

SUPPORTING INFORMATION

Independent validation of national satellite-based land-use regression models for nitrogen dioxide using passive samplers

Luke D. Knibbs^{1*}, Craig P. Coorey², Matthew J. Bechle³, Christine T. Cowie^{4,5,6}, Mila Dirgawati⁷, Jane S. Heyworth⁷, Guy B. Marks^{4,5}, Julian D. Marshall³, Lidia Morawska⁸, Gavin Pereira⁹, Michael G. Hewson¹⁰

¹ School of Public Health, The University of Queensland, Herston, QLD 4006, Australia

² School of Medicine, The University of Queensland, Herston, QLD 4006, Australia

³ Department of Civil and Environmental Engineering, University of Washington, Seattle, WA 98195, USA

⁴ South Western Sydney Clinical School, The University of New South Wales, Liverpool, NSW 2170, Australia

⁵ Ingham Institute for Applied Medical Research, Liverpool, NSW 2170, Australia

⁶ Woolcock Institute of Medical Research, University of Sydney, Glebe, NSW 2037, Australia

⁷ School of Population Health, The University of Western Australia, Crawley, WA 6009, Australia

⁸ International Laboratory for Air Quality and Health, Queensland University of Technology, Brisbane, QLD 4001, Australia

⁹ School of Public Health, Curtin University, Perth, WA 6000, Australia

¹⁰ School of Geography, Planning and Environmental Management, The University of
Queensland, St. Lucia, QLD 4067, Australia

* Corresponding author (e: l.knibbs@uq.edu.au; ph: +61 7 3365 5409)

Number of pages: 34

Number of figures: 5

Number of tables: 12

Adjustment of measurements to an annual mean

We used an approach based on three continuous monitoring sites in each city (Sydney and Perth) to determine ratios for adjusting the three 2-week measurements to an estimated annual mean. This approach captures the influence on pollutant levels of weather (e.g., temperature inversions) or sources that affect the entire airshed (e.g., bushfires), which tend to be high or low on the same days across a city.¹ We therefore selected background sites in order to account for temporal variation in NO₂ measured during the two week sampling periods. The continuous sites were regulatory chemiluminescence-based NO₂ monitors. While the two week measurements were done using passive sampling using Ogawa and Ferm-type samplers and the adjustment ratio was based on chemiluminescence, the active and passive methods agree well, particularly for two week sampling durations, and regression slopes are typically within $\pm 10\%$ of 1.0 and R² values above 0.85 (e.g., ^{2,3,4})

We used 3 sites in each city to determine an average ratio so that the adjustment was not dependent on a single site, and to improve the precision of adjusted concentrations. The sites were selected on the basis of (a) not being proximate to NO₂ sources (i.e., background sites); (b) spanning a wide area in different directions around the city where measurements were performed (i.e., creating a triangle centred on each study area); (c) being greater than approximately 20 km from other sites used to determine the ratio, and; (d) having 80% or more non-missing daily NO₂ data in a given two-week period, and in a given year. These criteria aimed to ensure that the ratios were representative of temporal trends in ambient NO₂ across the entire study area. If more than three sites in an area met the criteria, we used the sites with the most complete data. The sites we selected are given in Table S1.

Table S1. Characteristics of continuous monitoring sites used for determining annual mean adjustment ratios for each city.

Location	Distance to CBD (km) ^a	Distance to nearest monitor (km) ^b	Distance to nearest major road (m) ^c	Distance to nearest NO _x point source (km) ^c	Classification ^d
Sydney					
Site A (Bringelly)	41.5	30.3	2,810	2.4	Peri-urban background
Site B (Vineyard)	40.5	30.3	1,486	5.1	Peri-urban background
Site C (Rozelle)	4.1	37.2	301	3.4	Urban background
Perth					
Site A (South Lake)	17.8	18.5	257	2.4	Urban background
Site B (Caversham)	14.1	22.3	195	1.1	Peri-urban background
Site C (Swanbourne)	9.4	18.5	140	3.9	Urban background

^a CBD = central business district. ^b Distance to nearest site used to determine the adjustment ratio (i.e., sites A, B, or C). ^c Definitions and data sources for major roads and NO_x point sources are given in Knibbs et al.⁵ ^d Urban background sites are defined in the main article text. Peri-urban sites were located on the rural-urban fringe of the city.

Table S2. Descriptive statistics for daily mean NO₂ (ppb) measured at each continuous monitoring site used for determining ratios. Data are presented for years in which annual adjustment ratios were calculated (2006-08 and 2013-14 for Sydney; 2012 for Perth).

