CMAQ-Urban: UK FINE SCALE MODELLING FOR DYNAMIC EXPOSURE STUDY

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1. INTRODUCTION

Predicting people's exposure in the micro-environments, associated with their daily activities, is important in determining human health risks and to address the issue of exposure misclassification (HEI, 2010). Whilst personal exposure monitoring is increasingly used to estimate the air pollution exposure of individuals, the lack of spatial coverage leads to the need for additional tools that are capable of predicting outdoor ambient concentrations, where measurements are not available. A large number of techniques exist to estimate outdoor concentrations, including land use regression (Briggs, et al., 1997, Dons, et al., 2014), dispersion or chemical transport modelling (Nonnemacher, et al., 2014 and Bentayeb, et al., 2014), stochastic techniques using artificial neural networks (Ibarra-Berastegi, et al., 2008) and Monte Carlo simulation (McCreddin, et al., 2015). Here we use a dispersion modelling which accounts for the strength of emissions from different sources and the physical and chemical processes that influence transport, transformation and deposition of air pollutants (de Hoogh, et al., 2014). Dispersion models are attractive since they generate high temporal and spatial resolution air pollution concentrations and are suitable for both 'what-if' scenarios and for future air pollution and health forecasts (Batterman, et al., 2014).

With significant numbers of the UK population living or working near roads and epidemiological and toxicological evidence supporting the notion that transport related air pollution contributes to an increased risk of death from cardiopulmonary and respiratory disease (WHO, 2005), there is a need for street scale dispersion modelling. In response to this need, the CMAQ-Urban model was developed to predict outdoor air pollution at street level as part of the UK research council project, "Traffic Pollution and Health in London" (Beevers, et al., 2012a). The CMAQ-Urban couples the Community Multi-scale Air Quality (CMAQ) model (Byun and Ching, 1999) and ADMS-Roads model (CERC, 2006), and is capable of predicting hourly NO_x, NO_2, O_3, PM_{10} and $PM_{2.5}$, at 20m grid resolution. As such the CMAQ-Urban model can be used for predicting the exposure of cyclists and pedestrians outdoors and in combination with micro-environmental mass balance models to calculate indoor air pollution within vehicles, trains, buses and buildings.

For those people within the London population who travel beyond the capital, CMAQ-Urban has been extended to predict hourly concentrations at 20m grid resolution over the whole of the UK. To make this scale of prediction possible, the model Fortran code has been parallelized with a Message Passing Interface (MPI) to minimize the model's runtimes. The extension of CMAQ-urban for UK applications has been supported by the National Institute for Health Research (NIHR) project, "the Public health air pollution impacts of different pathways to meet the UK Climate Change Act commitment to 80% reduction on CO_2 and other greenhouse gas emissions by 2050". This paper discusses the performance of the CMAQ-urban at UK scale and its application to the London Hybrid Exposure Model (LHEM).

2. CMAQ-urban APPROACH

The CMAQ-Urban model interface was written using Fortran and has been parallelized with the Message Passing Interface (MPI) to improve model speed. The interface links meteorology from the Weather Research and Forecasting (WRF) model (Skamrock, et al., 2008), background concentrations from CMAQ, and dispersion of road transport pollutants from the ADMS-Roads model. A simple near road NO_2-NO_x-O_3 chemistry scheme (Carslaw and Beevers, 2005) is included within the interface. In the current version of the CMAQ-urban and close to traffic sources (5-225m), the exhaust component of PM_{10} and $PM_{2.5}$ is treated as an inert species.

An inline bottom-up road emissions module is integrated in the interface and is using the approach described in Beevers, et al. (2012b).

