COUPLING CMAQ-urban FOR FINE SCALE AIR POLLUTION AND ITS IMPACTS MODELLING FOR LONDON

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1. INTRODUCTION

Air quality models are one of the main tools providing evidence of the impact on air quality, of intergovernmental, national and local authority policies. Hence, model forecasts need to account for a range of policy options, including in Europe, compliance with NECD regulations (http://ec.europa.eu/environment/air/pollutants/ceilings.htm) and in the UK, policy's aimed at improving air quality and meeting climate change targets (http://www.defra.gov.uk/publications/2011/04/13/pb13378-air-pollution/). In the UK concerns are focused on meeting NO_2, PM_{10} and $PM_{2.5}$ EU limit values, on the impacts of short term climate forcing and on the impacts on sensitive ecosystems and crops. However, increasingly models are also being used as a source of human exposure information for epidemiological studies (Maheswaran et al., 2010, Tonne et al., 2010) and health impact assessments (e.g., Georgopoulos, et al., 2005., Isakov, et al., 2009 and Woodcock et al., 2011). Epidemiological requirements include annual mean concentrations to be made at fine spatial scales (post/zip code areas), and to look cross sectionally at health outcomes. However, increasingly there is a need for the epidemiological community to elucidate a combination of spatio-temporal influences and this places a further temporal demand on the models used. Finally, there is a need to take account space-time-activity data (Ashmore, 2005) in exposure assessments both for policy development and for example, to reflect the dose from pollutants that have a range of toxicity (PM) (Kelly et al., 2011) or of mixtures of pollutants (Molitor et al., 2011).

In an attempt to meet these demands in a large urban area, we describe the coupling of the Community Multiscale Air Quality (CMAQ) modeling system (Byun and Ching, 1999) and the ADMS model (CERC, 2006). We provide details of the models performance in predicting hourly NO_x-NO_2-O_3 concentrations over a detailed (20m x 20m) grid in London in 2006. The results for a similar run in 2008 have been reported elsewhere (Carslaw, 2011a).

2. CMAQ-urban COULPING

A tight coupled regional (CMAQ) and local (ADMS) model system was developed to model air quality for health and ecosystem impacts at fine spatial scale. A fortran interface coupled CMAQ v4.6, which provided urban background concentrations, with roadside concentrations based on the ADMS roads model (v2.3). Application of the ADMS model used methods similar to those described in Kelly et al. (2011). Six road categories were used in London including open (motorway), typical (average urban roads surrounded by low rise buildings) and 4 street canyons (classified by their orientation: north-south, east-west, southwest-northeast and southeast-northwest).

The CMAQ model was set up using 23 vertical layers with 7 layers under 800m and 3 horizontal nesting levels, downscaling from 81km over Europe to 9km over London. Anthropogenic and natural source emissions for CMAQ were derived from European Monitoring and Evaluation Programme (EMEP, http://www.ceip.at/), European Pollutant Release and Transfer Register (E-PRTR, http://prtr.ec.europa.eu), the National Atmospheric Emissions Inventory (NAEI, http://naei.defra.gov.uk/) and the London Atmospheric Emissions Inventory (LAEI, http://data.london.gov.uk) and were processed into gridded hourly chemical species using speciation and temporal profiles developed in AQMEII. Biogenic emissions such as isoprene and terpene, were estimated for both years using high resolution CORIN land cover data, meteorological data from WRF and methods described by Guenther et al. (1995) and Sanderson (2002).

For the ADMS model, road traffic NO_x and NO_2 emissions data was taken from the LAEI (http://data.london.gov.uk). Hourly emissions profiles of NO_x and NO_2 were derived from 37 automatic traffic counts in London.

For the NO_x, NO_2 and O_3 chemistry close to roads, the CMAQ-urban model adopted a simple

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chemical scheme, described in Carslaw and Beevers (2005), whilst v4.6 of the CMAQ model used CB-05.