	Site A (Bringelly)	Site B (Vineyard)	Site C (Rozelle)	Site A (South Lake)	Site B (Caversham)	Site C (Swanbourne)
2006						
min.	1.0	1.0	3.0	-	-	-
5 th	2.0	3.0	6.0	-	-	-
25 th	4.0	5.0	8.0	-	-	-
50 th	6.0	7.0	12.0	-	-	-
75 th	8.0	9.0	18.0	-	-	-
95 th	11.0	14.0	24.0	-	-	-
max.	15.0	17.0	30.0	-	-	-
mean	6.3	7.3	13.1	-	-	-
s.d.	2.8	3.2	5.8	-	-	-
missing (%)	3.8	8.8	2.5	-	-	-
2007						
min.	1.0	1.0	2.0	-	-	-
5 th	2.0	2.0	4.0	-	-	-
25 th	4.0	4.0	7.0	-	-	-
50 th	6.0	6.0	11.0	-	-	-
75 th	7.0	8.0	15.0	-	-	-
95 th	10.0	11.0	21.0	-	-	-
max.	14.0	15.0	28.0	-	-	-
mean	5.6	6.0	11.6	-	-	-
s.d.	2.6	2.7	5.4	-	-	-
missing (%)	2.7	5.8	6.0	-	-	-
2008						
min.	1.0	1.0	2.0	-	-	-
5 th	1.0	1.0	4.0	-	-	-

25 th	3.0	3.0	7.0	-	-	-
50 th	4.0	5.0	10.0	-	-	-
75 th	6.0	7.0	15.0	-	-	-
95 th	9.0	11.0	20.8	-	-	-
max.	13.0	15.0	26.0	-	-	-
mean	4.6	5.4	11.0	-	-	-
s.d.	2.3	2.7	5.2	-	-	-
missing (%)	10.1	9.3	17.2	-	-	-
2012						
min.	-	-	-	1.5	1.1	0.2
5 th	-	-	-	2.4	1.9	0.3
25 th	-	-	-	4.5	3.4	2.5
50 th	-	-	-	6.9	5.6	4.4
75 th	-	-	-	10.0	8.3	7.4
95 th	-	-	-	14.0	11.1	13.4
max.	-	-	-	18.5	15.6	19.2
mean	-	-	-	7.5	6.0	5.3
s.d.	-	-	-	3.6	3.0	3.9
missing (%)	-	-	-	1.6	3.6	0.3
2013						
min.	1.0	1.0	2.0	-	-	-
5 th	1.0	2.0	4.0	-	-	-
25 th	3.0	4.0	7.0	-	-	-
50 th	4.0	5.0	10.0	-	-	-
75 th	6.0	7.0	15.0	-	-	-
95 th	8.0	10.1	21.0	-	-	-
max.	11.0	14.0	27.0	-	-	-
mean	4.6	5.4	11.4	-	-	-
s.d.	2.1	2.6	5.4	-	-	-
missing (%)	3.6	2.2	5.5	-	-	-
2014						

min.	1.0	1.0	2.0	-	-	-
5 th	1.0	2.0	4.0	-	-	-
25 th	2.8	4.0	7.0	-	-	-
50 th	4.0	5.0	10.0	-	-	-
75 th	6.0	7.0	14.0	-	-	-
95 th	8.0	11.0	20.0	-	-	-
max.	11.0	13.0	25.0	-	-	-
mean	4.2	5.4	10.7	-	-	-
s.d.	2.1	2.6	5.0	-	-	-
missing (%)	6.3	1.9	2.2	-	-	-

Table S3. Mean, standard deviation, and standard error of the mean (SEM) for ratios used to adjust NO₂ measurements to annual means at the 123 validation sites. The adjusted and unadjusted annual mean NO₂ concentrations, standard deviation, and SEM are also shown. Each mean ratio was based on three separate continuous monitoring sites (above) repeated during typically 3 measurement campaigns. Note #1: site 43 did not require adjustment as it was a passive sampler monitoring site with a full year of data; some sites in the same data set were measured concurrently during each of the three sampling campaigns, and hence have the same adjustment ratios; the overall mean ratio presented below wasn't directly applied to the mean unadjusted NO₂ concentration to perform the adjustment, and each sampling period at a given site used a ratio based on three adjustment sites (it is given here to provide a single figure summary of the adjustment ratio). Note #2: Sampling dates for Sydney 1 campaign were 18/9/06 to 2/10/06; 23/10/06 to 6/11/06; 27/11/06 to 11/12/06; 17/09/07 to 1/10/07; 22/10/07 to 5/11/07; 26/11/07 to 10/12/07; 26/3/08 to 9/4/08; 12/5/08 to 26/5/08; 17/6/08 to 30/6/08; 15/9/08 to 29/9/08; 20/10/08 to 3/11/08; 24/11/08 to 8/12/08. Dates for Sydney 2 campaigns were 22/7/13 to 5/8/13; 28/11/13 to 12/12/13; 18/3/14 to 1/4/14. Dates for Perth 1 campaigns were 31/1/12 to 14/2/12; 16/2/12 to 1/3/12; 6/3/12 to 20/3/12; 22/3/12 to 5/4/12; 17/4/12 to 1/5/12; 3/5/12 to 17/5/12; 21/5/12 to 4/6/12; 6/6/12 to 20/6/12; 27/6/12 to 11/7/12; 13/7/12 to 27/7/12; 1/8/12 to 15/8/12; 17/8/12 to 31/8/12. Not all sites were measured simultaneously during all campaigns – see references in Table 1 for more information.