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The emissions factors are derived from a remote sensing device (RSD) for NO_x (Carslaw and Rhys-Tyler, 2013), from the UK Department for Transport (DFT) for exhaust PMs (http://www.dft.gov.uk/matrix) and for non-exhaust PMs from the London Atmospheric Emissions Inventory (http://data.london.gov.uk/dataset/ london-atmospheric-emissions-inventory-2010). The emissions model includes 11 vehicle types, with vehicle speed based upon the road types including motorway, dual carriageway, and single carriageway. The emissions are disaggregated into hourly values using the hourly profile of road traffic from 37 automatic traffic count sites in London. Currently emissions are calculated for over 17,000 UK major roads (Figure 1).

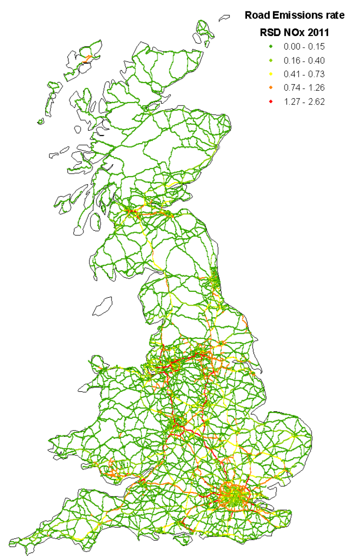

Fig. 1. NO_x emission rates for UK major road links (g km^{-1} s^{-1})

The CMAQ-Urban outputs include; (i) maps of mean concentrations of NO_x, NO_2, O_3, PM_{10} and $PM_{2.5}$ at 20m grid resolution, (ii) concentrations at selected receptors for model evaluation, and (iii) concentrations for exposure estimation following each individual travel routes (optional). The output of hourly concentration maps is also optional.

2.1 WRF/CMAQ model

The WRF v3.4.1/CMAQ v5.0.1 model uses a domain of 23 vertical layers with seven layers under 1km and one horizontal nesting level, downscaling from 50km over Europe to 10km over the UK. Lateral boundary conditions for the WRF model were taken from the Global Forecast System (GFS) model at 6hr intervals and at 1° grid resolution and USGS land cover data were used. The physics options used for the simulation include Rapid Radiative Transfer Model (RRTM) longwave radiation scheme (Mlawer et al., 1997), Dudhia shortwave radiation scheme (Dudhia, 1989), Kain-Fritsch cumulus scheme (Kain, 2004), WSM6 microphysics scheme (Hong and Lim, 2006), Pleim-Xiu surface layer scheme (Pleim, 2006), Rapid Update Cycle (RUC) land surface model (Benjamin, et al., 2004), and Asymmetric Convection Model 2 Scheme (ACM2) scheme (Pleim, 2007) for planetary boundary layer parameterization.

The anthropogenic emissions for CMAQ were derived from the European Monitoring and Evaluation Programme (EMEP, http://www.ceip.at) and the European Pollutant Release and Transfer Register (E-PRTR, http://prtr.ec.europa.eu) for Europe, and a combination of the National Atmospheric Emissions Inventory (NAEI, http://naei.defra.gov.uk) and the King's road traffic emissions for the UK. The annual emissions data were processed into gridded hourly chemical species using the speciation and temporal profiles from AQMEII (http://aqmeii.jrc.ec.europa.eu/). The biogenic emissions and plume rise for point source emissions were calculated using SMOKE v2.6 (https://www.cmascenter.org/smoke). The boundary conditions were derived from the Monitoring Atmospheric Composition and Climate project (MACC, http://www.gmes-atmosphere.eu). The CMAQ simulation was performed with CB-05 with aerosol and aqueous chemistry.

Analysis of CMAQ's PM predictions showed that secondary organic aerosol (SOA) was under predicted by approximately 1.7 μg m^{-3}; and so a correction of 1 μg m^{-3} was added to the background concentrations prior to CMAQ-Urban simulation. The value of 1 μg m^{-3} was also added to compensate a lack of biomass burning sources within the UK emissions model and was based upon the study on biomass burning contribution to aerosols in London and the UK Fuller, et al. (2014).

