COMPREHENSIVE ANALYSIS OF ANNUAL 2005/2008 SIMULATION OF WRF/CMAQ OVER SOUTHEAST OF ENGLAND

Nutthida Kitwiroon and Sean Beevers

Environmental Research Group (ERG), King's College London, London, United Kingdom

Abstract: A comprehensive evaluation was conducted on annual 2005 WRF/CMAQ simulations over the southeast of England to identify the cause of model deficiencies and to determine if the model is suitable for policy applications. The model performance was characterised through operational, dynamic and diagnostic evaluations. For operational evaluations, the model results, downscaled from a horizontal grid resolution of 81km to 3km, were compared against the observations from 120 air quality monitoring sites measuring NO_2 and O_3 concentrations across the southeast of England. The predicted surface and vertical profiles of temperature, relative humidity and wind components were also evaluated, as was the predicted atmospheric pressure at mean sea level, which was compared with the synoptic scale charts. Demonstration of a number of model diagnostics was made possible through the use of 'Openair' (http://www.openair-project.org/), AMET (http://www.cmascenter.org) and through development of R scripts. These included time series plots, scatter plots, diurnal error plots, Taylor diagrams and statistical measures.

The performance of WRF/CMAQ for 2005 showed that the model was able to capture seasonal trends, the magnitude of the observed meteorology, NO_2 and O_3, and the partitioning of oxidant (NO_2+O_3). The analysis presented indicates that overall CMAQ represents O_3 concentrations well, although WRF over predicts wind speeds during the night and this has an impact on NO_2 and O_3 concentrations during this time. The dynamic evaluation showed that the model responds to changes in emissions of NO_X and HC's and that these agree well with other results in the literature. Further sensitivity analyses between 2005 (typical UK weather) and 2008 (wet year) showed that the model is able to represent air pollution concentrations across a wide range of UK weather conditions. However possible areas for model improvement are also discussed. The diagnostic evaluation showed an indication of underprediction of local sources of the oxidant. Finally, the statistical measures presented here indicate that the WRF/CMAQ model is acceptable for policy applications in the UK.

Key words: *Model evaluation, photochemical model, model performance, WRF, CMAQ*

INTRODUCTION

CMAQ is a state-of-the-art Eulerian model developed for both scientific research and policy applications. The evaluation of CMAQ and other models of this kind have generally been against very limited observational data and for limited periods which is obviously not enough to clarify which processes or inputs are responsible for the deficiencies of the model. As such the US EPA has developed a more systematic and comprehensive model evaluation framework (http://www.epa.gov/AMD/ModelEvaluation/index.html) which includes the operational, dynamic, diagnostic and probabilistic evaluation. This framework does not only allow the model performance to be characterised, but is also capable of identifying the areas of model improvement. Operational evaluation is a first benchmark of the model performance and is used to identify performance deficiencies. The diagnostic evaluation is then used to identify the particular cause of the performance deficiency which would lead to improvement of model performance. The dynamic evaluation is used to demonstrate if the model is able to respond to changes in meteorology or emissions, which is a key use of an air quality model for air pollution control. The probabilistic evaluation attempts to characterise the uncertainties of the model.

Within this study, operational, dynamic and diagnostic model evaluations have been conducted on the meteorological model WRF (v3.0.1) for years 2005 (typical UK weather) and 2008 (wet year) and on CMAQ (v4.6) for 2005 over the UK. This study focuses on the performance of CMAQ for the criteria pollutants NO_2 and O_3 and for WRF, the evaluation of temperature (T2) and relative humidity at 2m (RH2) and wind speed (WS10) and direction (WD10) at 10m. For dynamic evaluation, the ability of the model to represent the effect of emission changes on ground-level O_3 concentrations and the ability to adapt to changes of meteorology were assessed. Further diagnostic evaluations to determine if CMAQ is able to reproduce observed oxidant partitioning was conducted and recommendations for further sensitivity studies and possible areas for model improvement discussed.

