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Supplement of

Spatiotemporal evaluation of EMEP4UK-WRF v4.3 atmospheric chemistry transport simulations of health-related metrics for NO_2, O_3, PM_{10}, and $PM_{2.5}$ for 2001–2010

Chun Lin et al.

Correspondence to: Mathew R. Heal (m.heal@ed.ac.uk)

Supplementary Information

A. Sites supplying measurement data used in this study

Table S1 lists the names and locations of the UK Automated Urban and Rural Network (AURN) stations used in this study. The percentage data captures for each pollutant at each site are also presented. The criteria for data capture are described in Section 2.2 of the main paper. More detail on each site is available online (uk-air.defra.gov.uk).

B. Long-term averaged model-measurement concentrations by temperature

Figure S1 presents an analogous figure to Figure 1 – i.e. scatter plots of the 10-y means of the modelled and measured pollutant daily metrics at each site, grouped by site type – but with data markers shaded according to the 10-y mean temperature at the measurement site. The correlations between the normalised model-measurement bias at each site of a given site type with temperature (for a given pollutant) are given in Table 2 of the main paper.

C. Analysis of model-measurement statistics averaged by hour of the day

The focus in the main paper is model-measurement comparisons at daily and annual averaging resolution, but concentration data were available at hourly resolution and figures and discussion of the comparison statistics for NO_2 and O_3 averaged by hour of day are presented in Figure S2 and Table S2.

The model-measurement statistics for NO_2 concentrations averaged by hour of day shown in Figures S2a-d reveal some diurnal variation in these statistic. Model-measurement negative bias for hourly NO_2 concentration at UB sites increased from 05:00-06:00 through the morning rush hours (Figure S2c), coincident with the increase in traffic movements (Figure S3a) and the consequent increase in NOx and VOC emissions (Figure S3b) imposed on the model. NO_x emissions decreased after the morning rush hours, and the model negative bias in urban areas continued to increase until midday. Model underestimation reduced steadily after the evening rush hours when both emissions and photochemical reactions are lower than in daytime. Model-measurement RMSE was also generally poorer (i.e. greater) during the day than during night (Figure S3d). The model NO_2 daytime lifetime may be too short, again likely due to the over-dilution of NOx emissions into the model grid (in more concentrated NO_2 environments OH is depleted to the main NO_2 loss process of HNO_3 formation is slower in the model than in the vicinity of the monitor). The model-measurement correlation for hourly NO_2 remained more consistent throughout the day (Figure S3a); correlations were similar at the two types of background sites (mean of median r = 0.64 and 0.60 at RB and UB sites, respectively). Correlation coefficients were slightly lower when emissions increased at the morning rush hour (Figure S3b), particularly at the urban sites, but due to the large inter-site variability, this reduction in correlation was not statistically significant (Figure S2a).

For hourly O_3, model-measurement correlation was similar at both types of background sites (mean of median $r = 0.68$ and 0.70 at RB and UB sites, respectively) (Figure S2e) and varied little during the day. Model positive bias for hourly O_3 concentrations at both RB and UB sites increased to peak in the morning rush hours (Figure S2g), and gradually reduced thereafter. Model RMSE also increased at UB sites during daytime, but not at RB sites (Figure S2h). The trend for bias in hourly O_3 is associated with the increased model underestimation of NO_2, for similar reasons, but is less pronounced because of the somewhat slower timescales for O_3 chemistry.

Overall, these data for model-measurement comparison by hour-of-day support the general trends presented in the main paper for the longer averaging periods, in particular that correlations are generally consistent throughout the day but that bias showed systematic variation, interpreted as a mismatch with reality of the hour-of-day emissions factors used to disaggregate the supplied annual NO_x emissions totals, and to over-dilution of the NO_x emissions into the model grid compared to the siting of the monitor for UB sites.

