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ADMS-URBAN: DEVELOPMENTS IN MODELLING DISPERSION FROM THE CITY SCALE TO THE LOCAL SCALE

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Abstract: ADMS-Urban, an advanced three dimensional, quasi-Gaussian model nested within a simple trajectory model, has been used to model urban air quality in many cities across the world, calculating street scale resolution of concentration over city-scale domains. It has been used for all the purposes described under the EU Air Quality Directive, namely: assessment of compliance with air quality limit values; planning and mitigation; source apportionment; short term forecasting. In assessing compliance with the PM10 air quality limit values, cities including London are increasingly looking into pollution hotspots where local effect such as street canyons and the street geometry are important. There is also increasing awareness of the importance of modelling spatial variations in the urban background and the influence of changes in meteorology on the urban scale on this background.

Since its initial development ADMS-Urban has modelled the local (street scale) impact of two-sided, symmetrical street canyons on dispersion within the canyon using a model based on OSPM (Operational Street Pollution Model) (*Kakosimos et al, 2011*). It has allowed for the impact on dispersion immediately downwind of a street of noise barriers on one or on both sides of a street. It has considered NO_x chemistry (NO, NO_2, O_3, VOC) and generation of sulphate using a local chemistry model and also a grid-based trajectory model to account for the chemical reactions on the city-scale.

This paper describes ongoing developments that extend the application of ADMS-Urban at both city and the local scale. At the city scale ADMS-Urban has been developed to use gridded meteorological and chemistry output from regional models (with grid scale down to 1km). This nesting of ADMS-Urban within a regional-scale numerical model allows seamless modelling from regional through to the local (street) scale. At the street scale ADMS-Urban is being extended to model explicitly a number of local effects including single-sided and asymmetrical street canyons, streets on embankments, streets in cuttings, elevated roads (flyovers) and tunnel exits.

Key words: *Air quality modelling, nesting, EU air quality directive, pollution hotspots*

INTRODUCTION

Regional models are essential tools for modelling the dispersion of pollutants over large distances. They are driven by spatially and temporally varying meteorological output from meso-scale models, and are able to model deposition and chemical processes that occur over a large range of temporal and spatial scales. These models are sometimes applied at relatively high resolution in urban areas, but even then they are unable to resolve the large concentration gradients that occur, for instance, close to roads. It is in these locations that air pollutant concentrations may be highest, so an alternative modelling approach is required.

Gaussian plume models are able to resolve the details of concentration fields within an urban area by explicitly representing the near-field features of the dispersion of emissions from all source types; for instance, point, line, area, volume, road and airport runway source types can be modelled. However, the most widely used models of this type (for example, the ADMS suite of models (*CERC, 2010a*), AERMOD (*Cimorelli et al, 2004*) and OML (*NERI*, 2011) are not applicable over large distances because they are limited by their use of stationary and usually spatially homogeneous meteorology, and by their inability to model the stagnation of emissions that occurs at low wind speed conditions.

Whilst it would be possible to develop local models to be applicable over larger areas, a simpler approach that accounts for the full range of temporal and spatial scales is the 'nesting' of a local model within a regional one. An example of this is presented in this paper, with the regional model selected being the US EPA Community Multiscale Air Quality, CMAQ model (*Byun and Schere*, 2006; *US EPA*, 2010), and the local model being ADMS-Urban (*CERC*, 2010b). Preliminary results are presented for the case where the CMAQ domain extends 60 km in all directions from the centre of London, covering the majority of south east England; the detailed ADMS-Urban modelling domain is a 27 km^2 area within central London, which contains 17 continuous monitors that can be used for model validation.

Other attempts have been made at nesting, for instance, some calculations of nesting ADMS 4 within CMAQ have been presented in the Review of Air Quality modelling by Defra (*Williams et al, 2011*); however that methodology is subject to 'double counting' of emissions.

A general overview of the way in which ADMS-Urban has been 'nested' within CMAQ is given in the first section below. This is followed by details of the way in which CMAQ and ADMS-Urban have been set up to model the region of interest. Comparisons of model predictions against measured concentrations are then presented, followed by a brief discussion of results.