A number of tools were used, such as time series and scatter plots, diurnal error plots and Taylor diagrams as were statistical measures such as the index of agreement (IA), correlation coefficient (CORR), root mean square error (RMSE), normalised mean bias (NMB) and mean bias (MB). Such a comprehensive analysis was undertaken using Openair (http://www.openair-project.org), AMET (http://www.cmascenter.org) and through developing R scripts. The formulae of the statistical measures are shown below. The ideal values for IA, RMSE, NMB, MB and CORR are 1, 0, 0, 0 and 1, respectively. C_p and C_o are the modelled and observed data, respectively. N is the total number of data.

$$IA = 1 - \frac{\sum_1^N (C_p - C_o)^2}{\sum_1^N \left(|C_p - \overline{C_o}| + |C_o - \overline{C_o}|\right)^2} \quad , \quad NMB = \left(\frac{\frac{1}{N}\sum_1^N (C_p - C_o)}{\overline{C_o}}\right) * 100 \quad , \quad MB = \frac{1}{N}\sum_1^N (C_p - C_o)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{1}^{N}(C_p - C_o)^2} \quad , \quad CORR = \sum_{i=1}^{n}(C_{o,i} - \overline{C_o})(C_{p,i} - \overline{C_p}) \Big/ \sqrt{\sum_{i=1}^{n}(C_{o,i} - \overline{C_o})^2 \sum_{i=1}^{n}(C_{p,i} - \overline{C_p})^2}$$

MODEL SETUP

The model made use of 4 nested domains as shown in Figure 1. The vertical domain consisted of 23 layers with 7 layers within 800 m of ground level. The top pressure level was 100mb. The physics setting in WRF includes the RRTM radiation scheme, the Kain-Fritsch (new Eta) scheme for microphysics, the YSU planetary boundary layer scheme and the NOAH land surface scheme. The dry deposition scheme is the Models-3 (Pleim) dry deposition (M3DDEP). The chemical scheme is CB-05 with aerosol and aqueous chemistry. The initial and boundary conditions for WRF were derived from the National Centres for Environmental Prediction (NCEP) FNL (Final) Global Tropospheric Analyses at 1^0 x 1^0 grid spacing and 6 hour temporal resolution. The initial and boundary conditions for CMAQ were derived from the UK Meteorological Office chemistry-transport model (STOCHEM).

The annual anthropogenic emissions (CO, NO_X, NH_3, SO_2, NMVOC and PM_{10}) data were obtained from a number of sources including the European Monitoring and Evaluation Programme (EMEP) at a grid resolution of 50km, the UK National Atmospheric Emissions Inventory (NAEI) at a grid resolution of 1km, the London Atmospheric Emissions Inventory (LAEI) at a grid resolution of 1km. The emissions from point sources were derived from the European Pollutant Emission Register (EPER) and the NAEI databases. The emissions from EMEP were used in CMAQ domain 1 and 2, domain 3 (UK) used the emissions from NAEI and domain 4 used a combination of the LAEI and NAEI. The annual primary emissions were disaggregated into hourly emissions using sources specific, chemical speciation profiles (Dick Derwent and Garry Hayman personal communication). Detailed temporal profiles for traffic emissions were derived from ATC (Automatic Traffic Counters) and for the remaining 10 CORINAIR/UNECE emission source categories use was made of the monthly, daily and hourly profiles from the City-Delta project (http://aqm.jrc.ec.europa.eu/citydelta/). The biogenic emissions, isoprene and terpene, were estimated using 100m grid resolution CORIN land cover data, incoming shortwave radiation and surface temperature, using methods described by Guenther et al. (1995) and Sanderson (2002).

MONITORING STATIONS

The location of meteorological and air quality monitoring sites are shown in Figure 1. Surface meteorological data was taken from 26 UK Meteorological Office stations, archived by the British Atmospheric Data Centre (BADC). Air quality monitoring data was taken from the London Air Quality Monitoring Network (LAQN) (http://www.londonair.org.uk/) and the UK Automatic Urban and Rural Network (AURN) (http://aurn.defra.gov.uk/). The LAQN database contains 65 urban background, 24 suburban and 15 rural sites, the AURN data 9 urban background sites, 2 urban centre sites and 5 rural sites.

