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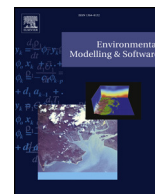
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Development and evaluation of the RapidAir® dispersion model, including the use of geospatial surrogates to represent street canyon effects

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ABSTRACT

We developed a dispersion model (RapidAir®) to estimate air pollution concentrations at fine spatial resolution over large geographical areas with fast run times. Concentrations were modelled at 5 m spatial resolution over an area of ~3500 km² in < 10 min. RapidAir® was evaluated by estimating NO_x and NO_2 concentrations at 86 continuous monitoring sites in London, UK during 2008. The model predictions explained 66% of the spatial variation (r = 0.81) in annual NO_x concentrations observed at the monitoring sites. We included discrete canyon models or geospatial surrogates (sky view factor, hill shading and wind effect) to improve the accuracy of model predictions at kerbside locations. Geospatial surrogates provide alternatives to discrete street canyon models where it is impractical to run canyon models for thousands of streets within a large city dispersion model (with advantages including: ease of operation; faster run times; and more complete treatment of building effects).

1. Introduction

The estimation of population exposures to air pollution is increasingly important as numerous studies highlight the detrimental effects of air pollution on human health (World Health Organization, 2013, 2016). The use of air pollution monitors allows direct measurement of ambient concentrations, and the on-going development of portable real-time monitors is providing improvements in temporally resolved concentration estimates (Dons et al., 2012; Spinelle et al., 2017, 2015). However, monitoring only provides concentration estimates at specific locations, whereas it has been observed that pollution concentrations can vary substantially over small areas (Gillespie et al., 2017; Lin et al., 2016). Models can overcome some of the limitations associated with monitoring as concentrations can be estimated at multiple locations within a study area. However, inherent uncertainties within models require to be quantified by comparison of predictions against air pollution measurements.

Two main types of models are commonly used to estimate urban air pollution – land use regression (LUR) models and dispersion models (we do not include discussion of Computational Fluid Dynamics (CFD) models in this paper as CFD models have not been used widely in operational predictions of spatial patterns of urban air pollution due to excessive computational constraints when operating over large geographical areas).

Land use regression (LUR) models use Geographical Information Systems (GIS) to quantify relationships between measured pollutant concentrations and land use variables (including traffic and population), which can then be extrapolated to estimate human exposure to air pollution at fine spatial resolution (Briggs et al., 1997). LUR models have been widely applied in in cohort epidemiological studies (Gillespie et al., 2016; Johnson et al., 2013; Wang et al., 2013) and in personal monitoring studies (Dons et al., 2014a, 2014b). LUR models are frequently used to estimate longer-term (e.g. annual) pollution exposure and often do not take into account the effects of meteorology. Additionally the transfer of LUR models between study areas has been shown have substantial limitations including differences in monitoring location type which can lead to model bias (Gillespie et al., 2016; Mukerjee et al., 2012; Patton et al., 2015). Many regulatory organisations are interested in source apportionment to inform policy on air pollution controls, which requires preparation of spatially accurate multi-source air quality emissions. However, LUR models seldom use direct quantitative estimates of emissions from sources (instead more commonly they assess the effects of receptor proximity to sources) and consequently LUR models have had limited application in air quality management policy development.

Dispersion models simulate atmospheric transport and transformation of air pollutants emitted from sources to allow estimation of concentrations at receptors. The most commonly used models are based on Gaussian plume concepts. Dispersion models can be used to estimate short term (e.g. hourly) variations in pollution concentrations (Gibson

Software availability

Name of software RapidAir®

DeveloperRicardo Energy and Environment

Hardware Information General-purpose computer (4–16 Gb
RAM, Intel(R) Core(TM) i5 processor, 64-bit operating
system)

Programming Language Python 2.6 and R

Availability Contact the developers

et al., 2013), and to estimate population exposures in cohort studies (Bellander et al., 2001; Nyberg et al., 2000). Additionally, projected emissions estimates (if available) can be used to estimate future concentrations. Commercially available software packages have been developed to simplify user inputs and modelling procedures, however this has often resulted in high license costs (Gulliver and Briggs, 2011), particularly when it is necessary to apply models over large geographical areas. Furthermore, Gaussian dispersion model run-times for large urban area can quickly become prohibitive due the computational demands of calculating concentrations at what can extend to millions of discrete locations. This may necessitate the use of GIS interpolation routines to increase the spatial resolution of the model estimates which may introduce other errors into estimated exposures (Wong et al., 2004).

Some studies have addressed these challenges to achieve fine spatial and temporal resolution by combining dispersion and LUR models (Korek et al., 2016; Michanowicz et al., 2016; Wilton et al., 2010); and/or including meteorological information within LUR models (Su et al., 2008a; Tan et al., 2016). A hybrid GIS-dispersion model (STEMS-AIR) has been developed to enable fine spatial and temporal resolution while minimising run times with readily-available computer software (Gulliver and Briggs, 2011). The STEMS-Air model estimates pollution concentrations from emission sources in 45° upwind 'wedge' shaped GIS-buffer areas, scaled by the distance between sources and receptors.

In built-up urban areas air pollution can become trapped in street canyons surrounded by tall buildings, especially if the wind is blowing from a direction perpendicular to the street, leading to recirculation of pollutants within the canyon. As a result, pollution concentrations in street canyons can become elevated and may be underestimated by 'standard' air pollution models, including LUR or Gaussian plume models. Exposure estimates may be improved by combining additional models that take into account urban topography in such locations with background pollution estimates from Gaussian-based air pollution models. Street canyon models range from complex computational fluid dynamic (CFD) models to simpler empirical (e.g. USEPA STREET box-model described by Dabberdt et al., 1973, and Johnson et al., 1973) and semi-empirical models (e.g. Danish Operational Street Pollution Model (OSPM) described by Vardoulakis et al. (2003). Some dispersion models include additional software modules for street canyon effects, however these may increase model run time (Fallah-Shorshani et al., 2017; Jackson et al., 2016).

Geospatial surrogates can be used to estimate the effect of street canyons on air quality in urban locations. Such metrics are commonly used in studies of urban climate where temperature, and hence comfort levels, are affected by building density and height. For example, sky view factor (SVF, which estimates the percentage of sky that can be observed using a fish-eye lens pointed vertically (Carrasco-Hernandez et al., 2015), with areas with low SVF corresponding to the presence of tall buildings) has been incorporated into a LUR model to estimate the presence of street canyons (Eeftens et al., 2013). Building height and/or volume information has also been observed to improve the accuracy of LUR model estimates (Gillespie et al., 2016; Su et al., 2008b; Tang et al., 2013). Geospatial surrogates can be readily applied across entire cities in automated processes which are likely to be more reproducible than

use of currently available GUI-based street canyon models, as the latter require user judgement to identify street canyon locations and detailed information (e.g. on traffic flow) for each location. The use of geospatial surrogates also has potential to improve the reproducibility of dispersion model pollution estimates as the number of model design choices is reduced substantially (with corresponding substantial reduction in manpower costs).