OVERVIEW

In the nesting of ADMS-Urban within CMAQ the key criteria which need to be followed are the utilization of the respective strengths of the two models but the avoidance of 'double counting' of emissions which will occur if the concentrations from a local model are simply added to those from a regional model. ADMS-Urban is therefore used for the dispersion of pollutant for a relatively short time scale after its release, whilst CMAQ is used for the longer timescales. More specifically ADMS-Urban is run using explicit representation of sources for pollutants with age (time since release) no greater than a time τ_m for

the pollutant to be well mixed over the CMAQ grid scale. The CMAQ model output is used to model the concentrations of pollutants with age greater than τ_m. At each output time CMAQ actually calculates dispersion of pollutants of all ages including emissions of age less then τ_m, so adjustment must be made to the CMAQ output before it is combined with the ADMS-Urban output; i.e. the contribution to CMAQ of pollutants with age less than τ_m needs to be subtracted from the CMAQ output. This contribution is estimated by using the grid model within ADMS-Urban run at the same spatial resolution as CMAQ.
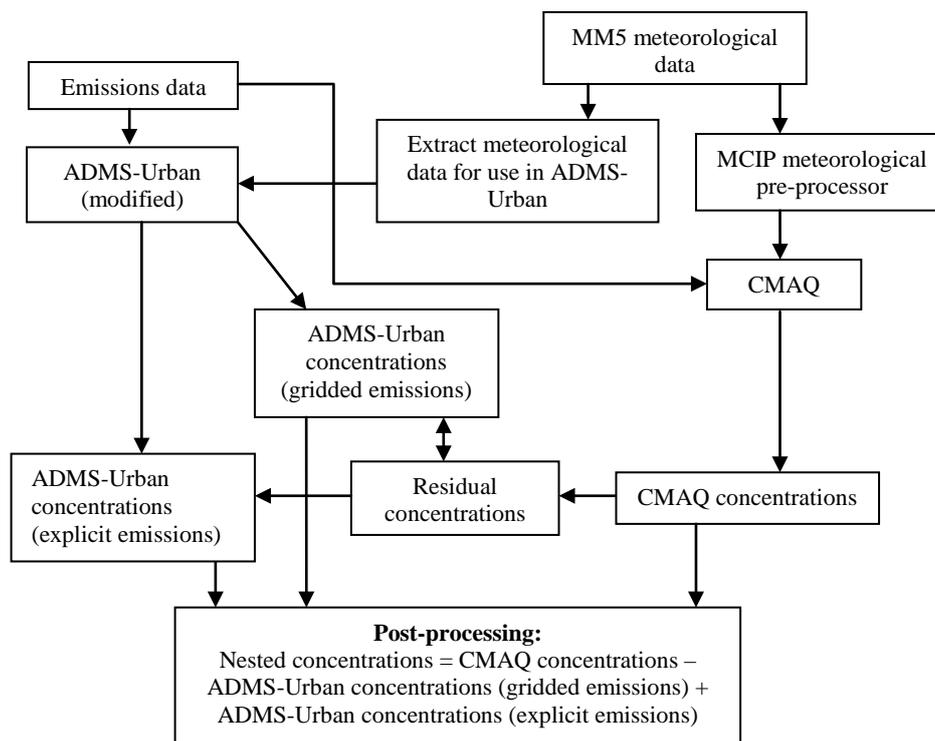
Figure 28. Flow chart showing the system used to nest ADMS-Urban within CMAQ.

Figure 28 gives an overview of the system used to nest ADMS-Urban within CMAQ. The same source emissions and meteorological data underlie both the local and regional models, with ADMS-Urban modelling the majority of emissions explicitly (for example, road sources), and CMAQ modelling emissions averaged over each grid cell; ADMS-Urban uses a single condition to represent the meteorology for each time step, whereas CMAQ models the spatial and temporal variation of meteorology over the domain.

ADMS-Urban is a steady state Gaussian plume model, which does not allow for any history of concentrations from previous time steps. In order to account for this, in the generally available version of the model, no limit is applied to the source-receptor travel time within the plume. This approach is reasonable if changes in emissions and meteorology over successive hours between time steps are small, but it is less accurate when conditions change significantly with time.

A modified version of the ADMS-Urban model has been developed that allows truncation of the plume based on the source-receptor travel time. This means that when nesting ADMS-Urban within CMAQ, it is possible to ensure that only concentrations from the initial dispersion of the emissions are taken into account, up to the time at which they become well mixed enough to be modelled as a grid source. This implementation of nesting a local model within a regional model avoids the 'double counting' of concentrations from previous time steps.

