THE DEVELOPMENT AND EVALUATION OF AN AUTOMATED SYSTEM FOR NESTING ADMS-URBAN IN REGIONAL PHOTOCHEMICAL MODELS

Jenny Stocker, Christina Hood*, David Carruthers, Martin Seaton and Kate Johnson
Cambridge Environmental Research Consultants, Cambridge, UK

Jimmy Fung
Division of Environment and Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong

1. INTRODUCTION

Within the regional air quality modeling community there is continual pressure to reduce the model grid scale, so that local variations in pollutant concentrations can be modeled. Whilst the scales have been reduced to as little as 1 km or even 500 m, such models will not, in the foreseeable future, be able to resolve high concentration gradients such as those found adjacent to roads. An alternative approach is to nest local-scale models, which explicitly represent pollution sources, within the regional models. Such an approach can be used with grid-based models operating at larger grid scales, for example 5-10 km.

This type of modeling approach is attractive for complex urban areas, where significant regional transport of pollutants is combined with local emissions. A nesting approach can allow the modeling of both fast local chemistry, such as the rapid reaction of NO emitted by vehicles, and slower long-range chemistry, for example the formation of secondary particulate species. The use of regional models in combination with local Gaussian-type models also allows modeling of local pollutant accumulation during low wind speed conditions.

The initial concept of nesting the Gaussian-type local dispersion model ADMS-Urban (McHugh *et al.*, 1997) in a regional photochemical model, so as to avoid double counting and exploit the advantages of each model type, is described in Stocker *et al.* (2012). The method has now been developed into a user-friendly and flexible automated system for nesting ADMS-Urban within CMAQ (Byun and Schere, 2006), CAMx (ENVIRON, 2014) or EMEP4UK (Vieno *et al.*, 2010) using meso-scale meteorological data from WRF (Dudhia *et al.*, 2005).

An outline of the concept of the nesting system is given in Section 2. The structure, components and procedures used in the automated system, known collectively as the ADMS-Urban Regional Model Link (RML), are described in Section 3. Section 4 covers an example use of the model with evaluation of concentration outputs for the Hong Kong Special Administrative Region (HK SAR), including comparisons between regional model-only, stand-alone ADMS-Urban and nested ADMS-Urban outputs. The system and results are discussed in Section 5.

2. NESTING CONCEPT

The concept of nesting ADMS-Urban in a regional air quality model without double-counting emissions is based on a separation of time-scales to which each model is applied. At short times after release of a pollutant from a source, concentration gradients due to releases from that source are high and a local model such as ADMS-Urban is most appropriate to capture the fine details of dispersion. At longer times after release, however, concentration gradients are reduced by mixing and a gridded regional model can be used to represent pollutant transport and chemistry. A ‘mixing time’ required for local emissions to become uniformly mixed over the scale of the regional model grid is defined as the threshold between local and regional calculations. In general this mixing time would vary with the size of the regional model grid, the meteorological conditions and the details of the local emissions, although a uniform value of one or two hours forms an adequate approximation.

The ADMS-Urban RML is an off-line system, meaning that the regional models can be run separately from the local modeling, which allows archived regional model data to be used as input. Meso-scale meteorological data from the WRF model drives both the regional and local dispersion models. Consistent emissions data are also used in both transport models.

Each regional model grid cell included in the nesting domain is treated separately within the

**Corresponding author:* Christina Hood, Cambridge Environmental Research Consultants, 3 King’s Parade, Cambridge CB2 1SJ, UK; e-mail: chood@cerc.co.uk

ADMS-Urban RML in order to ensure that the corresponding regional meteorological and concentration data are used in the calculations.

3. SYSTEM IMPLEMENTATION

The main components of the ADMS-Urban RML system comprise: the ADMS-Urban local dispersion model; Run Manager software for distributing ADMS-Urban runs across multiple machines; and the ADMS-Urban RML Controller, which consists of a simple graphical user interface, a control program and five utility programs, as illustrated in Figure 1.