The ADMS model in CMAQ-urban used the hourly meteorological inputs, wind speed and direction, temperature, surface sensible heat flux and planetary boundary layer height. All were predicted from the Weather Research and Forecasting (WRF) model (Skamrock et al., 2008). The urban model domain covered the whole of London with 3151x3151 cells of 20m x 20m grid resolution. Model outputs included hourly maps of NO_x, NO_2 and O_3 concentrations with 20m x 20m grid resolution

The results from the model were analysed using methods described in the UK Department of the Environment, Food and Rural Affairs (DEFRA) model evaluation protocol (AEA, 2009) and used the 'OpenAir' software (http://www.openair-project.org). The model results were compared against 85 monitoring stations from the UK and London monitoring networks (http://www.londonair.org.uk/LondonAir/Default.aspx), including 22 urban background, 16 suburban, 40 roadside and 7 kerbside sites. Statistical measures of model performance included fraction within factor of two of the observations (FAC2), mean bias (MB), normalized mean bias (NMB) and root mean square error (RMSE) and correlation coefficient (r).

5. RESULTS AND DISCUSSION

5.1 Annual 2006 results analysis

An example of annual mean NO_2 concentrations in 2008 is shown in Figure 1. From these results it is clear that the model is able to capture the spatial distribution of traffic related concentrations associated with London's road network and the M25 orbital motorway. NO_2 (and NO_x) concentrations decrease according to distance from central London, where the highest concentrations occur. As expected, the spatial distribution of O_3 concentration (not shown) shows the opposite of this NO_2 concentration pattern, with the minimum concentration being in the central urban area and close to road sources.

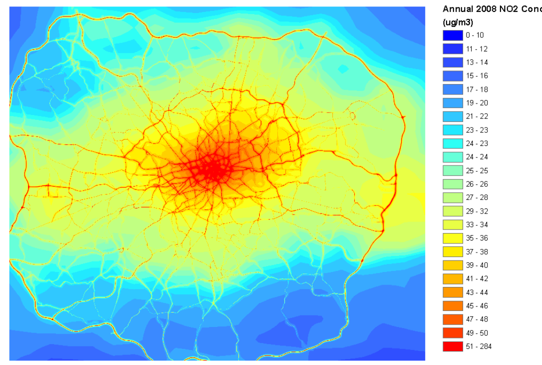

Fig. 1. Annual 2008 mean NO_2 concentrations for London

The suitability of combining the CB-05 mechanism with the simple NO_x-NO_2-O_3 roadside chemistry scheme was assessed by comparing the concentrations of NO_2 and O_3 as a function of NO_x in 2006 against measurements at curbside, roadside, suburban and urban background sites. An example of which is given for Marylebone road (Figure 2), a central London curbside, street canyon site. The analysis indicates that CMAQ-urban is able to capture NO_x-NO_2-O_3 relationship at this location reasonably well, although there is evidence of underprediction of NO_2 which is consistently seen at other curbside sites.

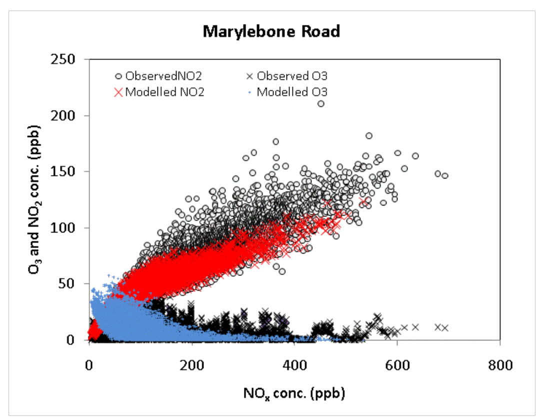

Fig. 2. Observed and modeled NO_2, O_3 and NO_x relationship at Marylebone Road in 2006

Scatter plots of the hourly model results were averaged into curbside, roadside, suburban and urban background locations. Figure 3 and 4 show the modeled vs. observed hourly NO_2 and O_3, respectively. Because it is difficult to distinguish the relationship in scatter plots that only use one color we have included a red to blue scale which indicates the frequency of hourly model-measurement pairs. The figures show that the highest density of data is within +/- FAC2 (dashed lines) for both NO_2 and O_3. As a consequence the model appears to predict NO_2 and O_3 reasonably well at most site locations. However, a large negative bias (NO_2) and positive bias (O_3) at kerbside sites was observed, especially at high concentrations.