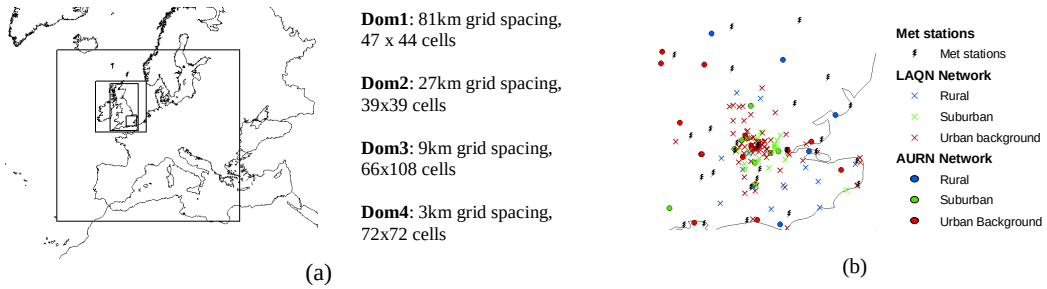

Figure 1. (a) Model domains and (b) meteorological and air quality monitoring stations

MODEL OPERATIONAL EVALUATION

At synoptic scale, the predicted atmospheric pressure was analysed during typical non-episodic conditions (7^{th} -15^{th} February 2005) and during elevated O_3 concentrations (9^{th} -17^{th} July 2005). The model captures the movement of atmospheric pressure systems well for the summer period although less so during winter. The vertical profiles of temperature and wind speed are also predicted well by the model during winter and summer periods although there is a tendency to overestimate surface (< 1 km above ground) wind speed by approximately 5 m s^{-1} during the night in winter (not shown here for the sake of brevity).

The comparison between measured and modelled surface data indicates that WRF/CMAQ reproduces the seasonal trends of observed T2, RH2, WS10 and WD10, NO_2 and O_3 well. The diurnal variation of the residual (modelled - observed) values of WS10, NO, NO_2, NO_X and O_3 are summarised in Figure 2. The Figure includes the diurnal variation of the residual (modelled - observed) by day of the week (top), 24-hour variation of the bias (bottom left) and daily average of the residual by day of the week (bottom right). The Figure shows that the model captures all the

parameters well during the afternoon period, but under predicts NO_X and over predicts O_3 during the night. This may be associated with the over prediction of wind speed at this time.

For NO_2, the results show that the measured concentrations are predicted well during the middle of the day but that the model overpredicts rush hour concentrations. The problems associated with predicting NO_2 are more complex and may be due to poorly predicted wind speeds and boundary layer structure in the met model, and the associated mixing of O_3 at ground level. Also the emissions estimates of directly emitted NO_2 from road traffic may have a role. The figures also shows that the bias varies by day of the week and is a maximum on Wednesday and this is currently under investigation.

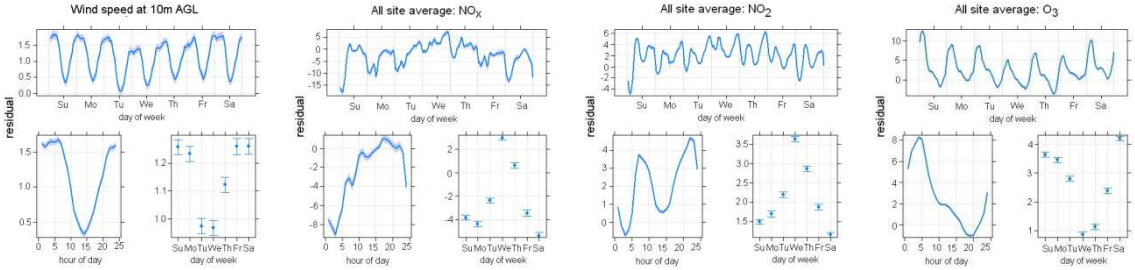

Figure 2. Diurnal variation of the residuals (modelled - observed) of WS10, NO, NO_2, NO_X and O_3 (2005)

