Workshop 6-10 December 2010 on Improving and Applying Air Quality Models *under the auspices of the Letter of Collaboration between the United States Environmental Protection Agency (USEPA), the United Kingdom's Department for Environment, Food and Rural Affairs (Defra), and the Environment Agency for England and Wales*

This is an introduction to the presentations given at the air quality workshop attended by US and UK scientists held in London on the 6 -10 December 2010, under the letter of collaboration on improving air quality models signed between the USA and UK. The valuable discussions between US and UK scientists at this meeting demonstrated the significant, recent developments in local, regional and global air quality modelling capability in the two countries.

The similarity in the approaches between the various groups is encouraging. This kind of meeting also enables modelling groups to identify where there are limitations in their models, providing a form of quality assurance that the methods used are at the forefront of international practice and can be fully justified, if challenged (presentation 2.05).

The air quality model evaluation protocol followed by the USEPA (presentations 2.02 and 5.03) is now well established and the model inter-comparison and evaluation under way in the UK, led by Defra, gives the modellers the tools to explore various kinds of scientific evaluation (presentation 1.02). Good performance when compared with current or past observations does not guarantee by itself that a model can be used for policy applications. Policy applications generally involve assessment of alternative emissions scenarios and the attribution of concentrations to specific sources. At some stage a judgement has to be made whether a model, or set of models, is fit for purpose and can be used to support policy decisions. The more important the decision, or the cost of getting the decision wrong, the more important is the quality of the set of models used to come to a decision, and the depth of their evaluation. The protocol is a framework towards satisfying this aim (presentation 1.03).

The driver for air quality studies is health and the need to improve the quality of the air quality analysis in epidemiological studies. As seen from the workshop presentations 3.01 and 4.01, air quality models will be used to improve the assessment of exposure. Mention was made at the meeting of the Twenty Third Conference of the International Society for Environmental Epidemiology, in Barcelona, Spain, September 13 - 16, 2011, (http://www.isee2011.org), which has a session on 'exposure assessment and air pollutants', as well as a number of sessions on outdoor air pollution and health outcomes.

The requirement to assess exposure, as well as the demonstration that transcontinental transport can have a significant influence on ozone (presentation 2.03), leads to the need for atmospheric models to be available on all spatial scales, from local to hemispherical, which inevitably increases their complexity and makes evaluation more difficult. The more complex a model is, the more difficult is the investigation of predictions, as a function of

emissions, and as a function of their dependence on the parameters in the model describing processes, such as chemical reactions and atmospheric transport. This further emphasises the need for a formal structure to model evaluation (see 2.02 for example). The need to consider the hemispherical scale in air quality assessments also suggests that a linkage should be made with the global modelling community, which is starting to include air quality effects in climate change predictions (4.11).

The workshop plan is to hold another US-UK Workshop in North Carolina in October 2011, in association with an AQMEII (Air Quality Modelling Evaluation International Comparison) workshop and the annual CMAS (Community Modelling and Analysis) conference.

The main themes to come out of the meeting were thus **evaluation** of the new, more detailed models (regional and local) to describe air quality on all scales and the improved assessment of human **exposure** to air pollution (4.01). The **exchange** of information is best done by scientists on a one-to-one basis, unless it involves cooperation over model development or is part of a model inter-comparison exercise, where the clear focus of the joint activity provides a convenient, common structure. In all cases joint publications between the groups at the workshop were encouraged, especially at the forthcoming 2011 AQMEII (2.03 and 2.04) and CMAS meetings.

The list of specific activities to be followed by participants at the workshop (summarised in presentation 5.04), includes the following:

(1) The AQMEII model evaluation will be continued. Comparison of CMAQ calculations against other models for the North American and European domains, with emphasis on the model boundary conditions, is under way (2.03 and 2.04). Participants should plan to present a joint paper at the CMAS conference in October 2011.