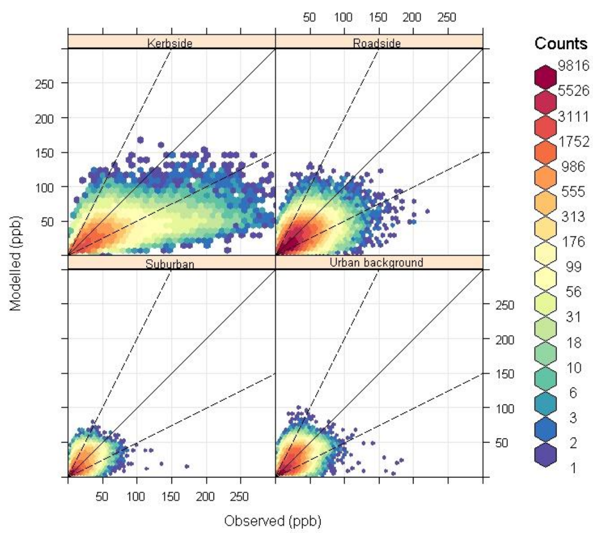

Fig. 3. Scatter plot of observed and modeled NO_2 concentrations at kerbside, roadside, urban background and suburban sites in 2006.

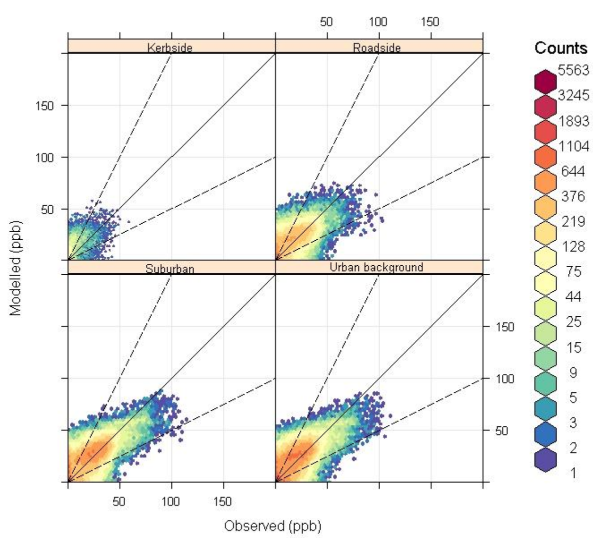

Fig. 4. Scatter plot of observed and modeled O_3 concentrations at kerbside, roadside, urban background and suburban sites in 2006.

Diagnostic measures of model performance are shown in Table 1 and include FAC2 values, which indicate that for the 'All sites' category, more than 70% of modeled of NO_2 results and 60% of modeled O_3 are within factor of two of the observations. The model under predicts NO_2 with a mean bias (MB) of approximately 5 ppb and a normalized mean bias (NMB) of -17%. The Root mean squared error (RSME) and R value for NO_2 are ~18% and 0.6, respectively. In contrast, O_3 is over predicted by approximately 3ppb giving a NMB of 15%, a RMSE of 12% and an r value of 0.64.

Table 1. Statistical measures of model performance in 2006.

