 5.0 includes a range of new features. Some improvements will be an advantage to Defra, other features relate to coupled modelling (WRF-CMAQ). These will take longer to evaluate and are less relevant to this project.

- Bi-directional NH_3 exchange will be an advantage. It is built on USA land maps and work would be required to fully activate this feature in the UK/Europe.

- The next planned version release will be in 2015; the main focus of this will be “coupled modelling” to maintain consistency between WRF and CMAQ.

- The TSSA methodology is under redevelopment and will be released in the future but it is unlikely to be called TSSA.

- Shawn Roselle's presentation on Source Apportionment at the meeting in Lancaster outlined the USEPA plans in this area. This includes a simplified user interface, chemical mechanism flexibility, compatibility with new CMAQ science processes and flexibility for defining regional sources. Implementation details will be given at the 2012 CMAQ meeting. The species to track in ambient concentrations, dry/wet depositions:
  - OC and EC
  - PM ammonium + precursor NH_3
  - PM sulphate + precursor SO_2
  - PM nitrate + precursor NO_x

- Guidance was given on the options used for WRF at the USEPA, this included options that reduce the southerly bias in the wind direction.

Actions following on from the meeting:

- More information on the methods used in the PCM (Pollution Climate Model) model used by the UK for EU Air Quality Directive compliance assessment modelling was sent to Vlad Isakov along with a link to the latest description. http://uk-air.Defra.gov.uk/reports/cat09/1204301513_AQD2010mapsrep_master_v0.pdf

- There are on-going discussions with Rob Gilliam related to the wind direction bias experienced using WRF in the USA. A similar bias is found using WRF for the UK daily air quality forecast.

- Following discussions with Rohit Mathur, Daiwen Kang has sent a copy of the bias correction code used by the USEPA for the air quality forecast.

4.2 UK Stakeholders meeting

Early draft copies of the two main project reports were circulated to a wide group of UK air quality modellers who were invited to provide feedback and attend a stakeholder meeting in London on 3rd July 2012.

The meeting was attended by: Martin Williams (KCL), David Carruthers (CERC), David Carslaw (KCL), John Stedman (AEA), Bernard Fisher (Environment Agency) , Noel Nelson (Met Office), Stephen Griffiths (E-ON), Paul Sutton (RWE npower), Christina Hood (CERC), Roger Barrowcliffe (RWDI), Samantha Lawrence (Defra), Michelle Cain (Defra), Emily Connolly (Defra), Sarah Honour (Defra), Tim Murrells (AEA), Andrea Fraser (AEA), Charles Chemel (UH), Ranjeet Sokhi (UH), Xavier Vazhappilly Francis (UH), Sean Beevers (KCL), Nutthida Kitwiroon (KCL) and Dick Derwent (rdscientific).

Some of the issues discussed are summarised below and where relevant comments received were taken into account in the final versions of the reports.

CMAQ-UK feedback

In addition to specific feedback, the group identified the need to verify what CMAQ is suitable for using now and verify its use. This should include the 'one atmosphere' features including PM and deposition (Critical Load). CMAQ is designed as a regional model, so are we pushing it too far to look at urban NO_2 (local) compliance?

Meteorology

The criteria used to establish the best options (e.g boundary layer scheme) in WRF for CMAQ-UK needs to be outlined. It is essential to look at the key met variables for air pollution dispersion.

Drawing from these discussions, the following recommendations have been included in the proposed Phase 2 plan:

- **WRF (surface layer/pbl) -** Boundary layer height (h), atmospheric stability (h/LMO) (LMO is the Monin Obukhov length), and a variable related to turbulence (TKE - for local scheme such as MYNN, ustar, wstar for non-local schemes) are important met variables for dispersion. The scheme proposed (MYNN) is a local scheme and has issues with counter gradient fluxes. CERC has conducted model runs with WRF using the local scheme, MYJ (similar to MYNN) and the non-local schemes ACM2 and YSU. Of the three ACM2 performed best for boundary layer height and turbulence variables. MYJ greatly underestimates TKE which may provide some explanation for the overestimate of NOx presented at the meeting as MYJ is similar to MYNN.