(2) The Defra modelling inter-comparison exercise involves the comparison of a range of UK models in the areas of urban, regional and trans-boundary modelling, and deposition modelling (1.02). The USEPA should be given the opportunity to comment on the inter-comparison review committee's draft report due in March 2011. Comparison of the outcome of the Defra modelling review (1.02) with conclusions from the AQMEII project would come later in the year.

(3) Similarly a report, under preparation, of the Environment Agency project CREMO (Comparison of REgional MOdels, presentations 2.06, 2.07, 2.10 and 2.11) focuses on messages for regulators as to how they should apply meso-scale chemical transport models. This would benefit from USEPA comments. There is interest in the interpretation of CMAQ predictions of speciated particulate matter, especially the component of particulate matter labelled as 'other'. An interim report for the Environment Agency is being drafted, which would outline for what purpose models should be used. Thus models might be applied in different ways in operational and policy contexts,

for assessing current and future budgets, when looking at future regulation and for assessing source apportionment.

(4) The proposed Defra contract to evaluate CMAQ should make use of the forthcoming CMAQ model version 5.0 (available from March 2011) before its general release (2.01 and 2.08). The emphasis of the Defra work is on source attribution.

(5) Similarly the proposed Environment Agency project to evaluate $PM_{2.5}$ exposure from industrial emissions in 2020 should apply CMAQ version 5.0.

(6) There should be some attempt to merge the evaluation of air quality and climate interactions from the air quality and climate change communities (4.09 and 4.10). The meeting heard about the Hadley Centre climate and air quality forecasts (4.11), which form part of the Atmospheric Chemistry and Climate Model Intercomparison Project (ACC-MIP), part of the atmospheric chemistry and climate activity of the International Global Atmospheric Chemistry programme (IGAC). This international model inter-comparison is working towards the fifth assessment report of the IPCC, using coupled climate chemistry models and emission projections based on Representative Concentration Pathways (RCPs). Linked to this programme, but not directly discussed at the meeting, are the activities undertaken by the Task Force on Hemispheric Transport of Air Pollution. These also involve multi-model comparisons emphasising inter-continental transport of ozone and particulate. One needs to explore how the evaluations might be linked, since the climate and air quality modellers have already set up structures for multi-model comparisons. Hemispheric transport, as the middle ground, might be the place to start (4.08).

(7) The evaluation of roadway models is an important link between exposure assessment and regional modelling (see presentation 3.02). Development of algorithms for the new US AERLINE roadway model is a key development, which would benefit from further analyses of the Las Vegas (3.04) and the Idaho Falls (3.06) tracer data sets using directional analysis (3.07) and data mining techniques (2.09). A joint US/UK team will focus on the following scientific issues:

1. Characterising the impact of vehicle-induced turbulence on dispersion of pollutants near roadways. The US/UK team will analyse the Las Vegas micro-meteorological measurements to investigate the relative importance of vehicle induced turbulence in the near-road environment, specifically the turbulent kinetic energy as a function of ambient meteorological conditions and traffic. The team will then examine if modelling tools can adequately account for vehicle-induced turbulence when simulating dispersion of pollutants near roadways.

2. Understanding the relative importance of the plume rise from highways on the near-road air quality. The US/UK team will analyse field data from the Las Vegas experiment to determine the relative importance of the plume rise effect on the dispersion of pollutants near roadways. The team will apply data

mining techniques to select subsets of data when the conditions were favourable for plume rise, to determine whether modelling tools should be improved.

3. Light wind conditions. The US/UK team will analyse field data from the Las Vegas experiment and the Idaho Falls tracer experiment to characterise the dispersion of pollutants under light wind conditions and examine the ability of existing modelling tools to simulate the dispersion of pollutants near roadways in such conditions, and provide recommendations for model improvements.