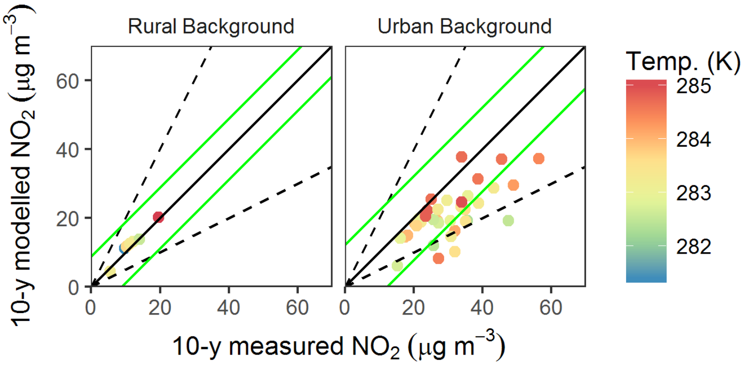
Table S1: The names and locations of the UK Automated Urban and Rural Network stations used in this study, with their measurement data availability, listed by site type (RB, rural background; UB, urban background). NA means no contributing measurements.

Site	Site type	Latitude (°)	Longitude (°)	Data Capture Proportion			
				NO_2	O_3	PM_{10}	$PM_{2.5}$ (2y)
Aston Hill	RB	52.50385	-3.034178	NA	92%	NA	NA
Auchencorth Moss	RB	55.79216	-3.2429	NA	NA	NA	84%
Bottesford	RB	52.93028	-0.814722	NA	99%	NA	NA
Bush Estate	RB	55.862281	-3.205782	NA	97%	NA	NA
Eskdalemuir	RB	55.31531	-3.206111	NA	96%	NA	NA
Glazebury	RB	53.46008	-2.472056	NA	90%	NA	NA
Harwell	RB	51.571078	-1.325283	97%	94%	94%	86%
High Muffles	RB	54.334944	-0.80855	NA	88%	NA	NA
Ladybower	RB	53.40337	-1.752006	87%	90%	NA	NA
Lough Navar	RB	54.43951	-7.900328	NA	90%	91%	NA
Lullington Heath	RB	50.7937	0.18125	97%	88%	NA	NA
Mace Head	RB	53.326444	-9.903917	NA	98%	NA	NA
Narberth	RB	51.781784	-4.691462	93%	NA	79%	NA
Rochester Stoke	RB	51.45617	0.634889	89%	92%	78%	NA
Sibton	RB	52.2944	1.463497	NA	92%	NA	NA
St Osyth	RB	51.77798	1.049031	84%	77%	NA	NA
Weybourne	RB	52.95049	1.122017	NA	84%	NA	NA
Wicken Fen	RB	52.2985	0.290917	90%	91%	NA	NA
Yarner Wood	RB	50.5976	-3.71651	NA	94%	NA	NA
Aberdeen	UB	57.15736	-2.094278	95%	NA	92%	NA
Barnsley Gawber	UB	53.56292	-1.510436	93%	93%	NA	NA
Belfast Centre	UB	54.59965	-5.928833	92%	93%	87%	91%
Birmingham Centre	UB	52.479724	-1.908078	76%	NA	NA	NA
Bournemouth	UB	50.73957	-1.826744	96%	76%	NA	NA
Bristol St Paul's	UB	51.462839	-2.584482	NA	NA	NA	93%
Canterbury	UB	51.27399	1.098061	98%	NA	NA	NA
Cardiff Centre	UB	51.48178	-3.17625	94%	92%	82%	90%
Chesterfield	UB	53.230583	-1.433611	NA	NA	NA	94%
Coventry Memorial Park	UB	52.394399	-1.519612	95%	85%	NA	93%
Cwmbran	UB	51.6538	-3.006953	89%	NA	NA	NA
Derry	UB	55.001225	-7.329115	96%	91%	89%	NA
Edinburgh St Leonards	UB	55.945589	-3.182186	NA	NA	NA	94%
Glasgow Centre	UB	55.85773	-4.255161	88%	96%	83%	99%
Glasgow City Chambers	UB	55.860414	-4.245959	99%	NA	NA	NA
Hull Freetown	UB	53.74878	-0.341222	76%	77%	NA	92%
Leamington Spa	UB	52.28881	-1.533119	87%	95%	90%	97%
Leeds Centre	UB	53.80378	-1.546472	95%	94%	94%	96%
Leicester Centre	UB	52.631348	-1.133006	96%	94%	89%	NA
London Bloomsbury	UB	51.52229	-0.125889	84%	92%	85%	88%
London Haringey	UB	51.58603	-0.126486	NA	90%	NA	NA
London Harrow Stanmore	UB	51.617333	-0.298777	NA	NA	NA	83%