The density-scatter plots in Figure 3 show the relationship between hourly results as well as number of points within each region of graph, coloured according to the data frequency. These plots show that the majority of hourly results of NO_2 and O_3 lie close the 1:1 line and more than 60% of the modelled results (as an average of all sites) are within factor of two of the observations although a slight positive bias is observed. In contrast, the Taylor diagrams in Figure 3 show how well the model predicts NO_2 and O_3 at individual monitoring site (coloured dot) and highlights how model bias varies from site to site. The diagrams depict the relationship between correlation coefficient, normalized standard deviations of the model output and observation (the radial distance from the origin) and normalized centred root mean square (RMS) error between the model output and observation (thin line contours). The shorter relative distance between coloured dot (monitoring sites) and observed point (purple dot) indicates the better agreement between model and observation. According to RMS, the biases of NO_2 prediction are observed at more sites than O_3 prediction which may be due to local emission influences on NO_2 observations. The plots also indicate that the model overpredicts the standard deviation of the observed NO_2 while opposite is observed for O_3 at various sites. It is worth mentioning here that the bias of model prediction at each site may be influenced by the uncertainties of the observations. Providing that the monitoring data has been through the quality control procedure, a lack of horizontal and vertical representativity of point measurements with respect to model grid cells still exists (Beekmann and Derognat, 2003 and Chang and Hanna, 2004). Selection of the sites prior to model assessment is therefore essential and a methodology to solve this issue is current being developed at ERG.

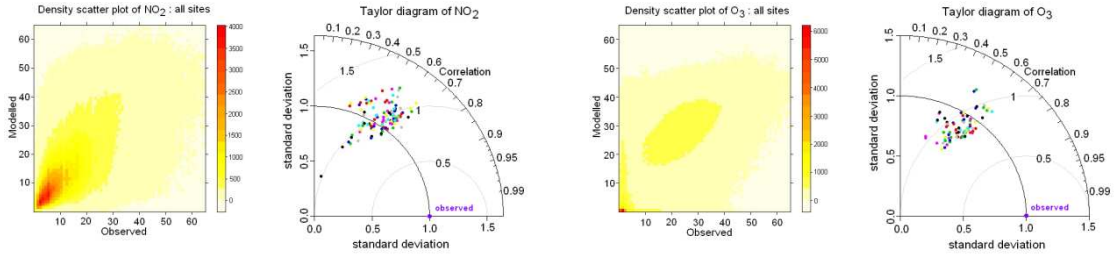

Figure 3. Density-scatter plots and taylor diagrams of NO_2 and O_3 (2005)

The statistical measures (Table 1) show that the model performs well particularly for temperature with a near perfect agreement and an IA of 0.95, a correlation coefficient of 0.9 and small negative error indicated the NMB and MB. The model slightly overestimates relative humidity but by less than 2% on average according to MB. The positive error in wind speed predictions, indicated by NMB and MB, is under investigation. The IA values of NO_2, NO_X and O_3 vary between 0.7 – 0.8 indicating that the model predicts exceptionally well the temporal and spatial pattern of the observations. The CORR of these pollutants falls between 0.5 – 0.6 and may be influenced by some outliers of that the observation for example NO, NO_2 and NO_X was measured as high as over 1000 ppb at a certain site and hour. These outliers may also be a reason of high values of RMSE. Nevertheless, the NMB values of these pollutants (within ±20%) suggest that CMAQ would satisfy the proposed UK Department for Environment, Food and Rural Affairs (DEFRA) protocol (AEA, 2009).

Table 1. Statistical measures of model performance years 2005

Statistics	IA	CORR	RMSE (%)	NMB (%)	MB
WS10 (m/s)	0.73	0.58	2.73	27.4	1.15
T2 (° C)	0.95	0.9	2.58	-1	-0.11
RH2 (%)	0.78	0.61	12.59	2.3	1.88
NO_2 (ppb)	0.77	0.61	11.08	13	2.17
NO_X (ppb)	0.68	0.52	34.23	-6	-1.77
O_3 (ppb)	0.75	0.56	12.4	14	2.84

MODEL DYNAMIC EVALUATION

Figure 4 shows the response of O_3 to 30% across-the-board reductions in the emissions of man-made NO_X (a) and VOC's (b) for the period 1-14 July 2005. This evaluation is to establish whether the modelled O_3 formation in the UK is VOC or NO_X limited, whether this agrees with the literature and whether CMAQ would be useful in developing effective policies.