Poll	Site	FAC2	MB (ppb)	NMB	RMSE (%)	r
NO_2	All	0.73	-4.73	-0.17	17.73	0.58
O_3	All	0.61	2.84	0.15	12.13	0.64
NO_2	KS	0.64	-19.0	-0.39	38.12	0.58
NO_2	RS	0.75	-4.98	-0.17	16.29	0.56
NO_2	SU	0.71	-0.79	-0.05	10.76	0.58
NO_2	UB	0.74	-2.09	-0.10	12.25	0.55
O_3	KS	0.37	5.63	0.68	11.12	0.50
O_3	RS	0.60	2.97	0.17	11.94	0.59
O_3	SU	0.66	2.70	0.13	12.41	0.65
O_3	UB	0.61	2.64	0.14	12.09	0.64

The results across the range of site categories show that the model performance deteriorates as you move from background to roadside locations, with the curbside sites showing the poorest model performance. The evaluation of NO_2 predictions at curbside sites give the FAC2, MB, NMB, RMSE and r results of 0.64, -19 ppb, 0.39, 38% and 0.58, respectively which represents an important reduction in performance, even when compared to the roadside results. Likewise the O_3 results at curbside locations are poor.

Hour of the day and day of the week temporal variations of NO_2 and O_3 were also analysed, although not shown here. These results showed that the model under predicts NO_x and NO_2 during midday and night time periods at urban background and suburban sites.

Finally, according to the DEFRA model evaluation protocol for 2008 (Carslaw, 2011a) and 2006 presented in this paper, the model performance is acceptable for regulatory purposes for all locations except at kerbside. At these locations further improvement is needed.

6. CONCLUSIONS

A tight coupled CMAQ-urban modelling system was developed for London to give fine temporal and spatial scale (hourly and 20mx20m) NO_X, NO_2 and O_3 concentrations. The model used a combination CMAQ v4.6 to predict background concentrations and the ADMS roads model (v2.3) to represent the dispersion from road traffic. Highly detailed road traffic emissions were taken from the LAEI 2006 and 2008.

Model predictions of NO_2 and O_3 were assessed using the DEFRA model evaluation protocol. The model was able to represent the observed NO_x-NO_2-O_3 chemistry at roadside sites such as Marylebone road reasonably well. The model also captured the spatial distribution of NO_2 and O_3 concentrations across London. Using observations from 85 monitoring sites at locations which included urban background, suburban, roadside and kerbside sites, the model predicted NO_2 and O_3 concentrations reasonably well, with 73% of hourly NO_2 concentrations within a factor of 2 of measurements and a RMSE of 17%. For O_3 similar results were obtained with 61% of hourly concentrations within a factor of 2 of measurements and a RMSE of 12%. However at at curbside sites the model under predicted NO_2 by a larger margin and especially at high hourly concentrations.

Average concentrations by hour of the day and day of the week show there to be a negative model bias at night time, associated with over predicted nighttime wind speed in WRF. During midday, the negative bias may be due to the fact that a total traffic temporal profile was used to scale the emissions into hourly values, rather than separate profile for individual vehicle types.

However, any number of reasons could be made for the errors occurring at locations close to road traffic, not least the uncertainty in emissions, the uncertainty in traffic estimates and breakdown of hourly vehicle flows on the roads closest to the measurement sites. In addition, the effect of multi-lane roads and the existence of tidal traffic flows are potentially influential. Furthermore, the simplicity of the street canyon model within ADMS roads and defining street canyon characteristics are other important sources of error, as are those associated with the WRF meteorological inputs, used in both CMAQ and ADMS.

Recent work on road traffic NO_X emissions estimates, Carslaw, et al. (2011b), show evidence that NO_X emissions trends for recent years and for light vehicles in particular are likely to be under predicted and that this is partly reflected in the results presented here.

Despite these potential sources of error, this paper demonstrates that the use of CMAQ-urban for the prediction of O_3 and NO_X/NO_2 concentrations in London is promising. And that at the spatial and temporal scale described it can be used for health impact assessments, epidemiological study, detailed human exposure assessments and to assess compliance with air quality legislation. Finally, forecasts of PM concentrations, using similar methods and version 5 of CMAQ, will be the subject of future work.

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