When run as a stand-alone model, ADMS-Urban uses hourly estimates of concentrations upwind of the model domain as boundary conditions for a trajectory model which in turn provides the urban background concentrations as boundary conditions for ADMS. When nesting ADMS-Urban within a regional model the urban background concentrations within the nested domain are calculated as the difference between the CMAQ concentrations and ADMS-Urban concentrations calculated using the grid model at the same spatial resolution as CMAQ for emissions of age less than τ_m using rural upwind concentrations as the upwind boundary condition. Ideally the background would vary spatially, but in the first implementation of the nesting system presented in this paper, an average over the nesting domain has been taken.

MODEL DESCRIPTION

This paper presents preliminary results from the system for a model set up in which a number of simplifications have been made. For instance, only detailed emissions of NO_x, NO_2 and ozone have been included, and emissions from large point sources have been neglected from the modelling. A single CMAQ domain only has been modelled, whereas ideally some nesting of the regional model should be implemented within the system. All calculations were performed in a Lambert conformal coordinate system. A five day period from July 2008 was considered for this an initial case study.

Emissions

The emissions for the model were taken from the London Atmospheric Emissions Inventory (*AEA*, 2010) and the UK's National Atmospheric Emissions Inventory (*Bush et al*., 2010). For the border region where these two inventories overlap, the detailed emissions from the LAEI were assumed to be more accurate. As mentioned above, the emissions from large point sources were omitted from both inventories.

Meteorology

Output from the meso-scale model MM5 (version 3.7) (*NCAR/Penn State University,* 2003) was used. The MM5 domain covered 75 km in each direction from the centre, but the outermost 15 km (5 cells) in each direction were not used for CMAQ in order to avoid meteorological boundary effects distorting the CMAQ dispersion results. The first 48 hours of the MM5 simulation were also neglected, for similar reasons.

Regional model set up

The emissions were aggregated onto 3 by 3 km^2 grid cells. The region extended 60 km in each direction from the centre of the nested domain. All emissions were assumed to be released within the lowest layer of the CMAQ vertical grid, approximately 0-14.4 m above the surface. As the model was not nested within a larger-scale regional model, simplified initial and boundary conditions were used. Specifically, time-averaged NO, NO_2 and ozone profiles were derived from the monitored concentrations at Lullington Heath, Rochester, Wicken Fen and Harwell for the southern, eastern, northern and western domain boundaries respectively. Although emissions of aerosols were not included within the modelling, it was necessary to include estimates of concentrations of these species in the initial and boundary conditions in order for the CMAQ model run to converge; similarly estimates of VOC concentrations were included.

The chemical mechanism used in CMAQ was CB-05, with the version 5 aerosol mechanism and aqueous chemistry. Dry deposition could not be calculated within the main chemistry-transport module of CMAQ due to the unavailability of suitable land-use fraction data, which also affected the minimum eddy diffusivity calculations.

Local model set up

Two ADMS-Urban model scenarios were developed: one for nesting within CMAQ and one as a stand-alone model for comparative purposes. For both runs, emissions from all major roads within the nested model domain were modelled explicitly. Other details of the model configurations are given in Table 3 below.

Table 3. Details of the ADMS-Urban model

Model feature	Nested ADMS-Urban model run	Stand-alone ADMS-Urban model run
Road emissions	Explicit within the nested domain	Explicit within the nested domain
Small point source emissions	Aggregated onto a 1 by 1 km^2 grid within the nested domain	Modelled explicitly
Other emissions	Aggregated onto a 1 by 1 km^2 grid within the nested domain	Aggregated onto a 1 by 1 km^2 grid over the whole of Greater London
Source-receptor travel time	Limited to 2 hours	Unlimited
Meteorological data	Local meteorological derived from the meso-scale data	Upwind rural meteorological data
Background concentration data	Urban (residual) concentrations	Upwind rural concentrations

MODEL PREDICTIONS AND COMPARISON WITH MEASUREMENTS

17 continuous monitors are located within the 27 km^2 nested modelling region. All recorded NO_x and NO_2 concentrations, whilst only 5 recorded ozone concentrations within the time period considered. The monitors are classified according to their locations: kerbside, roadside and urban background. Figure 2 a) to e) presents the modelled concentrations against the monitored values for NO_x, NO_2 and ozone, with values averaged over the five days included in the study; values at background sites are presented separately from those at kerbside/roadside sites for NO_x and NO_2 due to the difference in the magnitude of values at these locations.