In this example a reduction in NO_X emissions results in an increase in O_3 concentration by up to 31% in urban areas, whilst reducing O_3 in rural parts of the UK. A reduction in VOC emissions results in the reduction of O_3 of ~ 3% over urban areas and results in very small increases in Northern Scotland. These findings, which relate to VOC and NO_X sensitive chemistry, correspond with theoretical findings in Sillman (1999).

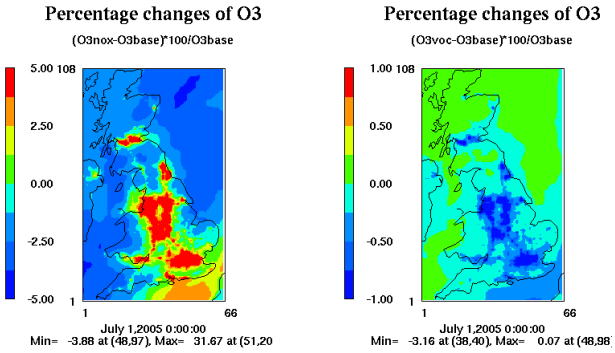

Figure 4. Percentage increase of O_3 due to 30% reduction across-the-board of man-made NO_X emissions (left) and VOC emissions (right)

As part of the dynamic evaluation, the model responses to changes of meteorological condition are investigated. Within this study, the results between CMAQ 2005 and 2008 are incomparable due to the difference of CMAQ versions used between these two years. However, the comparison between surface meteorological prediction for years 2005 and 2008 is conducted to provide an initial insight of how the CMAQ would perform. Statistical measures in Table 2 indicate that the model performs consistently between year 2005 and 2008 showing that the model is able to adapt to changes of weather conditions. Similar finding is observed between the two years runs that the model tends to overpredict wind speed under the stagnant condition. Further investigation on wind speed prediction under such condition is needed.

Table 2. Statistical measures of model performance on prediction of wind speed at 10m and temperature at 2m (2005 versus 2008)

Parameters	IA		CORR		RMSE		NMB		MB	
	2005	2008	2005	2008	2005	2008	2005	2008	2005	2008
WS10	0.73	0.75	0.58	0.6	2.73	2.75	27.4	23.2	1.15	1.06
T2	0.95	0.94	0.9	0.89	2.58	2.49	-1	-0.5	-0.11	-0.06

MODEL DIAGNOSTIC EVALUATION

Due to the chemical coupling of O_3 and NO_X, it is suggested that the relationship of the oxidant ($OX = NO_2 + O_3$) with NO_X can be used to gain some insight into the sources of OX (Clapp and Jenkin, 2001). This section demonstrates how this relationship is used to define the causes of prediction biases. The variation of NO, NO_2, O_3, OX (NO_2+O_3) as a function of NO_X mixing ratios was plotted both day and night, during winter (December-February), spring (March-May), summer (June-August) and autumn (September-November) periods. Figure 5 shows the results during the day in winter and summer. There was good agreement between observations and modelled results during daytime and night time (not shown here) although the model results are slightly less scattered than the observations. Further investigation is made by looking at the source contribution of OX.

Table 3 shows the observed and modelled daytime local OX and regional OX derived from the relationships between OX and NO_X mixing ratios at all monitoring sites. The model slightly underpredicts local OX in most seasons except in summer when a large negative bias is observed. This may be due to underprediction of one of the local oxidant sources such as direct NO_2 emissions, the thermal reaction of NO with O_3 at high NO_X or common- source emission of species which promote NO to NO_2 conversion (such as nitrous acid (HONO)).

For regional OX, the model captures the seasonal trend of the observation with a spring time maximum corresponding with Clapp and Jenkin (2001). Since the model underpredicts local sources of OX, it is not clear that the overprediction of O_3 is caused by overprediction of the boundary conditions. According to this result, it suggests that further investigation of input emissions should first be made.