In this paper we describe the development and evaluation of a new dispersion model (RapidAir®, Ricardo-AEA Ltd) that uses modern scientific computing methods based on open-source Python libraries (www.python.org). A key motivation for the development of RapidAir was our experience of a lack of a cost-effective operational city-scale dispersion model with convenient run times, which does not require large amounts of manpower to operate. We focused on operational convenience of the modelling process and accuracy of model predictions in a case study and compared our results to results from other published studies which evaluated other models in a similar geographical study area. The design concept for RapidAir is similar to the STEMS-Air model described by Gulliver and Briggs (2011) with some additional enhancements. RapidAir includes a dispersion model (AERMOD), with detailed treatment of boundary layer meteorology, and street canyon models. Additionally, we investigated the incorporation of geospatial surrogates to represent street canyon effects on spatial variations in pollution concentrations; and we established methods for efficient post-processing of the output from fine resolution dispersion models over large geographical areas using these surrogates.

2. Methods

2.1. Study area and receptor locations

We modelled concentrations of oxides of nitrogen (NO_x) in Greater London (urban conurbation approximately bounded by the M25 orbital motorway). Although NO_x and NO_2 were the pollutants of focus in this work, the RapidAir model can be run for any pollutants for which there are supporting emissions data, including $PM_{2.5}$. Greater London was chosen as the study area because it contains a large network of air pollution monitoring sites, and has detailed traffic and building height data. Additionally this was the study area used in a previous Department for Environment, Food and Rural Affairs (DEFRA) Urban Model Evaluation exercise, which evaluated several commercially available and industry accepted models (Carslaw, 2011). We modelled annual average NO_x and NO_2 concentrations for 2008, which was the same year as used in the DEFRA study to enable comparison between RapidAir and the models assessed in the DEFRA comparison. The RapidAir model can be run at higher temporal resolutions provided that the model input data (described below) is also available at the same higher temporal resolution.

We evaluated the RapidAir model at 86 continuous monitoring locations from the London Air Quality Network (LAQN) monitoring network (Fig. A1, Table A1) (London Datastore, 2016). All of these sites are maintained by the Environmental Research Group, Kings College London and local authorities in the city boroughs. The data collected were subject to national-ratification and detailed QA-QC procedures (DEFRA, 2017a,b; Targa and Loader, 2008). For model evaluation purposes the monitoring sites were classified as kerbside, roadside, suburban and urban background receptors according to proximity to road traffic: kerbside sites were located within 1 m of a busy road; roadside sites were located in 1–5 m of a busy road; suburban sites were located in a residential area on the edge of the urban conurbation; and urban background sites were located in urban areas but were free from the immediate influence of local sources to provide a good indication of background concentrations (DEFRA, 2016).

Similar to the DEFRA Urban Model Evaluation (Carslaw, 2011), we excluded sites which had less than 75% data during 2008. It was not possible to use exactly the same locations as the DEFRA Urban Model

Evaluation: when we imported the locations used in the DEFRA into a GIS programme some were incorrect, in a few cases up to several kilometres from their true location. We relocated receptors to a best approximation of their true location using aerial photography and street level photographs but small discrepancies in the locations may still persist. This may have affected our evaluation of the accuracy of model predictions at measurement sites, and comparisons of our estimates with the estimates of other groups in this paper.

2.2. Model description

A summary of the RapidAir model is provided below, and a technical description can be found in Appendix A. RapidAir uses open source python libraries to rapidly estimate concentrations at fine spatial resolution over extended geographical areas. RapidAir is conceptually similar to the STEMS-Air model (Gulliver and Briggs, 2011) with technical development primarily based on inclusion of open source AERMET and AERMOD software for automated processing of meteorological input data. In this evaluation study, surface and upper air meteorological data were obtained from the nearest meteorological stations to the study area: Heathrow Airport (National Climatic Data Centre NOAA, 2018) and Camborne (Earth Systems Research Laboratory NOAA, 2018) for surface and upper air data respectively.

AERMOD is used to produce dispersion model plume estimates (the kernel) for a small idealised area source. A theoretical source is located at the centre of the kernel in AERMOD, assigned with a nominal emission rate of 1 g/s, and a kernel of size 55 x 55 cells was produced. This kernel is rotated by 180° to represent the contribution of cells within the kernel to the central cell i.e. the cell in which we are trying to estimate the pollution concentration. This produces a plume which identifies pollution sources that contributed to the central cell and estimates a scaling factor for each source that falls within the plume based on its distance and location to the source.

The RapidAir dispersion model then uses a kernel convolution procedure which is similar to algorithms used in image processing software. The kernel produced above is passed over a road traffic emission raster at the same resolution pixel by pixel so the final city-wide model comprises millions of overlapping plumes from the road source emissions (Fig. A2).

For each receptor cell (in this case at 5 m resolution) the sum of concentrations falling within the kernel plume, weighted by their distance to the source, are written to the centre cell of the concentration raster (Fig. A3). In this way the pollution surface is created by the convolution step iterating over the gridded emission data. This means that model run time is linearly dependent on the spatial resolution of the output number of cells and is unaffected by the number of emissions sources in the domain. This is a key benefit compared with other Gaussian models whose run time is linearly dependent both on resolution/number of receptors and number of sources. Our experience suggests that run times in the order of several days/weeks can be expected for city-scale Gaussian models with only a few hundred thousand receptor locations, which are then interpolated to provide continuous pollution surfaces. In contrast, the RapidAir model computes concentrations at > 100 million discrete receptors in less than 10 min using a 64-bit Intel i5 8 Gb processor.

NO_x emissions data for each road link were obtained for London in 2008 from the London Atmospheric Emissions Inventory (LAEI) (London Atmospheric Emissions Inventory, 2008) (Fig. A1). Emissions from LAEI individual road links were converted to a 5 m raster using the ESRI ArcGIS 'Line Density' tool (ESRI, 2014) [subsequent versions of RapidAir use open source routines for preparing the emissions grid] and this emissions raster used in the convolution step described above.

1×1 km regional background concentrations calculated by the Pollution Climate Mapping (PCM) model (DEFRA, 2018) were added to the pollution raster (Fig. A4). Categorisations of the PCM model sources allowed us to remove road transport sources prior to adding the PCM model to the modelled pollution concentrations above to prevent double-counting of traffic related pollutants.