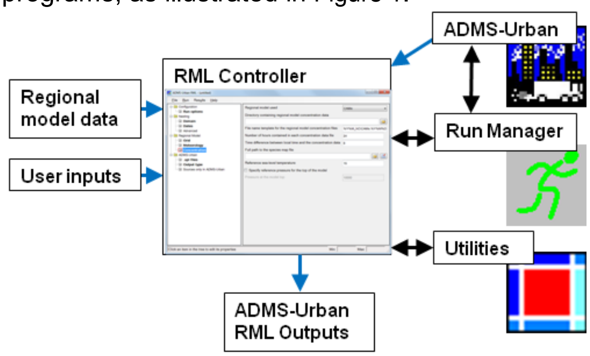

Figure 1 Illustration of system components. Blue arrows indicate input and output data, black arrows show data transfers during the system run.

The main procedures which are carried out by the system for a run with output at receptor locations for model validation purposes are as follows:

1) Initialization of the system, reading input parameters and calculating the number of regional model grid cells included in the nesting domain;
2) Extraction of ADMS-format meteorological data files from WRF for each regional model grid cell via a utility program;
3) Estimation of concentrations within each regional model grid cell in the middle of each hour for use as background to ADMS-Urban runs, by: extracting local upwind background concentrations via a utility program; running ADMS-Urban with gridded emissions equivalent to the regional model and calculations limited to 0.5 hours after emission; and running a utility program to calculate the difference between regional model concentrations at the end of the hour and the increment calculated by ADMS-Urban from half an hour of local emissions;
4) Runs of ADMS-Urban with gridded and explicit emissions, using the concentrations calculated in 3) as background for chemistry calculations and regional meteorological data, with dispersion limited to the mixing time after release;
5) Calculation of nesting output concentrations as:

$$RM - ADMS_G + ADMS_E \qquad (1)$$

where RM is the regional model concentration, $ADMS_G$ is the concentration from ADMS-Urban with gridded emissions and $ADMS_E$ is the concentration from ADMS-Urban with explicit emissions; and
6) Creation of final output files by combining results from each grid cell.

Two additional procedures are included if high-resolution contours of concentration are required, in order to create extra output points near explicitly-modelled road sources.

4. EXAMPLE USE OF SYSTEM

The ADMS-Urban RML system has been set up and run for example domains in the HK SAR for the whole of 2010. Results from stand-alone runs of the CAMx regional model and the ADMS-Urban local model are also presented alongside those from the ADMS-Urban RML system.

4.1 Input Data

Regional meteorological data were obtained from the WRF meso-scale model version 3.2. Regional concentration data were obtained from the CAMx model version 5.4. Both models were set up as described in Yao *et al.* (2014). Data files from the 1 km resolution domain, covering the whole of the HK SAR, were used as input to the ADMS-Urban RML system.

The gridded emissions data for diffuse sources in the HK SAR as used in CAMx were reformatted for use in ADMS-Urban. Both annual total emission rates and time-varying profiles of emissions were matched as closely as possible between the two models. Additional information about large industrial point sources and road traffic flow data was supplied by the Hong Kong Environmental Protection Department to enable explicit modeling of these sources in ADMS-Urban. A map of the emissions data used in ADMS-Urban is shown in Figure 2.

The stand-alone ADMS-Urban run uses as input measured meteorological data from Hong Kong airport and measured ‘background’ concentration data, which is taken to be the lowest measured concentration across all available monitors in the HK SAR on an hourly basis.