2.2 ADMS-Roads model

The ADMS-Roads v2.3 model has been used to estimate the dispersion of primary pollutants across regular grid with 5m spacing and within 225 m of the center of a road. The dispersion grid is estimated for six road categories initially using a constant road emission rate of 1 g km^{-1} s^{-1} and meteorological fields from WRF including wind speed and direction, temperature, surface sensible heat flux and planetary boundary layer height. The concentration from individual road is accounted for by scaling the 1 g km^{-1} s^{-1} value by each road's emission. The road categories include open (motorway), typical (average urban roads surrounded by low rise buildings) and 4 street canyons classified by their orientations (north-south, east-west, southwest-northeast and southeast-northwest).

3. RESULTS AND DISCUSSION

3.1 Model runtimes

Model runtimes have been measured using test simulations in London on a machine with 6 dual core 3GHz CPUs and 96GB RAM. Using the parallel code the CMAQ-Urban model runtime, using all 12 processors, was reduced by approximately a factor of 4, compared with a simulation using a single processor. Figure 2 shows the model runtimes against the number of processors indicating that the runtime can be reduced by about a factor of 3 using 6 processors with a small additional benefit gained by using a higher number of processors, and driven by the architecture of the machine and the CMAQ-urban code.

Within this study, the model runtime for UK annual simulations of NO_X, NO_2, O_3, PM_{10} and $PM_{2.5}$ is approximately 8 days on a Linux cluster with 8 slave nodes (6 dual core 3GHz CPUs and 48GB RAM on each node), plus 6 days for WRF/CMAQ simulations. Based on a small test on the NERC's ARCHER supercomputer, the model runtime can be further improved by a factor of 3-5.

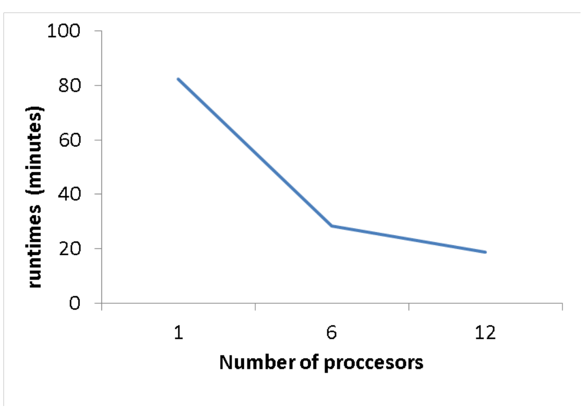

Fig. 2. Comparison of model runtimes for one day simulations for London against the number of processors

3.2 Model performance analysis

The predicted hourly NO_2, O_3, $PM_{2.5}$ and PM_{10} has been compared with measurements from 144 UK monitoring stations all having ≥75% data capture. The performance statistics (Table 2) indicate that 80% of modelled data are within factor of 2 of the measurement. The model yields small positive biases of 0.4 ppb (2%) and 1.5 ppb (7%), for NO_2 and O_3, respectively, and negative biases of 4 μg m^{-3} (16%) and 1 μg m^{-3} (7%) for PM_{10} and $PM_{2.5}$. The RMSE values are 11.8, 8.8, 13.0 and 9.3 for NO_2, O_3, PM_{10} and $PM_{2.5}$, respectively. The r values are 0.8 for both NO_2 and O_3 and 0.7 for PM_{10} and $PM_{2.5}$.

Table 2. Performance statistics of CMAQ-Urban in predicting NO_2 (ppb), O_3 (ppb), PM_{10} (μg m^{-3}) and $PM_{2.5}$ (μg m^{-3}), year 2011.