2.3. Street canyon models

Concentrations of NO_x within street canyons were estimated using two street canyon models: the STREET model (Dabberdt et al., 1973; Johnson et al., 1973) and the AEOLIUS Model (Buckland and Middleton, 1999). CFD models are complex, requiring very detailed emissions data which is difficult to obtain and have long run times. This means they are not an operationally feasible solution for large scale model correction for canyon effects, therefore were not considered during this study.

The STREET model estimates pollution concentrations empirically within a street canyon based on the emissions estimates within the canyon, and takes into account vehicle-induced turbulence and entry of air from the top of the canyon. Concentrations were calculated for the windward (C_W) and leeward (C_L) sides of the canyon using equations (1) and (2):

$$C_L = \frac{K*Q}{(U + 0.5) * \left[(x^2 + z^2)^{\frac{1}{2}} + L_0 \right]}$$ [1]

$$C_W = \frac{K*Q*(H - z)}{W*(U + 0.5)*H}$$ [2]

Where K is a scaling constant (set to 14 here); Q is the emission rate (g/m/s); U is the wind speed (m/s); L_0 is the length of individual vehicles (set to 3 m); W is the width of the canyon (m); H is the average building height of the canyon (m); x is the distance from emission source to receptor (m); and z is the receptor height (set to 1 m).

The AEOLIUS model was developed by the UK Meteorological Office in the 1990s (Buckland and Middleton, 1999) and the scientific basis for the model is presented in a series of papers (Buckland, 1998; Manning et al., 2000; Middleton, 1999, 1998a; 1998b). The AEOLIUS model shares many common features with the Operational Street Pollution Model (OSPM) (Berkowicz, 2000; Hertel and Berkowicz, 1989) which underpins many street canyon models included in commercial road source dispersion models. There are three principal contributions to concentrations estimated by the AEOLIUS model: a direct contribution from the source to the receptor; a recirculating component within a vortex caused by winds flowing across the top of the canyon; and the urban background concentration. The RapidAir model only takes the recirculating component from the canyon model and sums this with the kernel derived concentrations. The AEOLIUS model is written in python 2.7 and implements the equations as described in Appendix A.

2.4. Surrogates for street canyons

Building height data were used to calculate simple surrogates that could readily indicate locations that were located within street canyons, and consequently allow modelled concentrations in these areas to be corrected accordingly. A 5 m raster of maximum building height was created from building height data for London (Emu Analytics, 2018) derived by the suppliers from national scale LiDAR surveys (Survey Open Data, 2018). We investigated three surrogates for street canyons (Fig. A5):

- Sky view factor (*SVF*) representing amount of sky visible from each location when looking vertically up to the sky with a fish eye lens (dimensionless ratio between 0 and 1, where 1 is all visible sky). The Relief Visualization Toolbox (RVT) (Kokalj et al., 2011; Zaksek et al., 2011) was used to calculate SVF using building height raster as input and a search radius of 200 m (Eeftens et al., 2013).
- Hill Shading (*HS*) identifying areas in shade of surrounding topographical features (Zaksek et al., 2011). In our analysis we used

wind direction in place of the direction of the sun and the 'shading' identified was anticipated to represent areas of higher concentration on the windward side of a street canyon. The Analytical Hill-Shading option was run within RVT using an elevation angle of 45° (Kokalj et al. (2013) suggested this value to be most appropriate for steep terrain encountered in an urban environment). We calculated *HS* (dimensionless value between 0 and 255 representing shaded and unshaded areas respectively) for 8 sectors (i.e. every 45°) and averaged these calculated HS values for each 5 m raster cell in the study area.

- Wind Effect (*WE*) is a module in SAGA GIS (Conrad et al., 2015) which predicts if an area is wind shadowed or exposed, where dimensionless values below and above 1 represent shadowed and exposed areas respectively (Böhner and Antonić, 2009). *WE* was calculated for 8 sectors and averaged values calculated as above. A search radius of 200 m was used.

Surrogate *SVF*, *HS*, & *WE* values for 5 m buffers around each receptor location were calculated to allow for slight errors in the coordinates of receptor locations (e.g. receptors located 'within' buildings rather than on lampposts on the road).

2.5. NO_x to NO_2 conversion

Legislative limit values specified by the European Union and UK government are for NO_2, and not NO_x, therefore we converted RapidAir NO_x concentrations to NO_2 concentrations using the DEFRA NO_x to NO_2 model (DEFRA, 2017a,b) which is recommended for use in UK air quality assessment for statutory purposes. Further information about the DEFRA NO_x to NO_2 model is provided in the Appendix. Briefly, we derived a polynomial regression equation between predicted NO_x and NO_2 concentrations from the finite difference model within the DEFRA tool. The model was set to use the built-in fleet composition for London (which automatically sets the fraction of NO_x emissions as NO_2 (f-NO_2)) and the average NO_x background concentration over the study area from the PCM model. Estimated NO_2 concentrations were plotted against NO_x concentrations and fitted with a polynomial regression equation (Equation (3) and Fig. A6) subsequently applied to the kernel model output to estimate NO_2 concentrations over the study area:

$$NO_2 = -0.0001*(NO_x)^2 + 0.2737*NO_x + 18.648, \quad R^2 = 0.997 \quad [3]$$

where NO_x and NO_2 concentrations are in µg/m³. The expression is valid between the upper and lower NO_x concentrations in the curve in Fig. A6.

The calculator uses estimates of regional NO_2, NO_x and O_3 concentrations from the PCM model for individual local authority areas being modelled. Since London comprises many local authorities we compared NO_2 conversion estimates for two local authorities within our study area, which had different regional NO_2, NO_x and O_3 concentrations, and found little effect on the NO_x to NO_2 conversion rate (Fig. A6).

2.6. Model evaluation

Modelled concentrations of NO_x and NO_2 were extracted from the model outputs at the grid references for pollution monitoring sites to enable comparison. The R package OpenAir (Carslaw and Ropkins, 2012) was used to generate model evaluation statistics commonly used to evaluate pollution models, including FAC2, mean bias (MB), normalised mean bias (NMB), root mean square error (RMSE), coefficient of efficiency (COE) and index of agreement (IOA) (Carslaw, 2011; Chang and Hanna, 2004; Derwent et al., 2010). We used simple data assimilation methods to calibrate model output against observed pollution concentrations at monitoring sites (Gulliver and Briggs, 2011).

We present results of the evaluation of the kernel-modelled NOx *vs.* measured NO_x and kernel-modelled NO_2 *vs.* measured NO_2 below. This

Table 1
Model evaluation statistics for measured NO_x *vs.* unadjusted RapidAir modelled NO_x.