Data set	Site number	Adjusted	SD	SEM	Unadjusted	SD	SEM	Mean adjustment ratio (-)	SD adjustment ratio (-)	SEM adjustment ratio (-)
		annual mean NO2 (ppb)	adjusted annual mean NO2 (ppb)	adjusted annual mean NO2 (ppb)		unadjusted annual mean NO2 (ppb)	unadjusted annual mean NO2 (ppb)			
Perth 1	1	2.8	0.3	0.2	3.2	1.0	0.6	0.96	0.38	0.13
Perth 1	2	4.3	1.3	0.8	5.5	3.5	2.0	0.92	0.32	0.11
Perth 1	3	5.1	1.5	0.8	7.3	3.3	1.9	0.75	0.17	0.06
Perth 1	4	5.1	2.4	1.4	6.7	4.1	2.4	0.83	0.17	0.06
Perth 1	5	4.9	0.3	0.2	6.7	2.1	1.2	0.77	0.20	0.07
Perth 1	6	11.0	3.2	1.9	13.2	5.7	3.3	0.89	0.27	0.09
Perth 1	7	6.8	1.2	0.7	7.3	2.4	1.4	0.99	0.29	0.10
Perth 1	8	8.0	1.8	1.1	11.4	4.6	2.6	0.75	0.18	0.06
Perth 1	9	6.8	1.9	1.1	7.2	2.9	1.7	1.01	0.33	0.11
Perth 1	10	11.5	0.8	0.4	11.6	3.2	1.9	1.05	0.29	0.10
Perth 1	11	4.9	1.2	0.7	5.0	1.8	1.0	1.02	0.32	0.11
Perth 1	12	7.2	1.4	0.8	9.0	4.5	2.6	0.92	0.32	0.11
Perth 1	13	6.6	1.5	0.9	7.3	3.4	1.9	1.01	0.34	0.11
Perth 1	14	5.5	1.4	1.0	5.3	0.9	0.6	1.07	0.39	0.16
Perth 1	15	10.4	1.1	0.6	11.9	3.8	2.2	0.92	0.25	0.08
Perth 1	16	11.0	2.6	1.5	12.2	2.0	1.1	0.94	0.37	0.12
Perth 1	17	4.8	1.1	0.7	5.8	2.7	1.6	0.91	0.25	0.08
Perth 1	18	6.2	0.6	0.4	8.2	3.3	1.9	0.84	0.29	0.10
Perth 1	19	8.4	2.2	1.3	10.0	1.9	1.1	0.90	0.40	0.13
Perth 1	20	4.5	1.2	0.7	5.6	3.5	2.0	1.00	0.43	0.14
Perth 1	21	11.1	1.2	0.7	11.5	2.6	1.5	1.01	0.31	0.10
Perth 1	22	5.5	1.1	0.6	5.7	1.1	0.6	1.00	0.33	0.11
Perth 1	23	2.9	0.7	0.4	3.4	1.8	1.1	1.00	0.41	0.14
Perth 1	24	6.6	2.0	1.1	8.4	3.5	2.0	0.82	0.14	0.05
Perth 1	25	7.0	0.2	0.1	8.9	1.9	1.1	0.82	0.18	0.06

Perth 1	26	0.8	0.8	0.5	1.1	1.3	0.7	0.81	0.14	0.05
Perth 1	27	0.4	0.2	0.1	0.4	0.1	0.1	0.82	0.18	0.06
Perth 1	28	4.8	1.5	0.8	6.2	2.7	1.6	0.81	0.14	0.05
Perth 1	29	1.2	0.9	0.5	1.4	1.1	0.6	0.82	0.18	0.06
Perth 1	30	4.4	1.1	0.6	5.9	3.3	1.9	0.87	0.34	0.11
Perth 1	31	2.8	1.5	0.8	3.2	2.1	1.2	1.03	0.33	0.11
Perth 1	32	8.9	1.7	1.0	10.5	2.7	1.6	0.92	0.40	0.13
Perth 1	33	3.3	2.2	1.3	4.2	3.5	2.0	0.95	0.30	0.10
Perth 1	34	5.5	2.4	1.4	7.2	5.4	3.1	0.89	0.27	0.09
Perth 1	35	4.4	0.7	0.4	5.7	2.9	1.7	0.95	0.45	0.15
Perth 1	36	2.7	1.8	1.0	3.9	3.0	1.7	0.95	0.45	0.15
Perth 1	37	5.3	0.2	0.1	6.1	2.8	1.6	1.00	0.43	0.14
Perth 1	38	3.0	1.6	0.9	4.3	3.3	1.9	0.87	0.34	0.11
Perth 1	39	5.1	0.8	0.4	5.5	2.1	1.2	1.02	0.34	0.11
Perth 1	40	5.1	0.2	0.1	6.5	2.3	1.3	0.90	0.40	0.13
Perth 1	41	8.0	0.8	0.4	8.6	3.0	1.8	1.01	0.32	0.11
Perth 1	42	8.8	0.8	0.4	9.8	2.6	1.5	0.96	0.36	0.12
Perth 1	43	3.7	-	-	-	-	-			
Sydney 1	44	10.7	1.8	0.5	10.0	1.9	0.5	1.11	0.22	0.07
Sydney 1	45	12.4	2.2	0.7	11.5	2.3	0.7	1.11	0.22	0.07
Sydney 1	46	12.1	2.0	0.7	10.7	2.0	0.7	1.14	0.22	0.08
Sydney 1	47	10.7	1.8	0.6	9.3	1.3	0.4	1.15	0.52	0.14
Sydney 1	48	10.9	2.3	0.8	9.7	2.1	0.7	1.13	0.20	0.07
Sydney 1	49	16.5	2.3	0.7	15.5	2.1	0.7	1.10	0.23	0.07
Sydney 1	50	10.7	1.9	0.6	9.5	1.5	0.5	1.14	0.22	0.08
Sydney 1	51	11.4	1.6	0.5	10.1	1.6	0.5	1.14	0.22	0.08
Sydney 1	52	13.9	0.5	0.4	12.5	0.4	0.3	1.11	0.21	0.07
Sydney 1	53	10.1	1.3	0.5	9.2	1.3	0.5	1.11	0.22	0.08
Sydney 1	54	9.0	1.2	0.4	8.1	1.3	0.5	1.12	0.22	0.08
Sydney 1	55	11.7	1.9	0.6	10.3	1.8	0.6	1.14	0.22	0.08
Sydney 1	56	11.3	1.6	0.5	10.0	1.6	0.5	1.14	0.22	0.08