4. Complexity of road configurations. The US/UK team will focus on model evaluation and model improvements to account for the complexity of road configurations (such as noise barriers or depressed sections). The team will use observational data from the Las Vegas experiment and from the Idaho Falls tracer experiment to evaluate the ADMS and AERLINE models (3.02, 3.03 and 3.05).

(8) Under the exposure and health theme there is an opportunity to comment on the USEPA air quality and health synthesis report. There may also be the opportunity for the USEPA to have observer status under the forthcoming FP7 TRANSPHORM (Transport related Air Pollution and Health impacts - Integrated Methodologies for Assessing Particulate Matter) project (4.06). It may also be useful to compare the methods and the quality of the data sets used in the NEXUS project (to describe emissions and activity in Detroit, for example), with those applied in the forthcoming air quality epidemiological project in London, supported by the Medical Research Council and the Health Protection Agency. (A comparison of methodologies in the studies in Detroit and London could be conducted, see presentations 3.01, 4.03 and 4.05). Further links between the USEPA and the Health Protection Agency should be developed. Community engagement in relation to urban pollution is a topic which is thought to be neglected.

(9)The comparison of the photochemical schemes used in regional models, and in the different versions of each model, was discussed. In future developments, the EMEP model may include a number of photochemical scheme options (presentation 5.01) and so understanding of the performance of different schemes is important.

(10) NOx emission inventories were discussed in the context of improving regional and urban model performance (3.09). There is also the need for better speciated particulate matter inventories, and improved treatment of the temporal variability of ammonia emissions relating to farming practices. The informal exchange of information was encouraged.

(11) European and US air pollution policy drivers ultimately support air quality research. Current European concerns emphasise NO_2 and the health outcomes from high ground-level ozone concentrations (1.01, 3.08 and 4.02). The key point is whether the models are good enough for use in policy decisions. Evaluation for the scientists is through model inter-comparisons, but the wider outcomes from the models and subsequent decisions need to

be translated to policy makers through integrated assessments. NIAM (the Network for Integrated Assessment Modelling), FAIRMODE (the Forum for AIR quality MODelling) and air quality forecasting methodologies are relevant here (5.02, 2.13 and 2.12). **Independent** peer review of recommendations relating to 'fit for purpose' models would be enhanced by US-UK cooperation.

(12) There were a number of other topics, not fully discussed at the meeting, which should be followed up. One should not be complacent that the process descriptions within the regional models are appropriate in all situations. Limitations to the parameterisations of the urban boundary layer structure at night in the meso-scale meteorological models used to drive CMAQ, and of fine resolution rainfall in complex terrain (4.04 and 4.07) were discussed. Collaboration on the nocturnal boundary layer description using London observations and related urban modelling should be encouraged. Non-road sources in cities was also mentioned as a neglected topic.

List of presentations made at the meeting

A list of presentations given at the meeting is given below. These have been grouped into themes and are therefore not necessarily in the order in which they were given at the workshop.

Day 1 Theme USEPA and Defra Air Quality Policies and the Evaluation of Models used to support Policy

1.01 Air quality policy in the UK, Robert Vaughan, Defra.

1.02 Defra's atmospheric modelling capacity, Sarah Honour and Samantha Lawrence, Defra.

1.03 Model development for air quality management needs, S.T. Rao, USEPA.

Day 2 Theme: The use of CMAQ, the Community Multi-scale Air Quality modeling system

2.01 The Community Multiscale Air Quality (CMAQ) modeling system: On-going and planned developments, Rohit Mathur and the EPA CMAQ Development Team, Atmospheric Modeling and Analysis Division, NERL, EPA.

2.02 Using dynamic and diagnostic evaluation to probe the Community Multiscale Air Quality (CMAQ) modeling system, S.T. Rao, USEPA.

2.03 Part I: Overview of the Air Quality Model Evaluation International Initiative (AQMEII), Shawn Roselle, Kenneth Schere, Michael Moran, S.T. Rao and Stefano Galmarini.