Receptor site type	n	FAC2	MB (µg/m³)	NMB	RMSE (µg/m³)	r
All	86	0.65	−51.4	−0.46	73.2	0.81
Kerbside	8	0.38	−114.6	−0.53	150.2	0.71
Roadside	40	0.53	−66.8	−0.49	80.1	0.78
Suburban	13	0.69	−24.9	−0.46	27.0	0.92
Urban background	25	0.92	−20.2	−0.30	24.2	0.84

FAC2 = fraction of modelled concentrations falling within a factor of 2 of the measured concentrations; *MB* = mean bias; *NMB* = normalised mean bias; *RMSE* = root mean square error; and *r* = coefficient of determination.

is followed by description of the estimation of NO_x concentrations from the kernel and street canyons/surrogates and subsequent evaluation of modelled NO_2 concentrations after accounting for street canyon effects.

3. Results and discussion

3.1. RapidAir model evaluation - NO_x

The baseline RapidAir kernel model (i.e. model not including urban morphology effects) highlighted expected contributions to NO_x concentrations from major roads in London, and Heathrow airport in the west of the study area (Fig. A10). The modelled concentrations at the monitoring sites were extracted and showed that the RapidAir model systematically underestimated observed NO_x concentrations (Table 1). Possible causes of this model underestimation are discussed further below.

Using a similar conceptual approach to Gulliver and Briggs (2011), we corrected our modelled concentrations to account for potential systematic linear biases by linear regression between modelled and observed NO_x. The receptor locations were randomly split into *training* (n = 57) and *test* (n = 29) data sets, with the latter used as an independent verification data set. The linear regression using the *training* data (Fig. 1) was:

Measured NOx = 1.98∗*Kernel modelled NO$_x$*   [4]

Where *Measured NO$_x$* and *Kernel modelled NO$_x$* are concentrations in µg/m³.

A map of the modelled NO_x concentrations in the study area after correction for the systematic biases discussed previously is provided in Fig. A10.

3.1.1. Discussion of causes of systematic bias in air pollution models

Dispersion modelling involves multiple data inputs over several stages, any of which has potential to contribute to inaccuracies in pollution estimates. The under-prediction of NO_x concentrations in our analyses may be due to uncertainties in emissions and/or meteorological data, and/or uncertainties of representation of physical processes in AERMOD. The simplest errors to characterise are for road traffic emissions and meteorology data.

It is likely that road traffic NO_x emissions data are underestimated in LAEI inventory we used. This inventory was prepared by a statutory body (Greater London Authority [GLA]) and remains the officially recognised emissions dataset for London. The European Environment Agency's COPERT road traffic emissions model, which was used by GLA to create the LAEI, has been observed to under-predict historical NO_x emissions from diesel vehicles in the UK fleet (Carslaw et al., 2011). Consequently, it is likely that reported under-prediction of emissions in the diesel fleet biases the inventory towards under-prediction of atmospheric concentrations. NO_x emissions in the GLA inventory are reported to have been underestimated by approximately 31% in 2008 (Beevers et al., 2012b), consistent with predictions of a coupled regional CMAQ and road source dispersion model (CMAQ-urban)
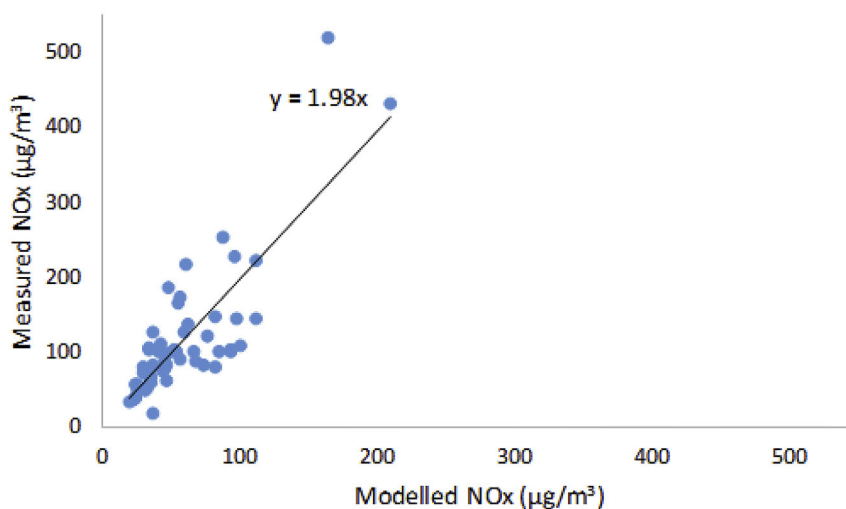
Fig. 1. Scatter plot of Measured vs. unadjusted RapidAir modelled NO_x concentrations for randomly selected training subset of receptors (n = 57).

developed by other researchers for London [average NO_x under-estimation by CMAQ-urban of 32% (Beevers et al., 2012a)]. A correction for 31% underestimated emissions in our analyses would change the slope of modelled vs. observed concentrations (= 1/1.98) in the training dataset regression analyses above from 0.51 (49% under-estimation of observations) to 0.73 (27% underestimation), which is of a consistent magnitude with the above underestimation of CMAQ-urban modelled *vs.* observed NO_x concentrations calculated by Beevers et al., (2012a). The effect of using the most recent release of COPERT road traffic emissions model on the emissions in London is discussed further in the Appendix (and Table A2).

Meteorological input data is a further potentially important source of systematic bias - concentrations are inversely proportional to wind speed in the Gaussian dispersion equation meaning uncertainties in wind speed estimates can lead to model bias. For example, Gulliver and Briggs (2011) noted that differences in windspeed measured at the