Sydney 1	57	12.9	1.5	0.5	12.6	2.5	0.8	1.10	0.26	0.10
Sydney 1	58	12.4	2.1	0.7	10.7	1.6	0.6	1.14	0.25	0.11
Sydney 1	59	14.6	2.5	0.9	12.6	1.9	0.7	1.14	0.25	0.11
Sydney 1	60	8.7	1.5	0.4	8.2	1.6	0.5	1.11	0.22	0.07
Sydney 1	61	10.5	1.5	0.5	9.3	1.5	0.5	1.14	0.22	0.08
Sydney 1	62	9.4	1.4	0.5	8.3	1.2	0.4	1.14	0.22	0.08
Sydney 1	63	11.2	1.4	0.5	9.9	1.5	0.5	1.14	0.22	0.08
Sydney 1	64	11.2	1.6	0.6	9.8	1.6	0.5	1.17	0.20	0.07
Sydney 1	65	11.3	1.4	0.5	10.0	1.5	0.5	1.14	0.22	0.08
Sydney 1	66	11.3	1.8	0.7	10.3	2.0	0.8	1.11	0.20	0.08
Sydney 1	67	9.7	2.2	0.7	8.6	1.7	0.6	1.12	0.22	0.08
Sydney 1	68	10.0	1.4	0.5	8.9	1.4	0.5	1.14	0.22	0.08
Sydney 1	69	19.3	5.2	1.6	18.1	4.0	1.2	1.09	0.22	0.07
Sydney 1	70	9.8	1.8	0.5	9.2	1.9	0.5	1.11	0.22	0.07
Sydney 1	71	10.6	1.7	0.5	10.0	2.2	0.6	1.11	0.22	0.07
Sydney 1	72	13.7	1.9	0.6	11.9	1.5	0.5	1.14	0.22	0.08
Sydney 1	73	16.5	2.8	0.9	15.4	1.9	0.6	1.10	0.23	0.08
Sydney 1	74	11.4	1.5	0.6	10.1	1.0	0.4	1.18	0.22	0.09
Sydney 1	75	11.8	1.4	0.5	10.4	1.4	0.5	1.15	0.22	0.08
Sydney 1	76	13.2	1.9	0.7	11.7	2.1	0.8	1.14	0.25	0.11
Sydney 2	77	11.9	1.6	0.9	11.7	3.0	1.7	1.05	0.21	0.08
Sydney 2	78	8.2	0.9	0.5	8.1	2.3	1.4	1.05	0.21	0.08
Sydney 2	79	9.7	0.0	0.0	10.5	1.2	0.9	0.92	0.14	0.06
Sydney 2	80	9.8	1.5	0.9	9.8	3.4	1.9	1.05	0.21	0.08
Sydney 2	81	17.7	2.3	1.3	17.3	3.2	1.8	1.05	0.21	0.08
Sydney 2	82	5.7	0.3	0.2	5.6	0.9	0.5	1.05	0.21	0.08
Sydney 2	83	12.1	1.9	1.1	11.8	1.3	0.8	1.05	0.21	0.08
Sydney 2	84	6.7	0.2	0.2	6.0	1.1	0.8	1.16	0.16	0.07
Sydney 2	85	8.3	0.6	0.4	8.3	2.0	1.1	1.05	0.21	0.08
Sydney 2	86	8.2	1.7	1.2	7.4	2.6	1.8	1.16	0.16	0.07
Sydney 2	87	16.8	2.8	1.6	16.9	5.9	3.4	1.05	0.21	0.08