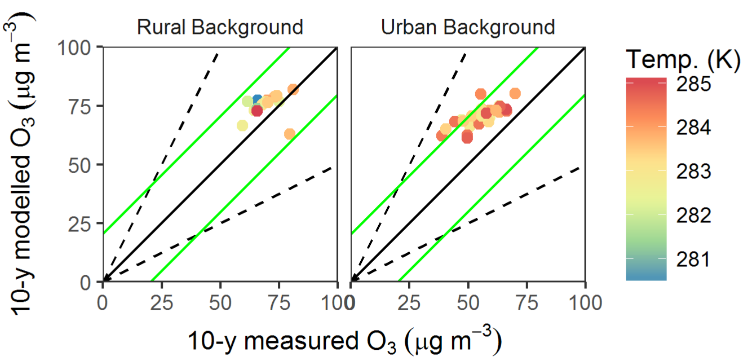
London Hillingdon	UB	51.49633	-0.460861	95%	94%	NA	NA
London N. Kensington	UB	51.52105	-0.213492	97%	96%	93%	95%
London Teddington	UB	51.42099	-0.339647	94%	96%	NA	87%
London Westminster	UB	51.49467	-0.131931	85%	85%	NA	NA
Manchester Piccadilly	UB	53.48152	-2.237881	88%	94%	78%	NA
Newcastle Centre	UB	54.97825	-1.610528	91%	94%	94%	93%
Newport	UB	51.601203	-2.977281	NA	NA	NA	99%
Northampton	UB	52.27349	-0.885933	90%	NA	NA	NA
Nottingham Centre	UB	52.95473	-1.146447	94%	97%	85%	81%
Oxford St Ebbes	UB	51.744806	-1.260278	NA	NA	NA	95%
Plymouth Centre	UB	50.37167	-4.142361	89%	76%	77%	NA
Portsmouth	UB	50.82881	-1.068583	99%	76%	82%	82%
Preston	UB	53.76559	-2.680353	92%	94%	77%	84%
Reading New Town	UB	51.45309	-0.944067	NA	NA	NA	90%
Sandwell West Bromwich	UB	52.52062	-1.995556	94%	95%	NA	NA
Sheffield Centre	UB	53.37772	-1.473306	91%	97%	94%	91%
Sheffield Tinsley	UB	53.41058	-1.396139	88%	NA	NA	NA
Southampton Centre	UB	50.90814	-1.395778	93%	92%	92%	85%
Southend-on-Sea	UB	51.544206	0.678408	89%	94%	NA	95%
Stoke-on-Trent Centre	UB	53.02821	-2.175133	98%	93%	90%	97%
Sunderland Silksworth	UB	54.88361	-1.406878	NA	NA	NA	78%
Thurrock	UB	51.47707	0.317969	94%	96%	91%	NA
Walsall Willenhall	UB	52.60821	-2.033144	85%	NA	NA	NA
Wirral Tranmere	UB	53.37287	-3.022722	89%	85%	NA	86%
York Bootham	UB	53.967513	-1.086514	NA	NA	NA	98%

Figure S1: Scatter plots of the 10-year means of the modelled and measured pollutant daily metrics at each site, grouped by site type, and with data markers shaded according to the temperature of the measurement site: (a) NO_2; (b) O_3; (c) PM_{10}; (d) $PM_{2.5}$. The values of *r*, FAC2, NMB and RMSE associated with the data in each plot are given in Table 1. The solid and dashed lines are the 1:1, and the 2:1and 1:2 lines, respectively. The green lines show values for model performance criteria for each pollutant taking account of variable measurement uncertainty using formulae and variable values published by the FAIRMODE project (fairmode.jrc.ec.europa.eu). See main text for further details.