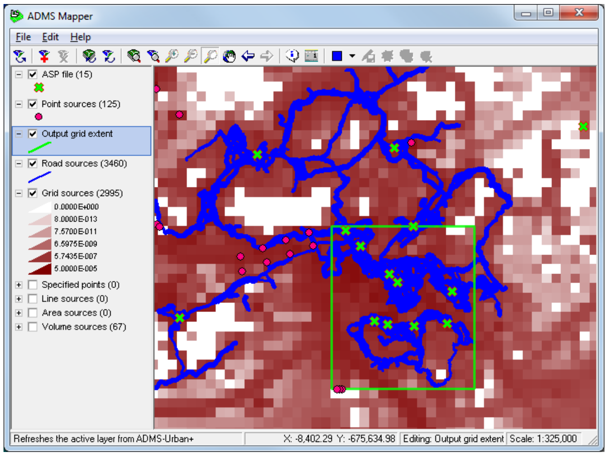

Figure 2 Map of sources and output locations for the HK SAR modeling domains displayed in the ADMS Mapper. The green crosses indicate monitoring sites while the green square shows the area in which contours of concentration have been calculated. Road sources are shown as blue lines and the grid source in shades of dark red, scaled by the NO_x emissions.

4.2 System Configuration

Two different nesting domains were defined for the ADMS-Urban RML system. A larger domain (72km x 49 km) was defined to cover all the monitoring locations in the HK SAR for the purpose of model validation, with an output receptor defined at each monitoring site. A smaller domain (15 km x 17 km) covering the main urban areas in the HK SAR, including most of Hong Kong Island and southern Kowloon, was defined for generating contours of concentration, with a regular grid of output locations supplemented by additional output points near road sources. Each full run of the system was preceded by a run in 'verification mode', which is an interface option to run the system for two model hours in order to test the validity of the input settings.

The mixing time used to separate regional and local effects in the ADMS-Urban RML system was set to one hour. As ADMS-Urban runs in local solar time whereas the regional models run in UTC, a time difference of 8 hours between the regional and local data was defined.

The ADMS-Urban RML system was run using seven desktop computers, one of which ran the RML Controller and the remaining six each performing up to three simultaneous ADMS-Urban model runs. The ADMS-Urban model runs were distributed between the available processors by Run Manager, to optimize run times by taking advantage of the available computing resources.

4.3 Evaluation Methodology

14 continuous monitors operate in the HK SAR, of which 3 are in roadside locations, 10 in 'urban background' areas and one in a rural area. The MyAir Model Evaluation Toolkit (Stidworthy *et al.* 2013.) was used to calculate model evaluation statistics for each of the three model cases. Additional data analysis and visualization was carried out in Microsoft Excel. Concentration contour plots were created in ArcGIS.

4.4 Results

Table 1 presents annual average NO_2 concentrations and model evaluation statistics at each monitoring site type for each of the models considered (ADMS-Urban RML, CAMx and stand-alone ADMS-Urban).

The scatter plots in Figure 3 compare the annual average modeled and observed concentrations of NO_2 and PM_{10} at each monitoring site for each of the three model cases.

Table 1 Model evaluation statistics for NO_2 concentrations in 2010 for the ADMS-Urban RML system, CAMx and stand-alone ADMS-Urban, with observed and modeled annual average concentrations, correlation coefficient (R), fraction of model predictions within a factor of two of the observed concentration (Fac2) and fractional bias of the model relative to the observed concentration (Fb).

Site type	Sites	Model	Observed ($\mu g/m^3$)	Modelled ($\mu g/m^3$)	R	Fac2	Fb
Roadside	3	RML (nested)	117.2	117.1	0.57	0.88	-0.002
		CAMx	117.2	58.5	0.49	0.45	-0.669
		ADMS-Urban	116.6	110.6	0.60	0.88	-0.053
Background	10	RML (nested)	55.6	47.7	0.56	0.73	-0.153
		CAMx	55.6	44.1	0.54	0.68	-0.231
		ADMS-Urban	54.7	48.0	0.58	0.81	-0.130
Rural	1	RML (nested)	12.7	9.0	0.30	0.52	-0.335
		CAMx	12.7	9.0	0.30	0.52	-0.335
		ADMS-Urban	12.5	19.0	0.57	0.86	0.415