Sydney 2	88	9.9	1.9	1.1	10.0	3.8	2.2	1.05	0.21	0.08
Sydney 2	89	7.8	0.9	0.5	7.7	1.3	0.7	1.05	0.21	0.08
Sydney 2	90	7.4	2.6	1.5	7.6	3.9	2.3	1.05	0.21	0.08
Sydney 2	91	9.1	2.2	1.3	9.2	3.9	2.3	1.05	0.21	0.08
Sydney 2	92	13.0	4.2	2.4	12.4	2.3	1.3	1.05	0.21	0.08
Sydney 2	93	11.4	1.7	1.0	11.0	1.2	0.7	1.05	0.21	0.08
Sydney 2	94	9.8	1.3	0.8	9.7	2.4	1.4	1.05	0.21	0.08
Sydney 2	95	8.4	0.6	0.3	8.3	2.0	1.1	1.05	0.21	0.08
Sydney 2	96	8.7	1.7	1.0	8.8	3.4	1.9	1.05	0.21	0.08
Sydney 2	97	8.1	0.6	0.4	7.8	1.5	1.1	1.06	0.25	0.10
Sydney 2	98	8.1	0.1	0.1	8.0	1.4	0.8	1.05	0.21	0.08
Sydney 2	99	6.0	0.5	0.3	6.0	1.6	0.9	1.05	0.21	0.08
Sydney 2	100	5.8	2.0	1.2	6.0	3.1	1.8	1.05	0.21	0.08
Sydney 2	101	13.4	1.7	1.0	13.4	4.3	2.5	1.05	0.21	0.08
Sydney 2	102	3.9	0.9	0.5	3.7	0.6	0.3	1.05	0.21	0.08
Sydney 2	103	9.5	0.7	0.5	8.5	1.9	1.3	1.16	0.16	0.07
Sydney 2	104	6.2	1.6	0.9	6.3	2.7	1.6	1.05	0.21	0.08
Sydney 2	105	7.1	1.7	1.0	7.1	2.7	1.6	1.05	0.21	0.08
Sydney 2	106	8.5	0.8	0.4	8.3	1.8	1.1	1.05	0.21	0.08
Sydney 2	107	7.5	1.8	1.0	7.2	1.7	1.0	1.05	0.21	0.08
Sydney 2	108	13.1	0.9	0.5	13.0	3.3	1.9	1.05	0.21	0.08
Sydney 2	109	14.5	1.1	0.6	14.3	3.6	2.1	1.05	0.21	0.08
Sydney 2	110	12.4	1.5	0.8	12.3	3.3	1.9	1.05	0.21	0.08
Sydney 2	111	15.3	0.6	0.3	15.1	3.0	1.7	1.05	0.21	0.08
Sydney 2	112	8.4	0.6	0.3	8.2	1.2	0.7	1.05	0.21	0.08
Sydney 2	113	9.2	2.2	1.3	9.3	3.8	2.2	1.05	0.21	0.08
Sydney 2	114	5.0	1.7	1.0	4.8	1.3	0.7	1.05	0.21	0.08
Sydney 2	115	7.6	2.2	1.3	7.6	3.3	1.9	1.05	0.21	0.08
Sydney 2	116	9.7	2.4	1.4	9.8	4.2	2.4	1.05	0.21	0.08
Sydney 2	117	7.0	0.6	0.3	6.9	1.9	1.1	1.05	0.21	0.08
Sydney 2	118	5.0	0.8	0.4	5.0	1.7	1.0	1.05	0.21	0.08

Sydney 2	119	5.9	2.1	1.2	6.0	2.7	1.6	1.05	0.21	0.08
Sydney 2	120	8.7	0.3	0.2	8.6	1.9	1.1	1.05	0.21	0.08
Sydney 2	121	6.1	5.3	3.1	5.9	5.2	3.0	1.06	0.25	0.10
Sydney 2	122	7.2	1.0	0.6	7.2	2.2	1.2	1.05	0.21	0.08
Sydney 2	123	5.9	0.8	0.5	5.9	1.9	1.1	1.05	0.21	0.08

Table S4. Percentiles of annual mean NO₂ concentrations measured at LUR development and validation sites.

Data set (<i>n</i> observations)	NO₂ concentration (ppb)					
	Min.	25th	50th	Mean	75th	Max.
development(358) ^a	1.3	4.9	6.6	7.1	9.0	17.8
validation (123)	0.4	5.9	8.5	8.6	11.2	19.3

^a Sixty-eight regulatory monitoring sites where NO₂ was measured were used to develop the model. Because the model was fit longitudinally to 6 years' monitoring (2006-11), the number of annual mean NO₂ observations was greater than 68 (=358). Not all sites had valid data for all years. See Knibbs et al.⁵ for a full description.

Table S5. Percentiles for annual mean NO₂ concentrations (ppb) measured at validation sites according to different site classification definitions.