(a)



(b)



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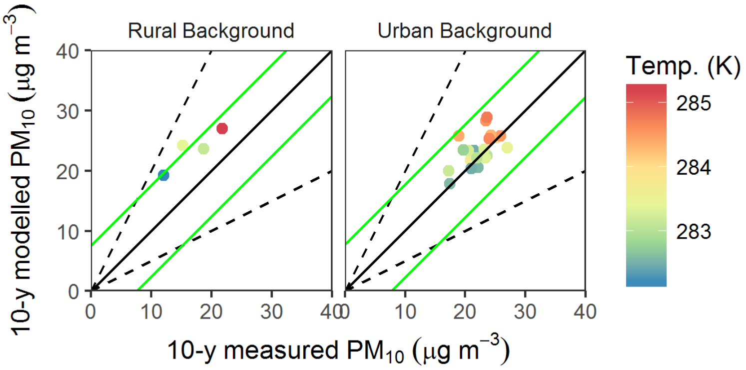


(d)

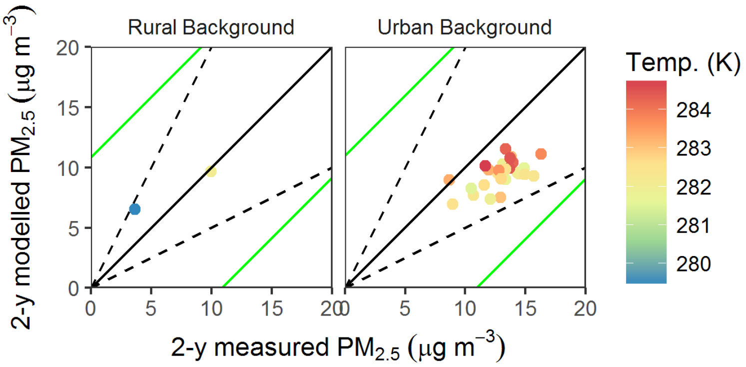


Figure S2: Model-measurement statistics per site for (a-d) NO_2 hourly and (e-h) O_3 hourly concentrations during 2001-2010, by site type, and by hour of day. (a) and (e) are correlation coefficient (*r*), (b) and (f) are fraction of data pairs within a factor of two (FAC2), (c) and (g) are normalised mean bias (NMB), and (d) and (h) are RMSE. Dots show individual site statistics, which are summarised in the superimposed box-plot whose shading demarcates the interquartile range (IQR) and whose whiskers extend to the largest and smallest value within 1.58 × IQR from the box hinges.