- **Vertical distribution -** There is concern that the vertical cloud distribution output by WRF is not consistent with the data expected by CMAQ. This could result in significant problems with CMAQ's wet deposition modelling which may be readily resolved by some simple investigation of the optimal WRF configuration, as was already done for other aspects of the WRF configuration. There was no scientific justification why 23 vertical layers have been used.

Other WRF features for consideration:

- Evaluation of the effects of one- or two-way nesting on continuity of variables at the boundaries of the nesting region should be considered.
- Use of UK specific land-cover data such as the CEH land cover map 2007.
- Cost of using ECMWF data was questioned - this project is evaluating the best option for Defra and this may involve purchasing data. All data recommended will need to be available for use by Defra and its contractors, including academic and commercial organisations now and for the foreseeable future. However there may be an associated cost.

Emissions

A general improvement to the emissions modelling in the UK was recommended. This should include improvements of the existing data in the models e.g. improvements to the temporal profiles and speciation of PM emissions rather than improvements to the core inventory.

Specific areas identified include:

- NAEI mapped emissions are available by species and SNAP sector. There may be advantages in producing sub-sector maps in order to produce better model emissions e.g. shipping and air transport are in the same SNAP sector but different temporal or speciation profiles apply. Ideally they should be available as separate maps.
- Ammonia and natural emissions were raised as areas for improvement.
- Temporal profiles based on UK and European activity
- PM speciation profiles based on UK and European activity

Deposition modelling

It was noted by RWE npower and E-ON that deposition modelling is a key component of the CMAQ model and has not been considered. Given the importance of critical loads assessments in relation to policy developments (NECD, Gothenburg, Habitats Directive) and the limitations of the current regulatory models, it should be included. Given that CMAQ is a "one-atmosphere" model, evaluating the treatment of deposition and PM would also inform the evaluation of the air quality performance. Consideration should also be given to the use of CMAQ to model deposition to specific habitat types.

Deposition and PM were less suitable indicators to use for model performance when looking at the interactions for WRF, emission, boundary condition and different CMAQ applications. They will be included in Phase 2 when the sensitivity tests are focused around CMAQ-UK.

Fine scale modelling (coupled CMAQ-ADMS urban models)

Fine scale modelling was identified as a requirement for several of the policy drivers. In discussion it transpired that the requirements for Health Protection and Ecosystem Impact Assessment are different from the requirements for Compliance with the Directives.

This is a complex area: CERC and KCL have examples of nesting fine scale dispersion modelling in CMAQ. AEA have experience of fine scale modelling for compliance assessment. Discussions will continue between the interested parties to investigate the best modelling applications for Defra. In this respect, CERC are interested in collaboration with the project in this area.

Assimilation of observations in CMAQ. It was considered that in applications where 'matching observations' was a requirement then observation assimilation should be considered.

5 Recommendations for Phase 2

Drawing on the experiences and findings of Phase 1 and feedback from stakeholders, the project partners have put together a recommended programme of work for Phase 2 of the project.

Collaboration with the wider community, started in Phase 1, will continue. The main part of the work in Phase 2 will focus on two key objectives: The first will focus on targeted **improvements** to CMAQ-UK developed in Phase 1 with scientific justification to support the application of CMAQ-UK for Defra policy development and analysis. The second will **demonstrate** the application of CMAQ-UK to assess compliance with regulatory air quality obligations for 2020.