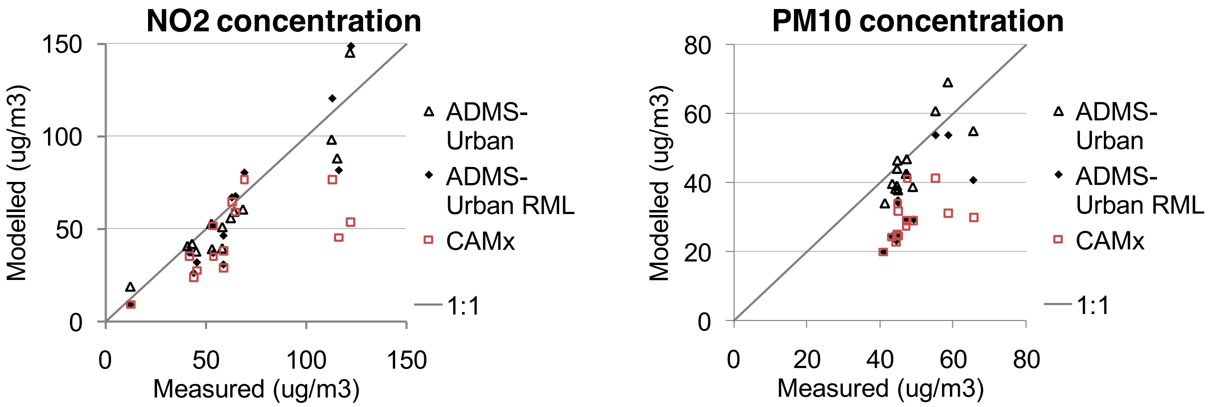

Figure 3 Comparison of observed and modeled annual average NO_2 (left) and PM_{10} (right) concentrations for each model configuration at each monitoring site in the HK SAR.

The contour plot in Figure 4 shows high-resolution nested NO_2 concentrations output from the ADMS-Urban RML system surrounded by the 1 km resolution concentrations output from the CAMx regional model for the whole nesting domain. Figure 5 compares areas where the annual average air quality objective for $PM_{2.5}$ is predicted to be exceded by the ADMS-Urban RML and CAMx.

5. DISCUSSION

In comparison to the preliminary implementation of nesting ADMS-Urban in a regional model described in Stocker *et al.* (2012),