Roadside ≤ 7.5 m^a	Min.	5th	25th	50th	75th	95th	Max.
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 10$)	6.2	6.6	9.1	13.0	15.7	18.2	19.3
urban traffic ($n = 33$)	4.8	4.9	6.8	9.8	11.7	15.3	17.7
urban background ($n = 80$)	0.4	2.8	5.2	8.2	10.0	12.4	15.3
Roadside ≤ 30 m^a							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 32$)	4.8	4.9	6.8	10.7	12.9	17.2	19.3
urban traffic ($n = 11$)	5.5	6.3	8.6	10.4	11.9	14.2	14.4
urban background ($n = 80$)	0.4	2.8	5.2	8.2	10.0	12.4	15.3
Major road definition changed^{b, e}							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 25$)	5.1	5.6	8.0	11.0	13.1	17.6	19.3
urban traffic ($n = 17$)	4.8	4.9	5.5	9.8	11.7	14.9	16.5
urban background ($n = 81$)	0.4	2.8	5.3	8.2	10.0	12.4	15.3
Urban traffic ≤ 50 m^c							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 25$)	5.1	5.6	8.0	11.0	13.1	17.6	19.3
urban traffic ($n = 11$)	4.8	4.9	5.0	6.8	9.6	15.5	16.5
urban background ($n = 87$)	0.4	2.8	5.6	8.4	10.6	12.8	15.3
Urban traffic ≤ 50 m + major road definition changed^{d, e}							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 25$)	5.1	5.6	8.0	11.0	13.1	17.6	19.3
urban traffic ($n = 10$)	4.8	4.9	4.9	6.1	10.3	15.6	16.5
urban background ($n = 88$)	0.4	2.8	5.7	8.4	10.6	12.8	15.3
Urban traffic ≤ 200 m^c							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 25$)	5.1	5.6	8.0	11.0	13.1	17.6	19.3
urban traffic ($n = 33$)	2.8	4.0	5.5	9.0	11.2	14.1	16.5

urban background ($n = 65$)	0.4	2.7	5.3	8.1	10.0	12.4	15.3
Urban traffic ≤ 200 m + major road definition changed^{d,e}							
overall ($n = 123$)	0.4	2.9	5.9	8.5	11.2	14.6	19.3
roadside ($n = 25$)	5.1	5.6	8.0	11.0	13.1	17.6	19.3
urban traffic ($n = 32$)	2.8	4.0	5.4	9.1	11.3	14.1	16.5
urban background ($n = 66$)	0.4	2.7	5.3	8.0	10.0	12.4	15.3

^a the effect of changing the definition of roadside while keeping other definitions constant (i.e., urban traffic are non-roadside sites ≤ 100 m from major road; urban background sites are > 100 m from a major road). ^b the effect of changing the definition of a major road while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 100 m from major road; urban background sites are > 100 m from a major road). ^c the effect of changing the definition of urban traffic sites while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 50 or ≤ 200 m from major road; urban background sites are > 50 or > 200 m from a major road). ^d the effect of changing both the definition of urban traffic sites and the definition of a major road while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 50 or ≤ 200 m from major road; urban background sites are > 50 or > 200 m from a major road).

^e major roads were originally defined as national/state highways, arterial roads (which are major connector roads for national and state highways) and sub-arterial roads (which are connectors between highways and/or arterial roads, or serve as an alternative for arterial roads).⁶ The definition change we assessed here was restricting major roads to only as national/state highways and arterial roads (i.e., dropping sub-arterial roads from the definition). The positional accuracy of roads data was ± 2 m in urban areas and ± 10 m in rural and remote areas. The attribute accuracy was 99.09% for key attributes (name and unique identifier).⁶

Table S6. Classification of LUR development and validation sites. The definitions of each category are presented in the main text.

Data set (<i>n</i> sites)	<i>n</i> roadside (%)	<i>n</i> urban traffic (%)	<i>n</i> urban background (%)
development (68)	2 (3)	10 (15)	56 (82)
validation (123)	25 (20)	18 (15)	80 (65)

Table S7. The number of sites in each category by data set. The definitions for each category are presented in the main text.

Data set	<i>n</i> roadside (%)	<i>n</i> urban traffic (%)	<i>n</i> urban background (%)	Total (%)
Perth 1	12 (28)	7 (16)	24 (56)	43 (100)
Sydney 1	5 (15)	6 (18)	22 (66)	33 (100)
Sydney 2	8 (17)	5 (11)	34 (72)	47 (100)
Total	25 (20)	18 (15)	80 (65)	123 (100)

Table S8. Percentiles of predictors at model development sites, validation sites, and census mesh block centroids.