The work plan recommended for Phase 2 is thus summarised as:

- Collaboration with the wider community (continuation from Phase 1)
- CMAQ-UK development and evaluation
- CMAQ-UK 2010/2020 $PM_{2.5}$ demonstration

Work for development and evaluation will be prioritised in the early stages of Phase 2 with the improved version of CMAQ-UK being used for the demonstration focused, but not limited to $PM_{2.5}$. The current version of CMAQ-UK developed in Phase 1 will be used to benchmark the improved version developed in Phase 2.

The work areas are described as core tasks, followed by a series of options. The core tasks will be shared within the project consortium, sharing knowledge and building on the individual areas of specialism so as to maintain the collaborative nature of this project.

5.1 Collaboration with the wider community

This is recommended to continue from Phase 1. The aim is to collaborate with the CMAQ and wider atmospheric modelling community, and to keep Defra and the consortium members up-to-date with developments.

This will include reporting back from any meetings with the USEPA or CMAS meetings held in the U.S. that members of the consortium attend outside this project. It will also include feedback from other CMAQ projects involving members of the project consortium in areas considered relevant to CMAQ-UK and its application to Defra policy.

A brief summary of significant developments in CMAQ and associated datasets within the external CMAQ community will be reported. This will consider the extent by which these developments may impact the development of CMAQ-UK. This may include:

- Fine scale modelling,
- Development in CMAQ decision support tools (TSSA, Adjoint models),
- European emissions, EMEP, TNO, MACC II,
- Boundary conditions,
- WRF-CMAQ and WRF-Chem coupled modelling,
- Other model intercomparison exercises and evaluation tools,
- Evaluation of CMAQ and other air quality model uncertainty analysis

- Issues raised in the CMAQ community.

Throughout the project the consortium will engage with the UK modelling community (in particular CERC, E-on, RWE and CEH) at regular intervals. To reduce the burden on the wider community, this will be as additional agenda items at the Defra Model Intercomparison Exercise (MIE) meetings.

5.2 CMAQ-UK development and evaluation

We recommend an efficient and transparent cycle of *development* and *evaluation* of CMAQ-UK to deliver a scientifically justifiable improved version. Performance will be evaluated using appropriate criteria for gaseous pollutants, PM and deposition. This is key to developing and maintaining a state-of-the-science application of CMAQ-UK for Defra.

The outcome of the core work, covering items we consider as high priority areas of development, will be a scientifically defendable version of CMAQ-UK, that has been evaluated for ozone, NO_2, PM, and deposition. The recommended options include larger individual pieces of work and development of tools that will be beneficial for CMAQ-UK implementation in this project.

Core work

The recommended core work comprises the essential work required to produce a scientifically defendable version of CMAQ for Defra applications. This includes optimising the three areas of input data: meteorology, emissions and boundary conditions and further optimising CMAQ itself. It is not considered necessary to test alternative options within CMAQ itself, although recent communications within the CMAQ community have raised a potential problem with treatment of ozone deposition over water.

Initial sensitivity studies should be run for January and July 2006 comparing with results from the provisional version of CMAQ-UK developed in Phase 1 in each of the main development areas. A final annual (2006) run would be performed using a version comprising all the developments and will be assessed for a series of Defra metrics.

The core work is described as a series of 3 main tasks for model optimisation:

- WRF optimisation
- Emissions optimisation
- Boundary conditions development

The model development tasks recommended reflect the lessons learned by the group and feedback from stakeholders in Phase 1.

The core work assumes that the existing dashboard and other tools from within the consortium will be used.

Options

Three tasks are recommended as additional options that would further enhance the performance of CMAQ-UK and its applications:

- Develop an emissions processing method for CMAQ-UK - A tool to improve CMAQ-UK implementation.
- Biogenic emissions for CMAQ-UK –improving the biogenic emissions data is a large piece of work, but we recommend reviewing available datasets for use in CMAQ.
- Dashboard developments – Some further developments are recommended. The dashboard is a tool to assist in evaluation of CMAQ but its development is not in itself

core to the developments of CMAQ-UK. The core work assumes that each group will use a range of existing tools and develop new ones as required.