2.04 Part 2: Progress with US-UK collaboration under the Air Quality Modelling Evaluation International Initiative (AQMEII), Charles Chemel, University of Hertfordshire.

2.05 Air quality modeling to support regulatory programs, David Mobley USEPA.

2.06 Application of CMAQ to regulatory issues in the UK power sector, Steve Griffiths, Environmental Modelling Team, E.ON New Build and Technology.

2.07 Application of CMAQ to regulatory issues in the UK power sector, Paul Sutton, RWE NPower.

2.08 CMAQ for research and policy application at ERG, Nutthida Kitwiroon and Sean Beevers, Environmental Research Group (ERG), King's College London.

2.09 Data mining for source and model performance of tall-stack sources, Roger Timmis, Environment Agency, Andy Malby and Duncan Whyatt, Lancaster University.

2.10 Assessment of regional effects using complex models, Bernard Fisher, Environment Agency.

2.11 Modelling the deposition of nitrogen and sulphur and the exceedance of critical loads and levels in the UK, Tony Dore, Małgorzata Matejko, Steve Hallsworth, Maciej Kryza, Bill Bealey, Jane Hall, Chris Dore, Ron Smith, Sim Tang, Massimo Vieno, Ulrike Dragosits and Mark Sutton.

2.12 AEA air quality forecasting WRF-CMAQ, Andrea Fraser, AEA Technology.

2.13 FAIRMODE Forum for air quality modelling in Europe, Keith Vincent, AEA Technology.

Day 3 Theme: Local Scale Pollution

3.01 Summary of a recent Air Quality and Exposure Modeling Workshop, David Mobley, USEPA.

3.02 Local scale air pollution in the US, Vlad Isakov, USEPA.

3.03 Local scale air pollution in the UK, David Carruthers, Celine Aulagnier, Cambridge Environmental Research Consultants.

3.04 Data mining of the Las Vegas roadway data set, Andy Malby, Lancaster University, Roger Timmis, Environment Agency, and Duncan Whyatt, Lancaster University.

3.05 The Raleigh 2006 field study, Vlad Isakov, USEPA.

3.06 The Idaho Falls tracer experiment, Vlad Isakov, USEPA.

3.07 Directional passive sampling of airborne pollutants, Roger Timmis, Environment Agency.

3.08 UK NOx and NO_2 modeling using the Pollution Climate Mapping (PCM) model, Susannah Grice, John Stedman, Sally Cooke, Andrew Kent, Daniel Brookes, Helen Walker and Keith Vincent, AEA Technology.

3.09 Analysis of NOx and NO_2 emissions inventory trends, Sean Beevers, Emily Westmoreland, David Carslaw, King's College, London.

Day 4 Theme: Exposure, and Air Quality and Climate

4.01 Air quality and exposure, Vlad Isakov, USEPA.

4.02 Should we be concerned about the health effects from ozone? Sotiris Vardoulakis and Clare Heaviside, Centre for Radiation, Chemical & Environmental Hazards, Health Protection Agency.

4.03 The Medical Research Council – Health Protection Agency Centre for Environment and Health: health effect of traffic project, Sean Beevers, King's College, London.

4.04 Urban boundary layer and inversion height, Julian Hunt, University College, London.

4.05 GENESIS: Air Quality London Pilot, Christine McHugh, CERC.

4.06 TRANSPHORM Transport related air pollution and health impacts - Integrated methodologies for assessing particulate matter, Ranjeet Sokhi and partners.

4.07 Improved treatment of rainfall and cloud in regional models and aviation induced cloudiness and climate forcing, Emma Ferranti, Roger Timmis and Duncan Whyatt, Lancaster University.

4.08 The WRF-CMAQ two-way coupled modeling system and hemispheric extensions: Development, testing and initial applications, Rohit Mathur, Jonathan Pleim, David Wong, Tanya Otte, Robert Gilliam, Shawn Roselle, Jeffrey Young, Atmospheric Modeling and Analysis Division, NERL, USEPA.