Model development sites (n = 68)	Min.	5th	25th	50th	75th	95th	Max.
impervious surfaces 1200 m (%)	0	0	7.5	15	26.5	45	54.8
major roads 500 m (km)	0	0	0	0.6	1.0	2.4	4.6
summer mean daily solar radiation (MJ/m ²)	21	21	22	23	24	28	29
open space 10,000 m (%)	14.4	16.3	25.6	51.2	72	96.2	99.9
industrial NO _x emission site density 400 m (sites/km ²)	0	0	0	0	0	0	2.0
industrial NO _x emission site density 1000 m (sites/km ²)	0	0	0	0	0	0.3	0.6
industrial land use 10,000 m (%)	0	0	2.3	6.1	9.9	22.8	37.5
OMI NO ₂ surface mean 2006 (ppb)	0.1	0.1	0.3	0.4	0.9	1.4	1.4
OMI NO ₂ surface mean 2007 (ppb)	0.1	0.2	0.3	0.4	0.9	1.1	1.2
OMI NO ₂ surface mean 2008 (ppb)	0.1	0.2	0.3	0.4	0.8	1.2	1.3
OMI NO ₂ surface mean 2009 (ppb)	0.1	0.2	0.3	0.4	0.8	1.3	1.3
OMI NO ₂ surface mean 2010 (ppb)	0.1	0.1	0.3	0.4	0.7	1.2	1.2
OMI NO ₂ surface mean 2011 (ppb)	0.1	0.1	0.3	0.4	0.8	1.1	1.2
OMI NO ₂ column mean 2006 (molecules × 10 ¹⁵ /cm ²)	0.7	1.0	1.3	2.0	3.2	4.0	4.0
OMI NO ₂ column mean 2007 (molecules × 10 ¹⁵ /cm ²)	0.7	1.0	1.3	2.0	3.0	3.7	3.9
OMI NO ₂ column mean 2008 (molecules × 10 ¹⁵ /cm ²)	0.7	1.0	1.3	1.7	3.0	3.3	3.3
OMI NO ₂ column mean 2009 (molecules × 10 ¹⁵ /cm ²)	0.7	1.1	1.3	1.8	2.7	4.0	4.2
OMI NO ₂ column mean 2010 (molecules × 10 ¹⁵ /cm ²)	0.6	1.0	1.2	1.7	2.7	3.4	3.4
OMI NO ₂ column mean 2011 (molecules × 10 ¹⁵ /cm ²)	0.8	1.0	1.2	1.7	2.8	3.4	3.6
Validation sites (n = 123)							
impervious surfaces 1200 m (%)	0	6.5	17.1	27	38.4	48	51.8
major roads 500 m (km)	0	0	0	0.8	1.4	3.2	4.6
summer mean daily solar radiation (MJ/m ²)	21.4	21.7	21.9	22	28.4	28.6	28.6
open space 10,000 m (%)	15.5	19.6	22.6	25.2	37.6	67.1	87
industrial NO _x emission site density 400 m (sites/km ²)	0	0	0	0	0	0	2.0
industrial NO _x emission site density 1000 m (sites/km ²)	0	0	0	0	0	0.3	0.6
industrial land use 10,000 m (%)	0	2.2	2.9	4.7	8.3	12.2	17
OMI NO ₂ surface mean 2006 (ppb)	0.3	0.4	0.4	1.0	1.1	1.1	1.1

OMI NO ₂ surface mean 2007 (ppb)	0.3	0.3	0.4	0.9	1.0	1.0	1.0
OMI NO ₂ surface mean 2008 (ppb)	0.3	0.3	0.4	0.8	0.9	0.9	0.9
OMI NO ₂ surface mean 2009 (ppb)	0.3	0.3	0.4	0.8	0.9	0.9	0.9
OMI NO ₂ surface mean 2010 (ppb)	0.3	0.4	0.4	0.8	0.8	0.8	0.8
OMI NO ₂ surface mean 2011 (ppb)	0.3	0.3	0.3	0.8	0.9	0.9	0.9
OMI NO ₂ column mean 2006 (molecules × 10 ¹⁵ /cm ²)	1.0	1.3	1.3	3.3	3.5	3.5	3.5
OMI NO ₂ column mean 2007 (molecules × 10 ¹⁵ /cm ²)	1.0	1.2	1.3	3.1	3.3	3.3	3.3
OMI NO ₂ column mean 2008 (molecules × 10 ¹⁵ /cm ²)	0.9	1.2	1.2	2.7	3.1	3.1	3.2
OMI NO ₂ column mean 2009 (molecules × 10 ¹⁵ /cm ²)	1.0	1.2	1.2	2.5	2.7	2.7	2.8
OMI NO ₂ column mean 2010 (molecules × 10 ¹⁵ /cm ²)	0.9	1.1	1.2	2.7	2.9	2.9	2.9
OMI NO ₂ column mean 2011 (molecules × 10 ¹⁵ /cm ²)	0.9	1.1	1.1	2.8	2.9	3.0	3.0
Mesh block centroids (n = 344,500)							
impervious surfaces 1200 m (%)	0	0	1.8	10	23.3	47.9	100
major roads 500 m (km)	0	0	0	0.7	1.1	2.3	10.8
summer mean daily solar radiation (MJ/m ²)	17	21	22	23	25	28	29
open space 10,000 m (%)	0.2	16	30.7	59.7	89.4	99.8	100
industrial NO _x emission site density 400 m (sites/km ²)	0	0	0	0	0	0	8
industrial NO _x emission site density 1000 m (sites/km ²)	0	0	0	0	0	0.3	2.6
industrial land use 10,000 m (%)	0	0	0.3	2.6	6.9	13.1	79.7
OMI NO ₂ surface mean 2006 (ppb)	0	0.1	0.2	0.4	1.0	1.4	1.4
OMI NO ₂ surface mean 2007 (ppb)	0	0.1	0.2	0.4	0.9	1.2	1.2
OMI NO ₂ surface mean 2008 (ppb)	0	0.1	0.2	0.3	0.9	1.3	1.3
OMI NO ₂ surface mean 2009 (ppb)	0	0.1	0.2	0.4	0.8	1.3	1.3
OMI NO ₂ surface mean 2010 (ppb)	0	0.1	0.2	0.4	0.8	1.2	1.2
OMI NO ₂ surface mean 2011 (ppb)	0	0.1	0.2	0.3	0.8	1.1	1.2
OMI NO ₂ column mean 2006 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.5	3.3	4.0	4.0
OMI NO ₂ column mean 2007 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.5	3.2	3.7	3.9
OMI NO ₂ column mean 2008 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.4	3.0	3.3	3.3
OMI NO ₂ column mean 2009 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.4	2.7	4.0	4.2
OMI NO ₂ column mean 2010 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.3	2.7	3.4	3.5
OMI NO ₂ column mean 2011 (molecules × 10 ¹⁵ /cm ²)	0.3	0.7	1.0	1.4	2.9	3.4	3.6

Table S9. The effect of different site classification definitions on model performance.