relatively open Heathrow airport meteorological station and wind-speeds measured during short duration periods at pollution monitoring sites in central London resulted in PM_{10} model predictions using windspeeds measured in central London being on average 67.5% lower than PM_{10} predicted using windspeeds measured at Heathrow. Similarly, Beevers et al. (2012a) noted that windspeeds measured at Heathrow were systematically higher than windspeeds forecast using the Weather Research Forecast (WRF) model. Specifically, Beevers et al. illustrate how average midday windspeeds for 2006 measured at Heathrow and modelled by WRF were ~5 m/s and ~3.5 m/s respectively (difference representing ~43% of WRF estimate approximated from Fig 7 in Beevers et al., 2012a). These differences suggest that use of measured Heathrow windspeed data could result in an approximate 30% underestimation of pollution concentrations compared to equivalent concentrations estimated using WRF windspeed data. The impact of using wind speeds from model *vs.* Heathrow for our study period and
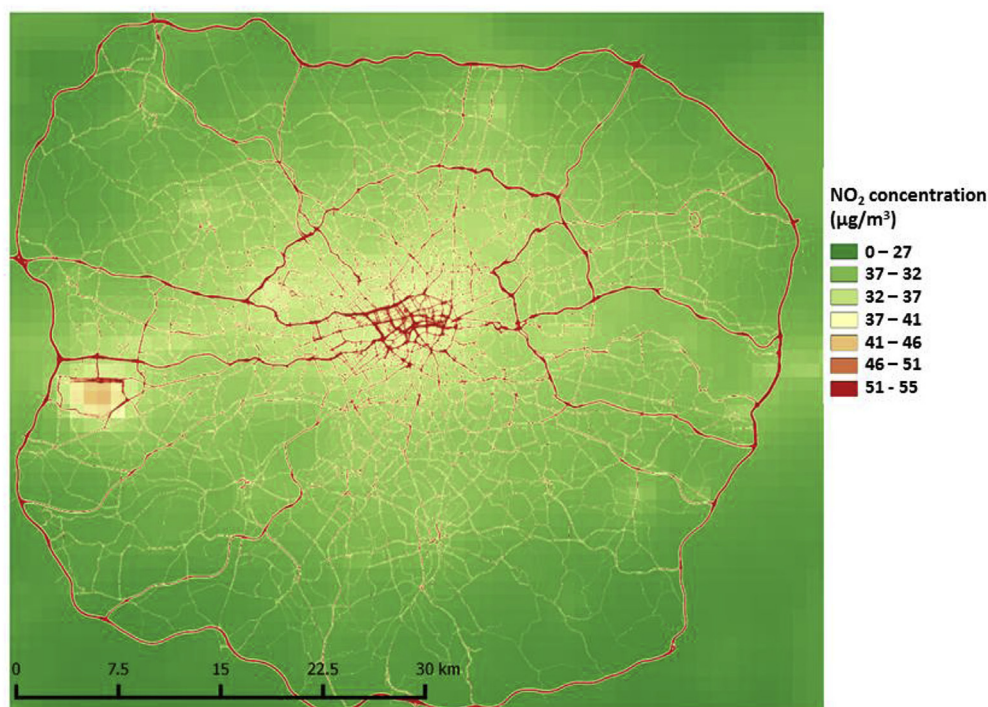

Fig. 2. NO_2 concentrations estimated by RapidAir for Greater London after correction for systematic biases.

the consequent impact on the kernels created is discussed further in the Appendix (and Figs A7 to A9, and Table A3).

The multiplicative combination of ~31% underestimated NO_x emissions from the LAEI and ~43% higher windspeeds from London Heathrow measurements (*cf.* WRF windspeed estimates used by Beevers et al., 2012a) suggests that the RapidAir pollution estimates in our analyses may have underestimated NO_x concentration observations in central London by approximately 48% ($\equiv$ 0.69/1.43) in context of above equivalent model-observation comparisons made for CMAQ-Urban (Beevers et al., 2012a). This difference is of similar magnitude to the underestimation of initial RapidAir model estimates compared to monitoring site observations (e.g. underestimation of 49% of observed concentrations represented in Fig. 1).

3.2. RapidAir model evaluation – NO₂

Concentrations of NO_2 estimated from RapidAir (Fig. 2) were compared to NO_2 concentrations measured at the receptor locations in Table A1.

NO_2 concentrations predicted by RapidAir were similar to measured NO_2 concentrations at most monitoring stations; however the model underestimated concentrations at some very high concentration kerbside measurement sites (Fig. 3, Table 2a). Underestimation by RapidAir model might be attributed to urban morphologies (including street canyon effects) or underestimation in the location-specific emissions rates used to predict the NO_x concentrations (Beevers et al., 2012b). The correlation between modelled and observed NO_2 concentrations ($r = 0.77$) was of similar magnitude to previous evaluations of dispersion models (e.g. $r = 0.74$ reported by de Hoogh et al. (2014) during evaluation of a NO_x dispersion model in the ESCAPE study).

DEFRA suggest that an air quality model is 'acceptable' for use if more than half of its observations fall within a factor of 2 of the observations (Williams et al., 2011). The NO_2 RapidAir model meets the *FAC2* criterion for all site types, with the lowest FAC2 value calculated for kerbside sites (FAC2 = 0.88) (Table 2a). Kerbside concentrations represent the worst-case exposure scenarios that are not representative of population exposures over extended periods, and consequently annual limit values do not apply at these sites (DEFRA, 2016). Similar findings were reported in the DEFRA urban model evaluation exercise

for NO_2 which found that *FAC2* values were lower for the kerbside sites than the three other site types tested, however all models met the above DEFRA criterion at the different site types (Carslaw, 2011). Another criterion suggested by DEFRA to indicate the acceptability of a model is that *NMB* values should lie between −0.2 and 0.2 (Williams et al., 2011). *NMB* values for RapidAir met this criterion when all sites were considered together; and for the individual site types, with the exception of the kerbside sites (Table 2a). None of the models tested during the DEFRA model evaluation exercise met the *NMB* 'acceptance values' proposed by DEFRA at the kerbside sites (Carslaw, 2011). The numbers of models meeting the criteria was progressively higher for kerbside, roadside and urban background site classifications – with all models meeting the *NMB* criterion at urban background locations (Carslaw, 2011).

3.3. Accounting for street canyon effects in RapidAir

We investigated the inclusion of two techniques within the RapidAir model to describe the effects of street canyons on pollution concentrations. The first technique used geospatial surrogates to account for building morphologies within a study area, and the second applied industry-standard street canyon models to user-defined street canyon geometries. These techniques are discussed in the following sub-sections.

3.3.1. GIS-surrogates for street canyons

We investigated if street canyon surrogates measured at each receptor could be used to estimate, and subsequently correct for, the effects of urban morphology on modelled NO_x concentrations, and NO_x concentrations converted to NO_2 concentrations using the method described above.

The NO_x receptors were split randomly into the same *training* ($n = 57$) and *test* ($n = 29$) datasets used to derive the OLS correction for bias described at the start of Section 3, with the former used to develop surrogate-correction equations and the latter used as an independent dataset to test the correction equations derived. A multiple-linear calibration equation was derived between *Unadjusted modelled NO$_x$*, *measured NO$_x$* and *Surrogate* for each of the three surrogate values investigated using the *training* dataset (Table 3a).