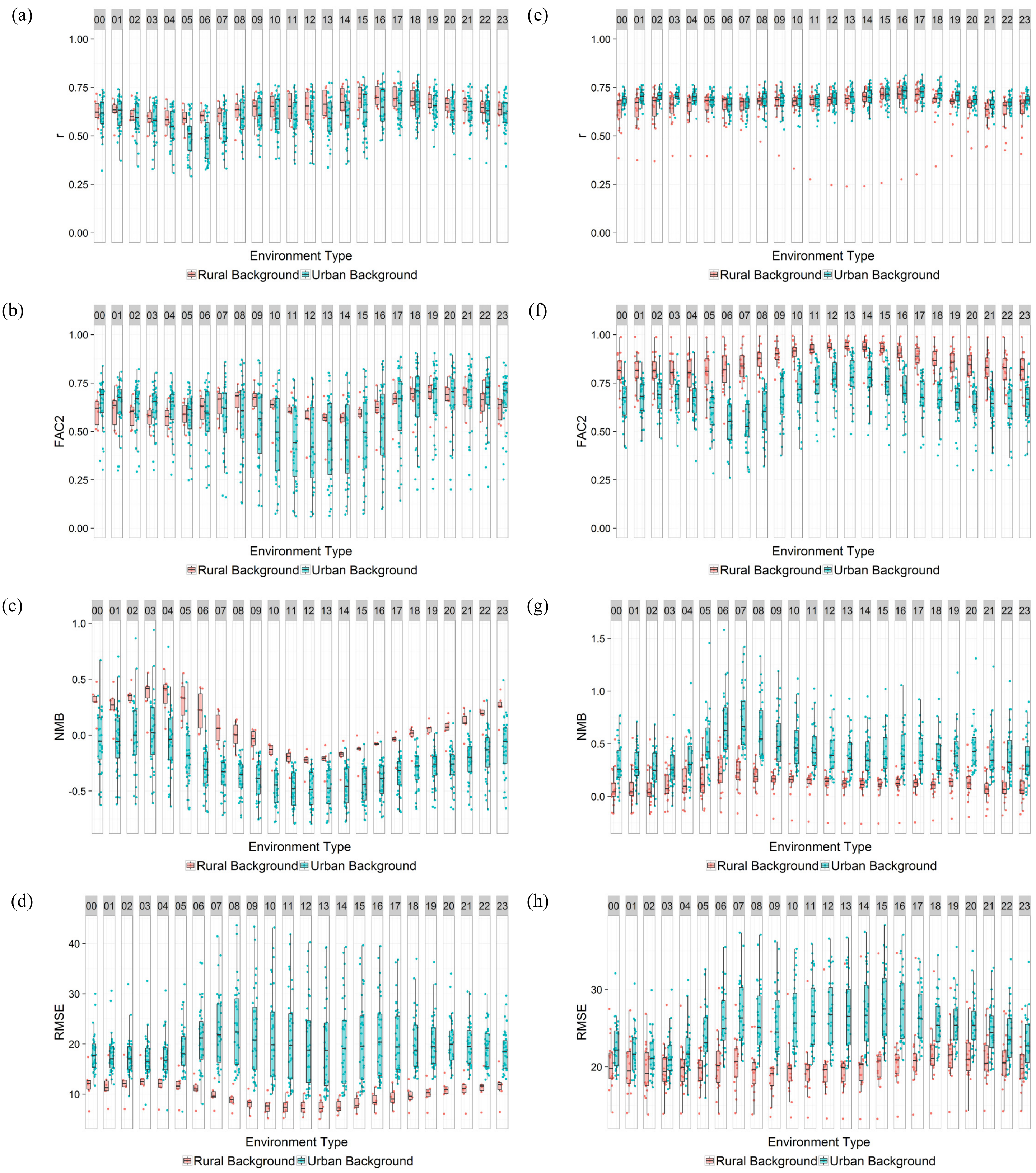
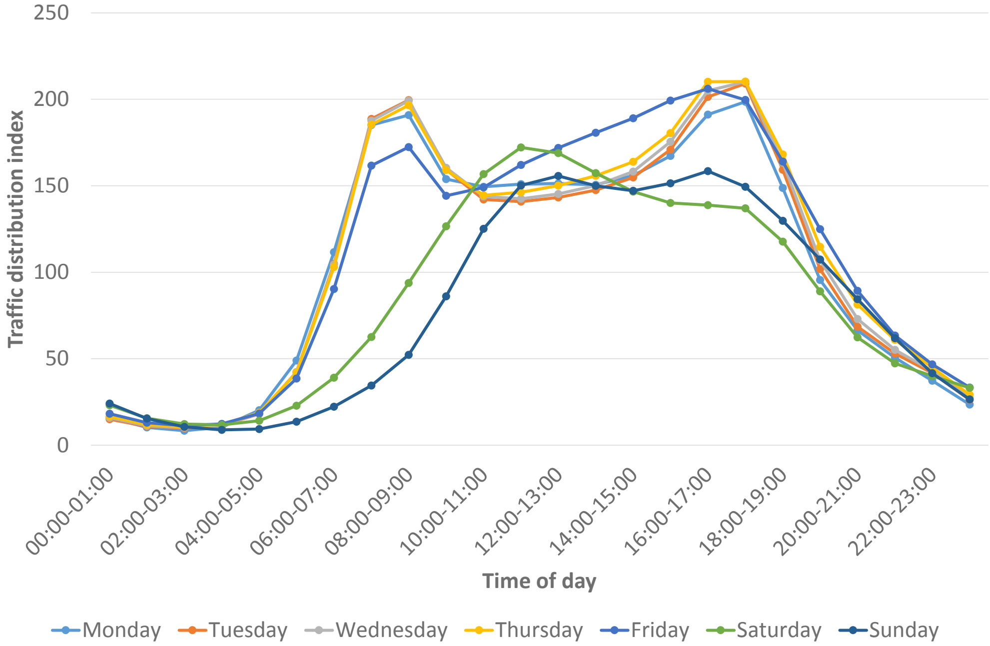