The results must be viewed as preliminary because of the short period considered in the calculations, however, as expected, the plots show that whilst the regional model, CMAQ, gives good estimates of the measured concentrations at urban background sites, it significantly underestimates the concentrations at the kerbside and the roadside sites. Both the nested and stand-alone versions of ADMS-Urban give reasonable estimates of the concentrations at all site locations. The local models have a tendency to slightly underestimate the NO_x and NO_2 concentrations, but this will in part be due to the lack of inclusion of the emissions from large point sources in the study. The differences in predicted concentrations between the two configurations of the local model are small for the scenario considered; however, for other meteorological conditions, for instance during low wind conditions, differences may be more significant.

In this preliminary implementation of the nesting of ADMS-Urban, the 'background concentrations' used as boundary conditions for the ADMS runs have been averaged over the local domain, for each time step. It would be more accurate for the model to include the spatial, as well as temporal, variation of these background concentrations.
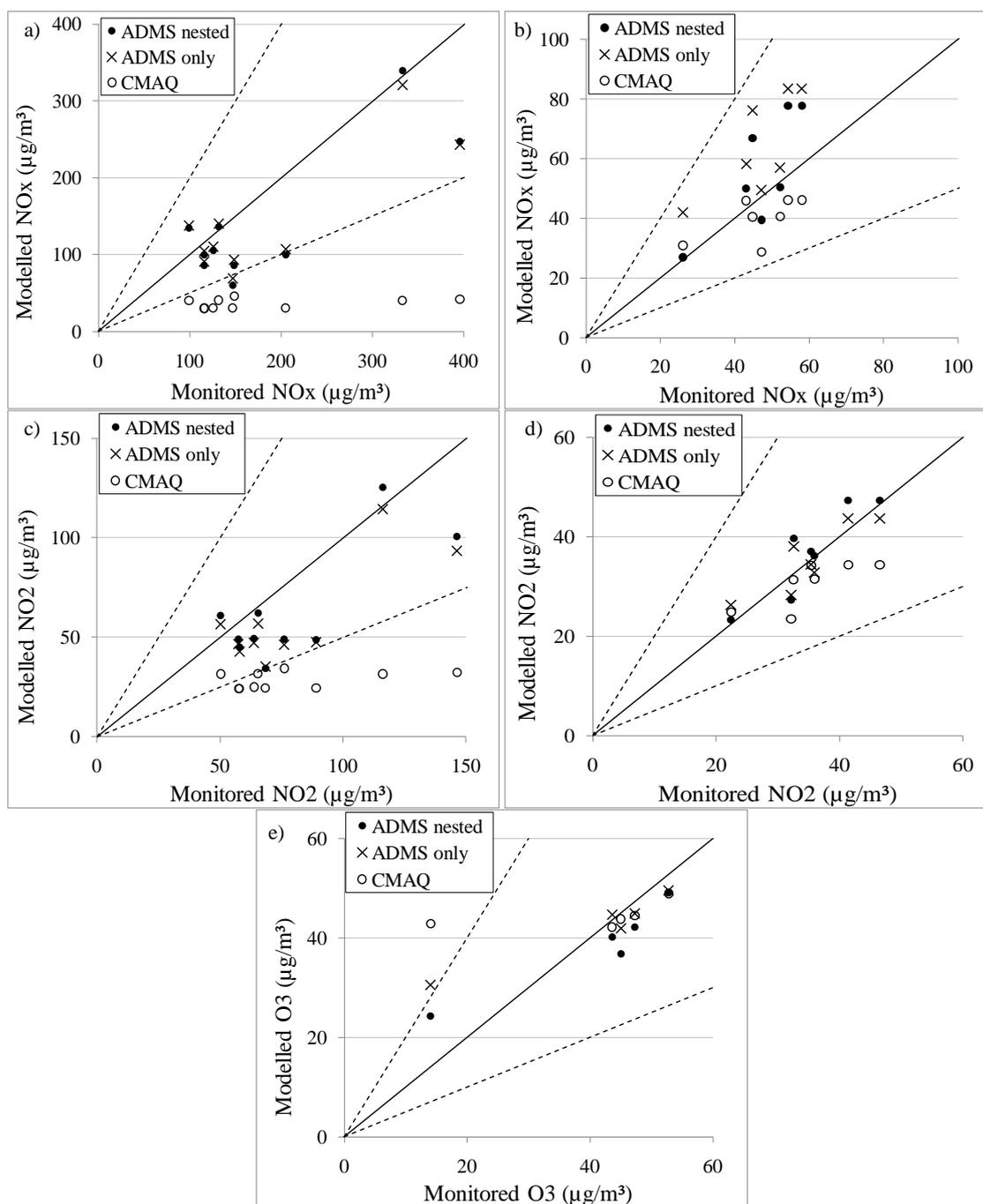
Figure 29. Scatter plots showing ADMS nested, ADMS only and CMAQ average concentrations against monitored values for the 5-day period in July a) NO_x roadside and kerbside sites, b) NO_x urban background sites, c) NO_2 roadside and kerbside sites, d) NO_2 urban background sites and e) ozone at all sites