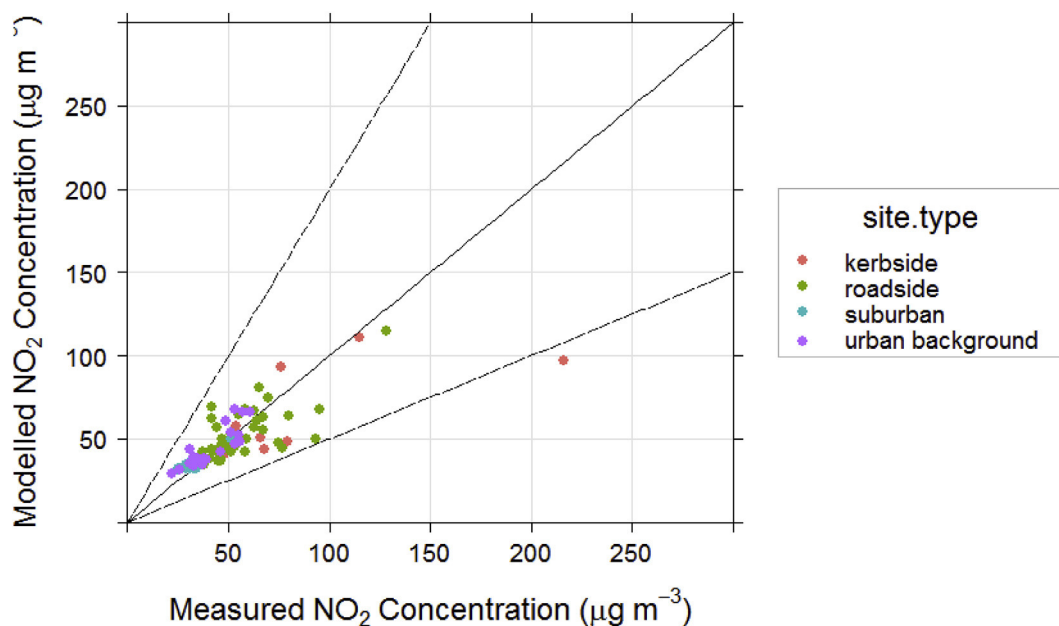**Fig. 3.** Scatter plot of NO_2 estimated by bias-corrected RapidAir kernel model *vs.* observed concentrations at measurement stations (n = 86). Receptors are colour coded to represent the different site types. Solid line represents 1:1. Dashed lines represent FAC2 values. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 2
Summary model evaluation statistics for annual mean NO$_2$ at receptor locations (*training* and *test* data combined) split by site type: (a) kernel model only (all sites); (b) kernel model with surrogate or street canyon correction (all sites); and (c) street canyon sites only. Statistics are given for the bias corrected Kernel only model, the kernel model after correction using the surrogates for street canyons and then bias corrected, and using the street canyon models with bias correction. See Table 1 caption for a description of the abbreviations used in the column headings.

Receptor site type	Model	n	FAC2	MB (µg/m^3)	NMB	RMSE (µg/m^3)	r	COE	IOA
(a) All sites:									
All	Kernel	86	0.99	−2.8	−0.05	17.1	0.77	0.46	0.73
Kerbside	Kernel	8	0.88	−22.6	−0.25	45.2	0.66	0.26	0.63
Roadside	Kernel	40	1.00	−4.0	−0.07	13.9	0.70	0.28	0.64
Suburban	Kernel	13	1.00	2.5	0.08	4.0	0.90	0.30	0.65
Urban background	Kernel	25	1.00	2.6	0.06	6.0	0.88	0.49	0.75
(b) All sites:									
All	SVF	86	0.99	−3.0	−0.06	16.3	0.80	0.50	0.75
	WE	86	0.98	−2.8	−0.05	17.0	0.78	0.47	0.74
	HS	86	0.99	−2.9	−0.06	17.0	0.77	0.47	0.73
	STREET	86	1.00	−4.4	−0.09	15.9	0.85	0.42	0.71
	AEOLIUS	86	0.99	−4.4	−0.08	16.4	0.83	0.46	0.73
Kerbside	SVF	8	0.88	−21.1	−0.23	44.0	0.67	0.31	0.66
	WE	8	0.88	−21.3	−0.24	44.9	0.65	0.28	0.64
	HS	8	0.88	−22.1	−0.24	45.3	0.65	0.27	0.64
	STREET	8	1.00	−22.0	−0.24	38.9	0.84	0.33	0.67
	AEOLIUS	8	0.88	−23.4	−0.26	42.8	0.76	0.29	0.65
Roadside	SVF	40	1.00	−4.0	−0.07	12.8	0.76	0.35	0.68
	WE	40	0.98	−3.6	−0.06	13.8	0.71	0.30	0.65
	HS	40	1.00	−3.8	−0.07	13.8	0.71	0.30	0.65
	STREET	40	1.00	−6.6	−0.11	14.3	0.72	0.21	0.61
	AEOLIUS	40	1.00	−6.2	−0.11	13.8	0.74	0.27	0.64
Suburban	SVF	13	1.00	1.1	0.04	3.4	0.90	0.35	0.68
	WE	13	1.00	2.0	0.06	3.7	0.90	0.33	0.66
	HS	13	1.00	2.0	0.06	3.7	0.90	0.30	0.65
	STREET	13	1.00	4.3	0.13	6.2	0.90	−0.16	0.42
	AEOLIUS	13	1.00	3.0	0.10	4.9	0.90	0.12	0.56
Urban background	SVF	25	1.00	2.3	0.06	5.2	0.90	0.55	0.77
	WE	25	1.00	1.8	0.05	5.5	0.87	0.54	0.77
	HS	25	1.00	2.0	0.05	5.6	0.87	0.53	0.77
	STREET	25	1.00	0.2	0.01	6.1	0.87	0.48	0.74
	AEOLIUS	25	1.00	0.7	0.02	5.3	0.87	0.54	0.77
(b) Street canyon sites only:									
	Kernel	19	0.95	−14.1	−0.18	32.4	0.68	0.22	0.61
	SVF	19	0.95	−11.6	−0.15	30.9	0.70	0.31	0.66
	WE	19	0.95	−12.9	−0.17	31.9	0.68	0.26	0.63
	HS	19	0.95	−13.4	−0.17	32.2	0.67	0.25	0.63
	STREET	19	1.00	−10.6	−0.14	28.1	0.80	0.28	0.64
	AEOLIUS	19	0.95	−13.0	−0.17	30.5	0.75	0.26	0.63

Table 3
(a) Linear regression equations between measured NO$_x$, kernel model NO$_x$ (*RapidAir_NO$_x$*) concentrations and the surrogate variables for the *training* data set (n = 59), used to obtain a surrogate-adjusted RapidAir NO$_x$ concentration ('*Surrogate' Adj_Mod_NO$_x$*); (b) Ordinary least squares regression equations between the measured (*Measured_NO$_x$*) and surrogate-adjusted kernel model NO$_x$ concentrations (baseline and after surrogate correction) for the *test* data set (the intercepts were insignificant therefore set to 0) (n = 29).