4.09 Megacities, air quality and climate change – MEGAPOLI, London case study, Xin Kong, Xavier Francis, Charles Chemel, Rong-Ming Hu, Ye Yu, Ranjeet Sokhi, Bill Collins and Maria Russo.

4.10 GEOS-Chem modelling capabilities and applications, Rong-Ming Hu and Ranjeet Sokhi, Centre for Atmospheric and Instrumentation Research (CAIR), University of Hertfordshire.

4.11 Air quality and climate change: Met Office modelling, Bill Collins, Hadley Centre, Met Office.

Day 5 Roundup of meeting

5.01 Comparison of photochemical mechanisms used in meso-scale models, Garry Hayman, Centre for Ecology and Hydrology.

5.02 An update on integrated assessment activities in Europe, Helen ApSimon, Imperial College.

5.03 A framework for evaluating regional air quality models, S.T. Rao, USEPA.

5.04 Summary of actions from the workshop, Bernard Fisher, Environment Agency.

A list of relevant, recently published papers by USEPA authors is given below.

List of recent, relevant USEPA papers

USEPA, Atmospheric Modeling and Analysis Division Strategic Research Plan (2011-2015).

Overview of the atmospheric model evaluation tool (AMET) v 1.1 for evaluating meteorological and air quality models. K. Wyat Appel, Robert C. Gilliam, Neil Davis, Alexis Zubrow and Steven C. Howard, Environmental Modelling and Software, 26 (2011) 434 - 443.

Lagrangian sampling of 3-D air quality model results for regional transport contributions to sulfate aerosol concentrations at Baltimore, MD, in summer 2004. T. Duncan Fairlie, James Szykman, Alice Gilliland, R. Bradley Pierce, Chieko Kittaka, Stephanie Weber, Jill Engel-Cox, Raymond R. Rogers, Joe Tikvart, Rich Scheffe and Fred Dimmick, Atmospheric Environment, 43 (2009) 3275 – 3288.

Assessing multi-year changes in modeled and observed urban NOx concentrations from a dynamic model evaluation perspective. James M. Godowitch, George A. Pouliot and S. Trivikrama Rao, Atmospheric Environment, 44 (2010) 2894 - 2901.

Ensemble and bias-correction techniques for air quality model forecasts of surface O_3 and $PM_{2.5}$ during the TEXAQS-II experiment of 2006. Djalalova, J. Wilczak, S. McKeen, G. Grell, S. Peckham, M. Pagowski, L. Delle Monache, J. McQueen, Y. Tang, P. Lee, J. McHenry, W. Gong, V. Bouchet and R. Mathur, Atmospheric Environment, 44 (2010) 455 - 467.

Dynamic evaluation of a regional air quality model: Assessing the emissions-induced weekly ozone cycle. Thomas Pierce, Christian Hogrefe, S. Trivikrama

Rao, P. Steven Porter and Jia-Yeong Ku, Atmospheric Environment, 44 (2010) 3583 – 3596.

A framework for evaluating regional-scale numerical photochemical modeling systems. Robin Dennis, Tyler Fox, Montse Fuentes, Alice Gilliland, Steven Hanna, Christian Hogrefe, John Irwin, S. Trivikrama Rao, Richard Scheffe, Kenneth Schere, Douw Steyn and Akula Venkatram, Environ. Fluid Mech., 10 (2010) 471 – 489.

Dynamic evaluation of long-term air quality simulations over the Northeastern United States. C. Hogrefe, K. Civerolo, W. Hao, E.E. Zalewsky, J.-Y. Ku, P.S. Porter, S.T. Rao, and G. Sistla, paper to 31st NATO/SPS International Technical Meeting on Air Pollution Modeling and its Applications, September 27 – October 1, 2010,Torino, Italy.