Pollutant	Number of data	Observed mean	Modelled mean	FAC2	MB	NMB	RMSE	r
NO_2	2681929	20.1	20.5	0.8	0.4	0.02	11.8	0.8
O_3	1605883	20.2	21.7	0.8	1.5	0.07	8.8	0.8
PM_{10}	2556574	23.4	19.7	0.8	-3.7	-0.16	13.0	0.7
PM_{25}	1860753	14.9	13.9	0.8	-1.0	-0.07	9.3	0.7

Note: FAC2 = factor of two of measurement, MB = mean bias, NMB = normalized mean bias, RMSE = root mean square error, and r = correlation coefficient

The temporal variation of modelled NO_2, NO_x, O_3, PM_{10} and $PM_{2.5}$ agree reasonably well with observations, although a large negative bias is observed in NO_x and PM_{10} predictions (Figure 3). The negative bias in PM_{10} particularly during daytime may be attributed to the missing emissions sources such as resuspended dust and the under prediction of SOA. The negative bias of NO_x is attributed to the under prediction at kerbside locations within 5m of the road. Figure 3 also shows diurnal and monthly variations of NO_2 at airport, kerbside, roadside, rural, suburban and urban background sites. Whilst the model is able to capture the magnitude of NO_2 well at most locations, a similar large negative bias occurs during the daytime at kerbside sites and a small positive bias is observed at rural and suburban sites. The monthly profiles also consistently show a negative bias at kerbside sites and a small positive bias at rural and suburban sites. The under prediction close to roads and over prediction at suburban and rural locations suggests that the bias in NO_x and NO_2 predictions may be due to a bias in the spatial distribution of the emissions.

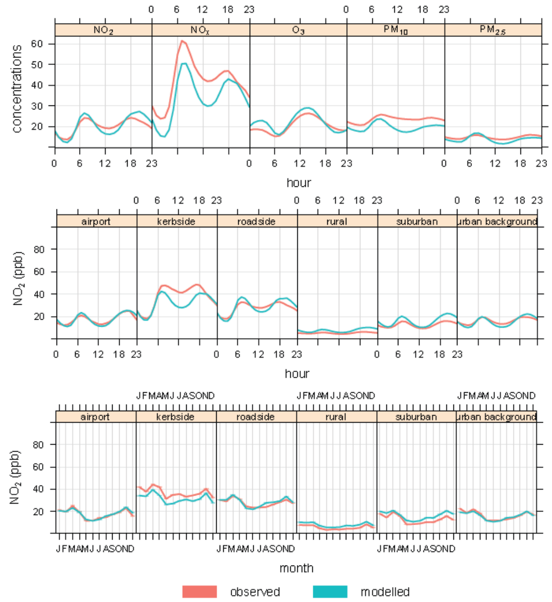

Fig. 3. 2011 annual average diurnal profiles of observed and modeled NO_2, NO_x, O_3, PM_{10} and $PM_{2.5}$ concentrations (top, ppb for gases, μg m^{-3} for PMs) and diurnal (middle) and monthly (bottom) profiles of NO_2 at airport, kerbside, roadside, rural, suburban and urban background sites.

However, as demonstrated in Figure 4 by the inset maps of London using 10km and 2km grids, the use of the coarse grid resolution may be partly responsible. To test this, a spatial analysis shows that increasing the grid resolution of background concentrations is important for NO_x and NO_2 with the spatial gradient of pollutant concentrations and the hot spots, such as Heathrow airport, much better captured using a 2km grid improving the negative bias at kerbside locations and negative bias at rural and suburban sites. Further investigation is required.

For the benefit of further development of the model, it is worth pointing out that the current results may slightly suffer from the double counting as traffic emissions were included in the CMAQ simulation. The double counting of traffic pollutant in background concentrations is estimated to be somewhat less than 1% (Beevers, et al 2012a). The double counting of traffic pollution can be eliminated using CMAQ-DDM to provide the more accurate background concentrations.