Surrogate	(a) *Training data:* Equations for surrogate-adjusted RapidAir NO$_x$ (µg/m^3)	r
RapidAir	RA_Adj_Mod_NO$_x$ = 1.98*RapidAir_NO$_x$	0.93
SVF	SVF_Adj_Mod_NO$_x$ = 1.87*RapidAir_NO$_x$ − 70.61*SVF + 55.90	0.84
WE	WE_Adj_Mod_NO$_x$ = 2.00*RapidAir_NO$_x$ − 90.99*WE + 85.43	0.84
HS	HS_Adj_Mod_NO$_x$ = 2.01*RapidAir_NO$_x$ − 54.04*HS + 49.57	0.83

Surrogate	(b) *Test data:* Measured vs Modelled NO$_x$ (µg/m^3)	r
RapidAir	Measured NO$_x$ = 0.79*RA_Adj_Mod_NO$_x$	0.86
SVF	Measured_NO$_x$ = 0.79*SVF_Adj_Mod_NO$_x$	0.87
WE	Measured_NO$_x$ = 0.78*WE_Adj_Mod_NO$_x$	0.85
HS	Measured_NO$_x$ = 0.78*HS_Adj_Mod_NO$_x$	0.85

The multiple linear calibrations developed were then applied to the *test* NO$_x$. Table 3b shows the *Measured* vs. *Modelled* NO$_x$ after application of the surrogate calibrations for the *test* dataset. The correlation between the concentrations and surrogates was unaffected by the surrogate used (*r* = 0.75).

3.3.2. Street canyon models

Of the 86 receptor locations we identified 19 sites that were located within urban street canyons through observations of the urban morphology using GIS and Google Maps Street View (Map data ©2017 Google) (Table A1).

A representative subset of the annual hourly meteorological data was used in the street canyon models to reduce model run times (discussed in Appendix A). The effect of using a subset of meteorological data on computed annual average concentrations compared to the whole dataset was minimal for both canyon models. AEOLIUS was slightly more sensitive to the use of a sampled meteorological record (STREET model: slope = 1.00, intercept = −0.21, R^2 = 1.00; AEOLIUS model: slope = 0.91, intercept = 0.71, R^2 = 0.99) (Fig. A11).

The windward and leeward concentrations predicted by each of the street canyon models were averaged on the assumption that over a year concentrations are well mixed within the street canyon. The concentrations predicted within by the canyon model were then added to the baseline NO$_x$ concentrations predicted by the RapidAir model (representing the urban background in the area), and the models corrected

for systematic bias following the guidance in DEFRA Technical Guidance 2016 (DEFRA, 2016) (Table 4).

3.3.3. Evaluation of RapidAir NO₂ estimates after accounting for street canyon effects

At the receptor locations in street canyons the underestimation of the receptor concentrations was lowest for the street canyon models, with the surrogates model and kernel models similarly under predicting the concentrations (NO₂ NMB = −0.18 for kernel, average NMB -0.16 for surrogates, −0.14 for STREET and −0.17 for AEOLIUS models (n = 19)) (Table 2b (NO₂) and Table A4 (NO$_x$)). The STREET model predicted higher concentrations than the AEOLIUS model which resulted in the smaller NMB values (Fig. A12). The difference in modelled concentrations between the STREET and AEOLIUS models was very small which is similar to previously published findings (Ganguly and Broderick, 2011, 2010; Gualtieri, 2010; Zhu et al., 2015).

When all types of receptor locations were considered, there was little difference between the pollution concentrations estimated at the receptor locations for the RapidAir model, surrogates and the street canyon models (Fig. A13). Consequently, there was limited difference in the model evaluation statistics when the surrogates and street canyon models were included (Table 2b (NO₂) and Table A4 (NO$_x$)). Inclusion of the street canyon models reduced the NO₂ NMB values compared to the standard kernel model, however inclusion of the surrogates had little impact on NMB values at the kerbside sites (Kernel = −0.25, Surrogates = −0.24, STREET = −0.24 and AEOLIUS = −0.26) (Table 2b (NO₂) and Table A4 (NO$_x$)). LUR models for NO₂ incorporating *SVF* street canyon surrogates also found little improvement in coefficient of determination values after surrogate inclusion (R^2 = 0.76 *vs.* 0.78) (Eeftens et al., 2013).

Despite the negligible change in model evaluation statistics the combined kernel-canyon models required less adjustment for systematic bias than the uncorrected kernel model (Table 4). Therefore, when a combined kernel-canyon model is applied to areas of the city which do not have any measurements the model may be subject to less over or under estimation than the kernel model which does not attempt to address urban morphology. For instance, the combined kernel-STREET model required adjustment using the linear regression equation *Adjusted NO$_X$ = 1.04 * Modelled NOx + 34.45*. The slope here is significantly lower than the regression equation used to correct the kernel-only model (*i.e.* 1.04 *vs.* 1.98). Predicted concentrations were similar for the combined kernel-STREET and combined kernel-AEOLIUS models. The inclusion of the street canyon models is therefore an important step in accounting for urban morphology which can in practice be as influential to air pollution concentrations as spatial variations in emissions in an urban setting.

The use of surrogates to account for urban morphology effects,

including street canyons, has computational simplicity advantages over street canyon models. Surrogate values can be rapidly calculated in a GIS across a large study area. Canyon models require user selection of canyon locations, and require additional information about canyon widths, heights, and traffic information such as speed (and therefore cannot be easily computed for large areas).

Additionally, the transition from 'built up' to 'open' within the city (for example at boundaries between buildings and parkland) is treated in a gradual manner in surrogate models - unlike street canyon models which impose a hard boundary at the canyon edge which is 'smoothed' artificially in a GIS with interpolation routines. Currently surrogates do not take wind speed into account which, for annual averages, we anticipate to have little influence on the model accuracy. However, if the surrogates were to be applied to a dispersion model with higher (e.g. hourly) temporal resolution then some modification of the surrogates to account for wind speed effects may be required in order to obtain similar modelled and measured pollution concentrations.

3.4. Advantages and limitations of RapidAir

The main aim of this work was to evaluate an air quality modelling platform designed for operational settings where time is often a priority and manpower/computational resources are limited. An example of an operational use of RapidAir is given in Appendix A. RapidAir succeeds as an operational air quality model in the context of very large urban areas and as a decision support tool but its efficiency comes with some drawbacks. Therefore, it is appropriate to outline the key benefits and limitations of the approach to enable practitioners to interpret this work in light of their current experiences in running city scale dispersion models.