Figure S3: (a) Normalised traffic distribution (all vehicles) on all roads by time of day and day of week in the UK in 2010 (DfT, 2011). Road traffic statistics in Years 2008 and 2009 showed similar diurnal variation to this figure. (b) Normalised emission factors used by EMEP4UK to disaggregate road-traffic NO_x emissions by time of day and day of week. Road-traffic VOC emissions in the model use the same factors.

(a)



(b)

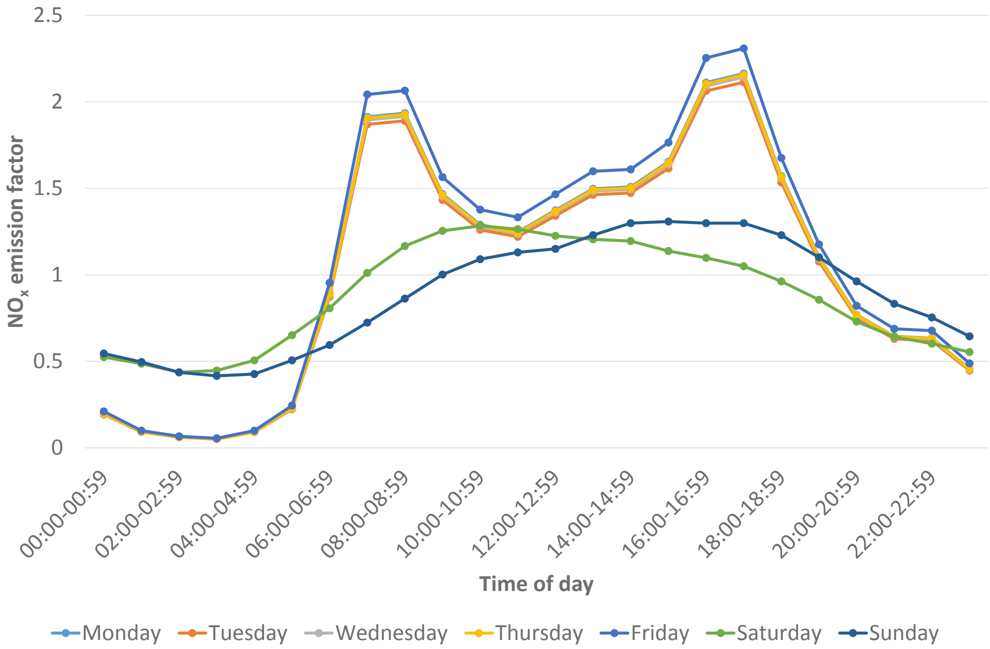


Table S2: Median (25th percentile, 75th percentile) values of the *n* individual-site model-measurement statistics of hourly NO_2 and O_3 for the full 10-y period, grouped by site type: RB, rural background; UB, urban background.

	n	*r*	FAC2	NMB	MB / μg m^{-3}	RMSE / μg m^{-3}
NO_2_hourmean						
RB	6	0.63 (0.60, 0.68)	0.63 (0.59, 0.66)	0.10 (0.05, 0.12)	1.12 (0.82, 1.31)	10.19 (9.48, 10.58)
UB	35	0.56 (0.51, 0.65)	0.60 (0.50, 0.69)	−0.28 (−0.42, −0.15)	−9.22 (−15.06, −3.19)	19.40 (15.16, 24.21)
O_3_hourmean						
RB	17	0.70 (0.68, 0.73)	0.86 (0.82, 0.90)	0.13 (0.09, 0.19)	6.61 (5.34, 7.84)	20.09 (18.96, 21.44)
UB	31	0.71 (0.69, 0.74)	0.67 (0.62, 0.75)	0.37 (0.25, 0.51)	14.88 (11.95, 20.09)	24.69 (22.34, 27.89)