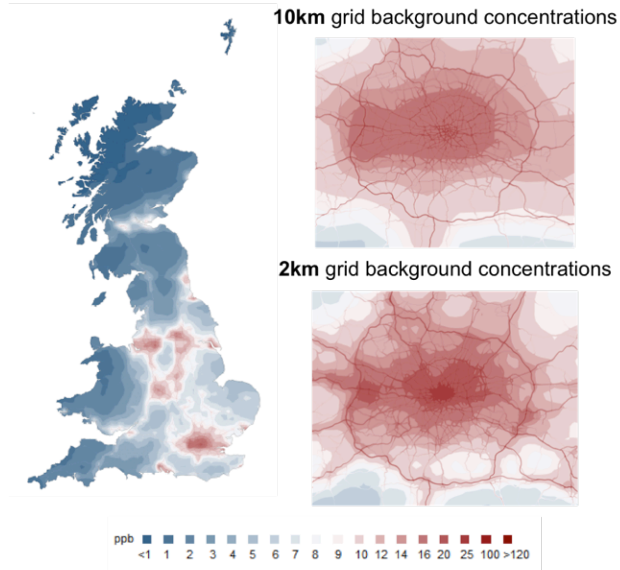

Fig. 4. 2011 Annual mean NO_2 concentrations for UK using 10km grid background concentrations (right) and for London using 10km and 2km grid background concentrations (left).

3.3 Application in hybrid exposure model

The CMAQ-Urban prediction in combination with micro-environmental mass balance models have been used to estimate the indoor concentrations within vehicles, trains, buses and buildings, and outdoors for the exposure of cyclists and pedestrians. In combination with space-time activity data taken from the London Travel Demand Survey and provided by Transport for London (David Wilby, personal communication) the time-activity based exposure to $PM_{2.5}$ and NO_x has calculated for 45,079 individuals. Figure 5 shows an example of the $PM_{2.5}$ exposure of a person during their daily journey. In this case the person started their journey by walking to an underground station at 8am and then travelling on an underground train for about half an hour before taking a bus to their destination. After spending some time at their destination, they returned home at lunchtime via the same route, using the same transport modes and then stayed at home from 12:30pm onward. The calculation shows that his exposure to $PM_{2.5}$ varies significantly across the journeys and in different locations. The highest level exposure to $PM_{2.5}$ is approximately 94 μg m^{-3} when they travelled via the underground.

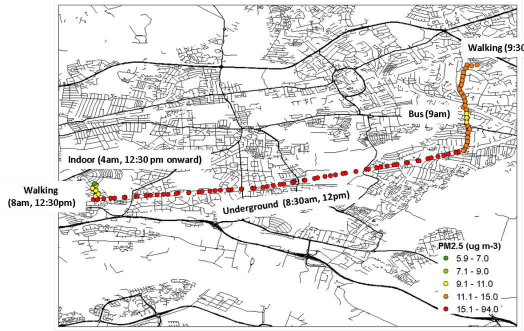

Fig. 5. Sample of exposure to $PM_{2.5}$ of a person during the course of the day

The exposure estimates of all individuals within the sample population of 45,079 can then be aggregated up to represent the entire London population. When compared with the exposure estimated using the residential address, the average exposure to NO_x and $PM_{2.5}$ using time-activity exposure model is ~60% and ~40%, respectively, less. This is a combination of the London population spending 90% of their time indoors and the effect of indoor/outdoor ratios. Note that this analysis does not include the effect of indoor sources. These differences highlight the exposure misclassification encountered using residential address and emphasize that the time-activity approach has the capability to produce accurate estimates of exposure, provided the ambient concentrations in different microenvironments are robust.

4. CONCLUSIONS

CMAQ-Urban has been extended to predict fine spatio-temporal scale of outdoor air pollution at UK national level for time-activity human exposure studies. An annual simulation can be accomplished within an acceptable time frame using the parallel CMAQ-Urban model code.

The model evaluation shows that the model results are in good agreement with the measurements, although some improvements are needed such as for SOA, biomass burning and re-suspended aerosols at background locations. The spatial distribution of model output can be further improved using a finer grid resolution of background concentrations and this may also reduce the negative bias at kerbside sites and positive bias at rural and suburban sites. Although a small error of less than 1%, double counting in CMAQ-Urban can be eliminated using CMAQ-DDM. The study has demonstrated that the output from CMAQ-Urban can be used in time-activity population exposure studies to provide more realistic exposure estimates.

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6. ACHKNOWLEDGEMENT

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