Clearly a significant benefit with RapidAir is reduced computational burden. Run times of 10 min or less for a very large city with > 8 million inhabitants present a significant benefit for the operational modeller and decision makers who require fast but robust analyses. The RapidAir platform allows extremely efficient policy testing and other "what if" model runs for new emission scenarios to be undertaken in a few minutes on a standard office computer which is to our knowledge not possible using existing platforms.

The model performance metrics for RapidAir in Table 2 are very similar to those computed for other dispersion modelling systems in the DEFRA inter comparison exercise. For example, the RapidAir outputs for kerbside locations in London have NO₂ RMSE values of 38.91–45.26 μg/m³ depending on the method taking street canyons into consideration (r = 0.65–0.84, n = 8) where the models in the inter comparison have RMSE values ranging from 29.39 to 67.09 μg/m³ (r = 0.15–0.93, n = 7). At roadside locations the RapidAir outputs have NO₂ RMSE values of 12.78–14.28 μg/m³ (r = 0.70–0.76, n = 40) where

Table 4
(a) Linear adjustment equations to account for systematic bias in kernel model performance. This data was derived from the *training* dataset (n = 59). Equations are shown for the kernel model; and kernel model including street canyon model. The intercept was not significant for kernel and therefore the intercept was forced through the origin. (b) Ordinary least squares regression equations between the measured (*Measured_NO$_x$*) and canyon-adjusted kernel model NO$_x$ concentrations (baseline and after canyon correction) for the *test* data set (the intercepts were insignificant therefore set to 0) (n = 29).

Model	(a) *Training data:* Equations for canyon model-adjusted RapidAir NO$_x$ (μg/m³)	r
Kernel	RA_Adj_Mod_NO$_x$ = 1.98*RapidAir_NO$_x$	*0.94*
STREET	STREET_Adj_Mod_NO$_x$ = 1.16*(RapidAir_NO$_x$ + STREET) + 29.80	*0.88*
AEOLIUS	AEOLIUS_Adj_Mod_NO$_x$ = 1.64*(RapidAir_NO$_x$ + AEOLIUS) + 8.94	*0.87*

Model	(b) *Test data:* Measured vs. Modelled RapidAir NO$_x$ (μg/m³)	r
Kernel	Measured_NO$_x$ = 0.79*RA_Adj_Mod_NO$_x$	*0.86*
STREET	Measured_NO$_x$ = 0.85*STREET_Adj_Mod_NO$_x$	*0.97*
AEOLIUS	Measured_NO$_x$ = 0.80*AEOLIUS_Adj_Mod_NO$_x$	*0.97*

the models in the inter comparison have RMSE values ranging from 9.94 to 19.69 μg/m^3 (r = 0.38–0.89, n = 30). Some of the variation between RapidAir and the other models will be due to the different number of receptors in each category (which in reality may help or hinder our model performance) but it is impossible for us to match the locations exactly for the reasons explained earlier. The model results also yielded good results for the COE and IOA when compared with the definitions for these metrics provided by Carslaw and Ropkins (2012). The key model metrics for the 2008 model run in London are very similar to standard modelling suites used in the UK and which are used and accepted by DEFRA for use in compliance assessments at the highest level of statutory European air quality reporting. The high spatial resolution possible with the RapidAir model makes it a suitable candidate for use as an exposure metric for epidemiology studies for example.

In our view the potential drawbacks of the model must be balanced against the benefits described above. There may be the suggestion that the kernel based model represents a significantly simplified treatment of urban dispersion compared with models currently in use in the UK which iterate over thousands of receptors and calculate contributions at those receptors as a function of those sources (with very significant run times). In fact, all Gaussian and empirical models are already a greatly simplified picture of reality in urban settings and the methodology in RapidAir does not significantly alter the overall level of simplification compared with the real situation. In any case the model results are compared against pollution measurements as with all other models using the same metrics and the results of that performance assessment are comparable with other platforms.

The performance statistics for the surrogates for urban morphology are reasonably close to those from the models which treat canyons discretely. Again our focus is on operational modelling where reproducible and efficient workflows are as important as the tools selected for use. Based on this work we would suggest that for compliance assessment RapidAir is used with either the STREET or AEOLIUS model options included as the run times are not significantly impacted by including these models. The model results should be compared with measured concentrations and the modeller may choose the best performing street canyon model for their case. The surrogate models should be used as screening tools and perhaps to spatially delineate locations where the street canyon models should be invoked, which is often difficult for a large and complex urban environment where resources do not permit thorough investigation and spatial treatment of the morphological conditions.

4. Conclusions

We developed a kernel-based dispersion model (RapidAir) combining AERMOD and open-source scientific computing methods to estimate pollution concentrations at fine spatial resolution. Model input data was obtained from public sources to allow comparison with pollution models for the same location with the same input data. The RapidAir dispersion model took approximately 7 min to model the Greater London conurbation (~3500 km^2) at 5 × 5 m resolution using an Intel i5 64-bit laptop with 8 Gb RAM.

We evaluated NO$_x$ and NO$_2$ model predictions at 86 sites across London. After correction for systematic under estimation bias in the initial RapidAir model, FAC2 values for modelled concentrations were > 0.85 at the 86 evaluation sites. RMSE values decreased through the site categories: Kerbside, Roadside, Urban Background and Suburban (RMSE = 45, 14, 6 and 4 μg/m^3 respectively). This finding is consistent with results from other modelling groups participating in the DEFRA inter comparison, whose RMSE values ranged from 3 to 70 μg/m^3 respectively.

The larger RMSE values at the sites in proximity to traffic sources may have resulted from the presence of street canyons that trap pollutants leading to elevated concentrations – an effect that cannot be

described in dispersion models unless urban morphologies are taken into consideration. Correspondingly, we used geospatial surrogates (sky-view factor, hill shading and wind effect) and separate street canyon models (STREET and AEOLIUS) to improve modelled concentrations at roadside sites. The STREET canyon model and street canyon surrogates improved the model RMSE at kerbside sites: RapidAir base-kernel = 45.2, sky-view factor surrogate = 44.0, STREET model = 38.9 and AEOLIUS = 42.8 μg/m^3. When all sites were considered the lowest RMSE values were observed for the kernel model combined with the STREET canyon model (RMSE RapidAir base-kernel = 17.1 *vs.* STREET model = 15.9 μg/m^3). Consequently, the combined models may be anticipated to provide more accurate estimates when extrapolated to locations without monitoring. The geospatial surrogates have potential as simple means of incorporating canyon effects into a large city scale dispersion model. The advantage of using simple geospatial surrogates for street canyons instead of modelling canyons discretely include: reduced run times, smaller user input required and the transition from 'built up' to 'open' environments is treated gradually.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx. doi.org/10.1016/j.envsoft.2018.05.014.

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