Modeled watershed runoff associated with variations in precipitation data, with implications for contaminant fluxes: Initial results. Heather E. Golden, Christopher D. Knightes, Ellen J. Cooter and Robin L. Dennis, The Third Interagency Conference on Research in the Watersheds, 8 -11 September 2008, Estes Park, CO.

Dynamic model evaluation of NOx emissions reductions on ozone concentrations in the presence of uncertain emission inventories. Sergey L. Napelenok, Kristen M. Foley, Daiwen Kang, Thomas Pierce, Rohit Mathur, and S. Trivikrama Rao, paper to 31st NATO/SPS International Technical Meeting on Air Pollution Modeling and its Applications, September 27 – October 1, 2010,Torino, Italy.

List of participants:

Andrea Fraser	Andrea.Fraser@aeat.co.uk
Beevers, Sean	sean.beevers@kcl.ac.uk
Bill Collins	bill.collins@metoffice.gov.uk
Celine Aulagnier	Celine.Aulagnier@cerc.co.uk
Christine McHugh	Christine.Mchugh@cerc.co.uk
Chemel, Charles	c.chemel@herts.ac.uk
David Carruthers	David.Carruthers@cerc.co.uk
Diane Brooke	Diane.Brooke@rwenpower.com
Dore, Anthony	tony.dore@ceh.ac.uk
Duncan Laxen	duncanlaxen@aqconsultants.co.uk
Garry Hayman	garr@ceh.ac.uk
Griffiths, Stephen	Stephen.Griffiths@eon-uk.com
Helen ApSimon	h.apsimon@ic.ac.uk
Helen Ainsworth	helen.ainsworth@defra.gsi.gov.uk
Honour, Sarah	sarah.honour@defra.gsi.gov.uk
Julian Hunt	jcrh@cpom.ucl.ac.uk
Jenny Stocker	jenny.stocker@cerc.co.uk
Daniel Instone	daniel.instone@defra.gsi.gov.uk
Vlad Isakov	Isakov.Vlad@epamail.epa.gov
Kavanagh, Miranda	Miranda.Kavanagh@environment-agency.gov.uk

Kitwiroon, Nutthida	nutthida.kitwiroon@kcl.ac.uk
Lawrence, Samantha	Samantha.Lawrence@defra.gsi.gov.uk
Malby Andrew	a.malby@lancaster.ac.uk
Mobley David	mobley.david@epa.gov
Powlesland, Colin	colin.powlesland@environment-agency.gov.uk
Ravindra Khaiwal	r.khaiwal@herts.ac.uk
Robert Vaughan	robert.vaughan@defra.gsi.gov.uk
Roger Barrowcliffe	roger.barrowcliffe@erm.com
Rohit Mathur	mathur.rohit@epa.gov
Rong-Ming Hu	r.hu@herts.ac.uk
Sarah Honour	sarah.honour@ defra.gsi.gov.uk
Shawn Roselle	Roselle.Shawn@epamail.epa.gov
Sokhi, Ranjeet	r.s.sokhi@herts.ac.uk
S T, Rao	Rao.ST@epamail.epa.gov
Susannah Grice	Susannah.Grice@aeat.co.uk
Sutton, Paul	paul.sutton@rwenpower.com
Tim Murrells	tim.p.murrells@aeat.co.uk
Tim Williamson	tim.williamson@defra.gasi.goc.uk
Timmis, Roger	roger.timmis@environment-agency.gov.uk
Vieno Massimo	mvieno@staffmail.ed.ac.uk
Vincent, Keith	Keith.Vincent@aeat.co.uk
Whyatt, Duncan	D.Whyatt@lancaster.ac.uk
Williams, Martin	martin.williams@kcl.ac.uk
Willows, Robert	robert.willows@environment-agency.gov.uk
Wright, Ray	Ray.Wright@RWEnpower.com
Xin Kong	X.Kong@herts.ac.uk

Bernard Fisher 10 January 2011