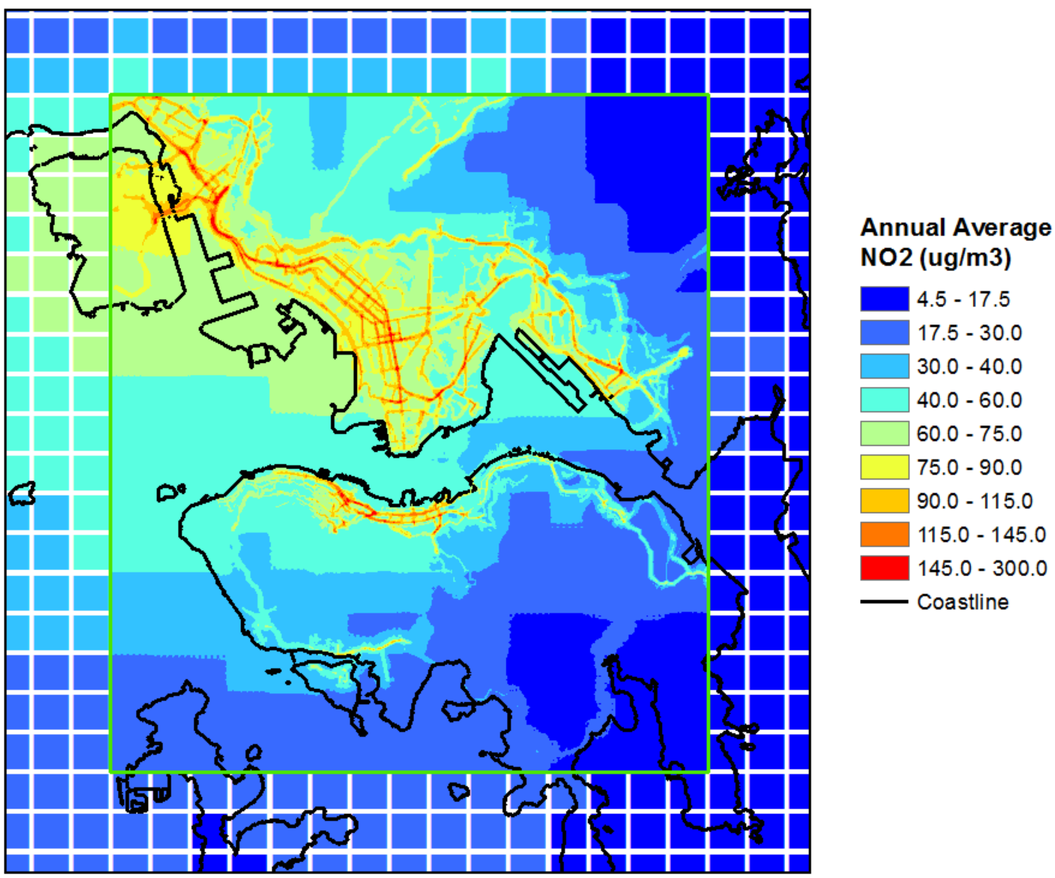

Figure 4 Contours of annual average NO_2 concentration from the ADMS-Urban RML system (within the green rectangle) and from the CAMx regional model, for the central urban areas of Hong Kong Island and Kowloon within the HK SAR.

the system developed for the current work is now fully automated, making it more practical for use in larger modeling domains. It has been applied to a different modeling location and uses meteorology and concentration outputs from different regional models. The regional air quality modeling used in the current study has a much less restricted set-up, with a full range of gaseous and particulate pollutant species, sources at a range of heights and multiple modeling domains. The nested modeling of sources within each regional model grid cell in the nesting domain now uses meteorological and background concentration data from the corresponding regional model cell rather than a single set of data for the whole nesting domain.

The results presented in Section 4 use regional model data run in one place at one time in an ADMS-Urban RML system run by a different group at a different time, which highlights the offline nature of the nesting system which has been developed.

At rural locations the ADMS-Urban RML results are identical to those from the regional model CAMx, as there are no local sources. Conversely, at roadside locations in very dense urban areas the effects of local sources and street canyon morphology dominate the monitored concentrations, with less influence from the regional modeling. The ADMS-Urban RML results at urban background locations concentrations lie between these two extremes, with a varying balance of regional and local influences. It can be seen from the NO_2 contour plot that there is a smooth transition of background concentrations between areas with few and many explicitly-modeled sources.

The balance between regional and local influences also varies between pollutants, for example particulate concentrations are dominated by regional industrial and shipping emissions whereas NO_2 concentrations are dominated by local traffic emissions.

As expected, the ADMS-Urban RML performs better than CAMx for roadside monitoring sites, due to the inclusion of the local dispersion of road emissions. The superior model performance in terms of the prediction of NO_2 concentrations indicates that the interaction between regional O_3 and local NO_x emissions via local and regional chemistry is adequately represented in the ADMS-Urban RML system.

The plot of predicted areas of exceedence of an air quality objective for $PM_{2.5}$ shows the ADMS-Urban RML system's inclusion of detailed spatial variation due to road sources which is not captured by the regional modeling. Exceedence of both short- and long-term air quality objective