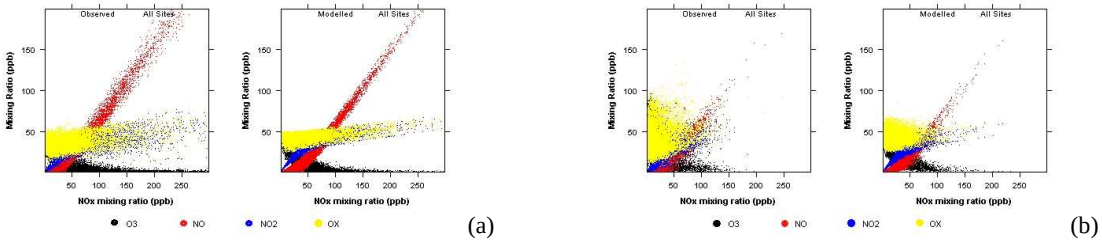

Figure 5. Observed and modelled partitioning of the oxidant between NO_2 and OX (O_3+NO_2) at daytime winter (a) and summer (b) 2005

Table 3. Observed and modelled daytime local and regional contribution to oxidant at all sites (2005)

Season	Observed local OX (ppb ppb-1 NO_X)	Modelled local OX (ppb ppb-1 NO_X)	Observed regional OX (ppb)	Modelled regional OX (ppb)
Winter	0.07	0.06	34.02	39.68
Spring	0.05	0.03	42.55	42.85
Summer	0.13	0.01	37.33	42.16
Autumn	0.09	0.07	33.33	40.05

CONCLUSIONS

The WRF/CMAQ mode performance has been conducted through a set of model evaluation routines, including operational, dynamic and diagnostic evaluation, developed by the USEPA and recommended by the UK DEFRA. Such an evaluation led to a better picture of model deficiencies and areas of model improvement which would not be obvious from just comparing averages across sites. The evaluation involved a large dataset of modelling results and the observations from the full 2005 (typical UK weather) and 2008 (wet year) simulations and is made possible by using the Openair, AMET and through developing R scripts.

The performance of WRF/CMAQ in 2005, through the operational evaluation, shows that the WRF model predicts synoptic scale features, vertical profiles of meteorology and surface meteorology well, although importantly it over predicts night time wind speed. The model reproduces the seasonal trend of the observed temperature, relative humidity, wind fields, NO_2 and O_3 well. Small biases of afternoon NO_2 and O_3 concentrations predictions is observed while large biases is observed during the night. The over prediction could be for a number of reasons particularly the oveprediction of nighttime wind speed. The bias of model prediction may also be influenced by the site representativeness issue, especially in urban areas, in which the site selection should be conducted prior to model evaluation. A methodology to resolve this issue is being developed at the ERG. Although the statistical measures indicate that the model is applicable for NO_2 and O_3 related policy applications, a few model improvements, such as the prediction of wind speed under stagnant condition, should be made. The dynamic evaluation indicates that the model is able to respond to changes of meteorology and emissions well while the diagnostic evaluation highlights the impact of underestimation of input emission on CMAQ prediction. A probabilistic evaluation which will provide a better insight of model deficiencies and further areas for model improvement is underway.

REFERENCES

AEA, 2009: Evaluating the Performance of Air Quality Models. AEAT/ENV/R/2793.

Beekmann, M. and C. Derognat, 2003: Monte Carlo uncertainty analysis of a regional-scale transport chemistry model constrained by measurements from the Atmospheric Pollution Over the Paris Area (ESQUIF) campaign. *J. Geophys. Res.*, **108**, D17, 8559.

Clapp, L.J and M.E. Jenkin, 2001: Analysis of the relationship between ambient levels of O_3, NO_2 and NO as a function of NOx in the UK. *Atmospheric Environment*, **35**, 6391-6405.

Chang, J.C. and S.R. Hanna, 2004: Air quality model performance evaluation. *Meteo. Atmos. Phys.* **87**, 167-196.

Guenther, A., C.N. Hewitt, D. Erickson, R. Fall, C. Geron, T. Graedel, P. Harley, L. Klinger, M. Lerdau, W.A. McKay, T. Pierce, B. Scholes, R. Steinbrecher, R. Tallamraju, J. Taylor and P. Zimmerman, 1995: A global model of natural volatile organic compound emissions. *Journal of Geophysical Research*, **100**, 8873–8892.

Sanderson, M.G., 2002: Emission of isoprene, monoterpenes, ethene and propene by vegetation, Hadley Centre Technical Note 40, UK Meteorological Office.

Sillman, S., 1999: The relation between ozone, NO_X and hydrocarbons in urban and polluted rural environments. *Atmospheric Environment*, **33**, 1821-1845.