We recommend that developing a common tool for preparation of emissions data and emissions scenarios be given high priority. This will not only make the demonstration tasks, which will require new years of emissions data to be prepared, to be undertaken more efficiently in this project, but will bring benefits to Defra's future users of CMAQ. Developing new sets of emissions data is time consuming, so developing a common approach will ultimately save time and costs.

5.3 CMAQ-UK demonstration for 2020 EU Air Quality Directive compliance assessment

We recommend a programme to demonstrate the application of the further optimised version of CMAQ-UK to assess compliance with regulatory obligations for 2020. This is a key date for achieving the $PM_{2.5}$ exposure reduction target and limit values, required by EC Directive 2008/50/EC.

The exposure reduction targets relate to the percentage reduction in the average concentration at approximately 47 specified sites. The baseline concentration is based on the concentrations at the specified sites averaged over the three-year period 2009-2011: the future year concentration target is the average over the three-year period 2019-2021.

Although we recommend a demonstration focused on $PM_{2.5}$ the same approach can be adapted for other pollutants for an alternative case suggested by Defra e.g. a demonstration on air quality impacts to support the revision to the Gothenburg Protocol.

We recommend a demonstration designed to provide Defra with confidence and evidence to support the use of CMAQ-UK for policy development and assessments. The evaluation would cover $PM_{2.5}$, but will include gas species and deposition to demonstrate the strengths of using a "one atmosphere" model.

Within the focus of a demonstration for regulatory compliance, our recommendations include a core task and a range of supplementary options. The core task focuses on two years: 2011 and 2020.

Core work

We recommend a core demonstration work plan as follows:

- Run CMAQ-UK for 2011 taking into account the refinements in Phase 2. 2011 has been selected to maximise the observational data available for evaluation and include the PM episodes in March/April.
- Run CMAQ-UK for 2020 using meteorology prepared based on a 2020 climatology model and current UK and European emission projections
- Model evaluation for 2011, using standard dashboard and evaluation for specialist observations.
- Demonstration for 2011 and 2020, with post-processing tools to evaluate compliance metrics e.g. population weighted metrics, limit value compliance.
- Evaluation of the 2020 obligations for achieving the $PM_{2.5}$ exposure reduction target and limit values.
- Demonstration of the differences in concentrations of gas species, PM species and deposition between 2011 and 2020.

The outcome of this would be:

- CMAQ-UK ready input datasets for 2011 and 2020 including WRF meteorology, emissions data and CMAQ outputs.
- An evaluation of the changes in air quality between 2011 and 2020.
- A set of post processing tools for developing compliance metrics.

Options

We recommend the following supplementary options:

- Demonstrating extra features of CMAQ-UK
    - Decision support tools – these may provide a powerful tool for Defra's policy applications. The tools have not been used in the UK. As a first step we need to get an appreciation for data produced using these tools and how they can be applied.
- Extending the demonstration
    - Extend the demonstration of CMAQ-UK for 2009, 2010 and 2011 – extending the demonstration to 3 years complies with the regulatory obligation and addresses the uncertainty associated with inter-annual variability as highlighted by RWE npower during the stakeholder meeting.
    - Extend the demonstration of CMAQ-UK for 2019, 2020 and 2021
    - Model Uncertainty Analysis
    - Source apportionment
    - Secondary Organic Aerosol

We recommend running CMAQ-UK at 10km resolution at the UK national scale. The low spatial resolution for annual modelling at UK scale (within a reasonable timescale) has been identified as a limitation of CMAQ for use in the context of Defra's evidence needs and this task investigates the possibility for final scale modelling.

There are different requirements for fine scale modelling for urban and national scale compliance modelling. KCL and CERC have been working on different methods to include fine scale road traffic emissions within a CMAQ-ADMS model. At this stage the nesting of fine scale models within CMAQ will not be developed within Phase 2 of this project.

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