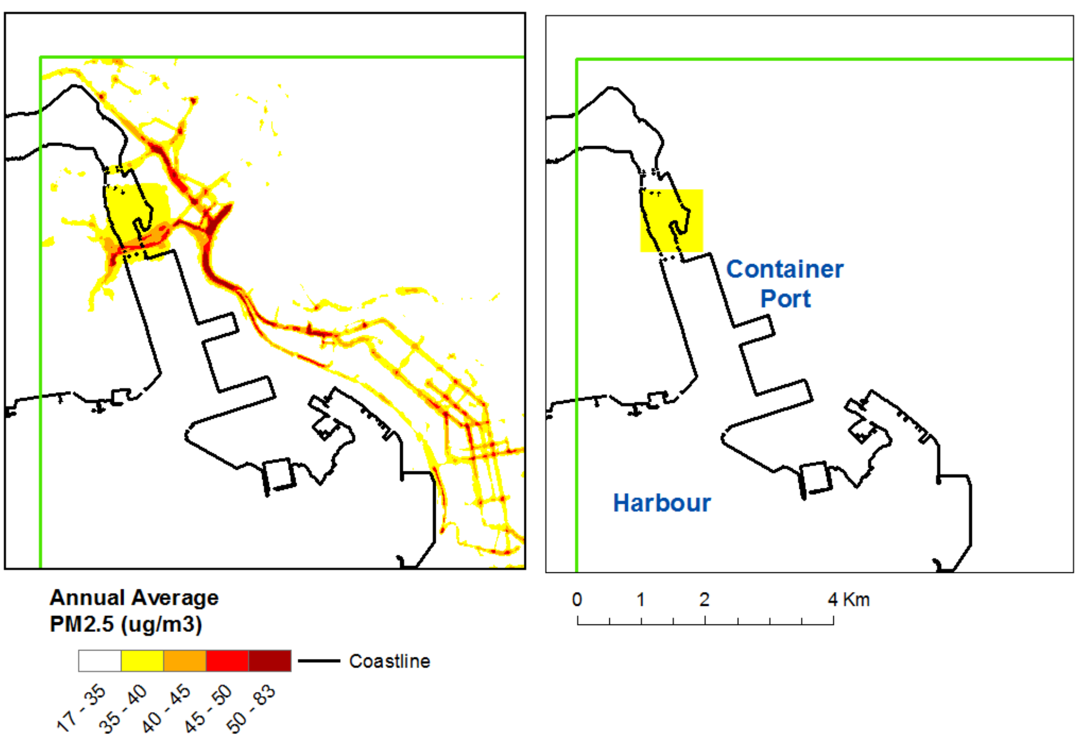

Figure 5 Contours of annual average $PM_{2.5}$ concentration from the ADMS-Urban RML system (left) and from the CAMx regional model (right), focused on the north-west corner of the nesting domain, with coloured areas indicating concentrations above the air quality objective level of 35 µg/m^3.

thresholds is of interest for regulatory air quality modeling applications. Output from the ADMS-Urban RML is in the form of hourly concentrations which can be post-processed to assess compliance with standards.

Running ADMS-Urban as a stand-alone model using measured meteorological and background concentration data removes some of the uncertainty associated with using regional model data and hence can give better results than nesting for historic concentrations, particularly for particulate pollutants and at rural locations. However the use of measured data limits the applicability of this approach to forecasting or testing future emissions and/or climate scenarios. The advantage of using measured meteorological and background concentration data rather than modeled data is less significant for urban background and roadside locations and for pollutants more associated with local sources.

The ADMS-Urban RML system has manageable run times. The results presented, with the full year of high-resolution modeling suitable for plotting concentration contours required approximately one week of computing time to run. This compares favorably with typical regional model run times. Validation runs, where model output is only required at monitor locations, take significantly less time to run.

Further work on the ADMS-Urban RML will include testing the effects of varying regional model resolution and mixing time on nested concentrations. The effects of extracting different combinations of met variables from WRF outputs for use in ADMS-Urban will also be investigated. At present the system is not optimized for modeling the effects of large elevated industrial sources, which will be investigated for future development.

The ADMS-Urban RML system has been designed to be run either interactively, from the user interface, or automatically, for use in complex applications such as part of a forecasting system. It is proposed that the model set up described in this paper will be integrated into the existing regional model air quality forecasting system run by the Hong Kong University of Science and Technology, in order to generate a street-scale pollution forecast.

In conclusion, an automated system for nesting ADMS-Urban in regional air quality models has been developed. The results presented for an example configuration in the HK SAR demonstrate that this system is able to model the high concentration gradients close to roads, whilst maintaining consistency with the regional model data used as input.

6. ACKNOWLEDGEMENTS

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