Figure 29e) presents the modelled ozone concentrations. In this figure, the local model prediction of the concentration at the one roadside location is significantly improved by the nesting within the regional model. This result is of particular interest as the spatial variation of ozone predicted by the model is solely a product of chemical reactions, because emissions of ozone are not included in the study, and so this result implies the combination of the regional and local model may improve the overall model predictions. However, in the absence of further monitored ozone data at near-road sites, firm conclusions cannot be drawn. Ozone concentrations at the urban background sites are well predicted by all models.

Figure 30 shows a spatial representation of the average NO_2 concentration over central London; the 9 x 9 km^2 nested model domain is shown in the centre of the output grid. The CMAQ model results (outside the nested model domain area) are presented as constant values over each modelled grid square using the same contour levels as the local model. The fine

resolution of model output within the nested domain highlights how much detail is missing from the regional model output; specifically CMAQ clearly underestimates the concentrations close to roads.
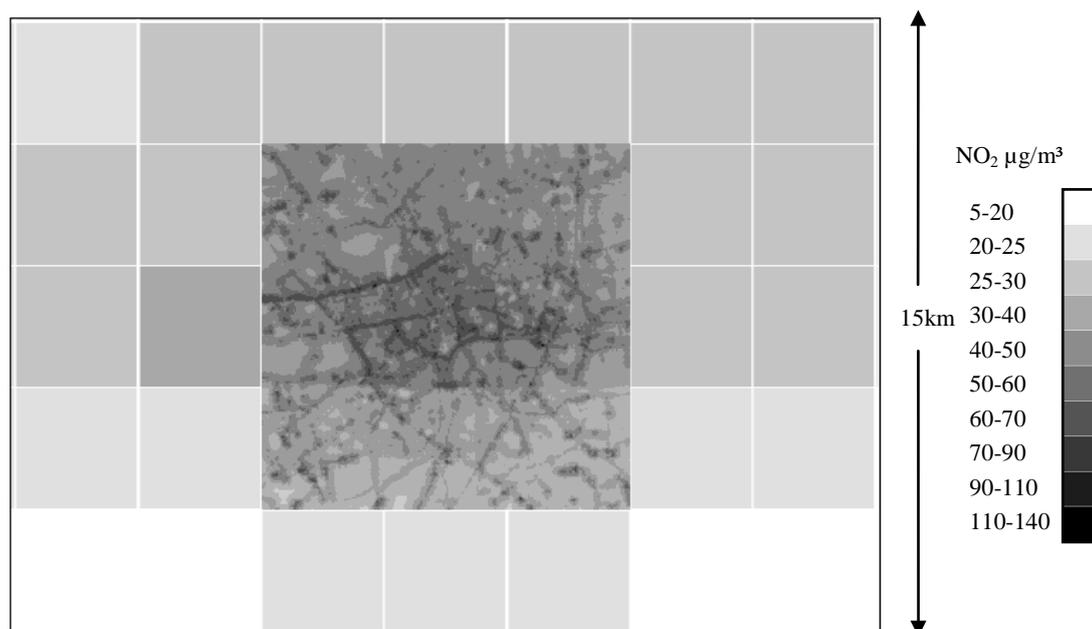
Figure 30. Five-day average NO_2 concentrations within the central London area

DISCUSSION

This paper demonstrates a consistent approach to nesting a local Gaussian-type plume dispersion model within an Eulerian regional model. This preliminary work makes a number of simplifications both in terms of the model input (for instance, large point sources are neglected and simplified initial and boundary conditions are applied for the regional model) and the model calculations (for instance, the local dispersion calculations are all assumed to be well mixed within a two hour time step). Despite these assumptions, the nested model concentrations compare favourably with monitored concentrations; they are also show consistency to the 'ADMS only' concentrations but are larger than the 'CMAQ only' as anticipated.

The advantage of nesting a local model within a regional model in this way is that it allows the modelling of high concentration gradients close to road sources in addition to obtaining good estimates for 'urban background' concentrations. Detailed modelling of source geometries that may significantly affect concentrations, such as street canyons and noise barriers, can be included, whilst also accounting for deposition and chemical processes that affect concentrations over large temporal and spatial scales.

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