Roadside ≤ 7.5 m^a	R²	β (95% CI)	MSE-R²	RMSE (ppb)	RMSE (%)	Bias (ppb)	FB (-)
<i>Surface model</i>							
overall ($n = 123$)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
roadside ($n = 10$)	0.39	0.56 (0.10, 1.02)	0.03	4.1	32.4	-2.2	-0.19
urban traffic ($n = 33$)	0.42	0.70 (0.45, 0.94)	0.08	3.3	33.9	-1.4	-0.15
urban background ($n = 80$)	0.68	0.74 (0.65, 0.84)	0.66	1.9	24.6	-0.5	-0.06
urban traffic + urban background ($n = 113$)	0.59	0.72 (0.62, 0.81)	0.51	2.4	28.7	-0.7	-0.09
<i>Column model</i>							
overall ($n = 123$)	0.55	0.64 (0.55, 0.72)	0.52	2.6	29.5	-0.6	-0.07
roadside ($n = 10$)	0.32	0.47 (0.02, 0.92)	0.02	4.1	32.5	-2.0	-0.17
urban traffic ($n = 33$)	0.39	0.64 (0.40, 0.88)	0.16	3.1	32.5	-1.0	-0.11
urban background ($n = 80$)	0.64	0.67 (0.57, 0.76)	0.64	2.0	25.3	-0.2	-0.03
urban traffic + urban background ($n = 113$)	0.55	0.66 (0.56, 0.75)	0.52	2.4	28.5	-0.4	-0.05
Roadside ≤ 30 m^a							
<i>Surface model</i>							
overall ($n = 123$)	0.58	0.69 (0.61, 0.78)	0.51	2.5	29.6	-0.8	-0.10
roadside ($n = 32$)	0.49	0.65 (0.44, 0.85)	0.16	3.8	36.6	-2.2	-0.23
urban traffic ($n = 11$)	0.43	0.74 (0.22, 1.27)	0.20	2.4	22.9	0.2	0.02
urban background ($n = 80$)	0.68	0.74 (0.65, 0.84)	0.66	1.9	24.6	-0.5	-0.06
urban traffic + urban background ($n = 91$)	0.67	0.78 (0.68, 0.87)	0.64	2.0	24.4	-0.4	-0.05
<i>Column model</i>							
overall ($n = 123$)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
roadside ($n = 32$)	0.43	0.58 (0.37, 0.79)	0.21	3.7	35.5	-1.7	-0.18
urban traffic ($n = 11$)	0.42	0.71 (0.20, 1.23)	0.21	2.3	22.7	0.3	0.02
urban background ($n = 80$)	0.64	0.67 (0.57, 0.76)	0.64	2.0	25.3	-0.2	-0.03
urban traffic + urban background ($n = 91$)	0.64	0.71 (0.61, 0.80)	0.63	2.0	25.0	-0.2	-0.02
Major road definition changed^{b, e}	R²	β (95% CI)	MSE-R²				FB (-)

				RMSE (ppb)	RMSE (%)	Bias (ppb)	
<i>Surface model</i>							
overall (<i>n</i> = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
roadside (<i>n</i> = 25)	0.36	0.55 (0.29, 0.81)	-0.18	4.1	37.5	-2.5	-0.26
urban traffic (<i>n</i> = 17)	0.70	0.96 (0.68, 1.25)	0.60	2.3	24.2	-0.2	-0.02
urban background (<i>n</i> = 81)	0.68	0.74 (0.65, 0.84)	0.66	1.9	24.5	-0.5	-0.06
urban traffic + urban background (<i>n</i> = 98)	0.69	0.80 (0.71, 0.89)	0.66	2.0	24.5	-0.4	-0.06
<i>Column model</i>							
overall (<i>n</i> = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.6	29.5	-0.6	-0.07
roadside (<i>n</i> = 25)	0.29	0.47 (0.21, 0.74)	-0.13	4.1	36.7	-2.1	-0.21
urban traffic (<i>n</i> = 17)	0.70	0.90 (0.63, 1.17)	0.64	2.2	23.0	0.1	0.01
urban background (<i>n</i> = 81)	0.64	0.67 (0.58, 0.76)	0.64	2.0	25.2	-0.2	-0.03
urban traffic + urban background (<i>n</i> = 98)	0.66	0.73 (0.65, 0.82)	0.65	2.0	24.8	-0.2	-0.02
Urban traffic ≤50 m^c							
<i>Surface model</i>							
overall (<i>n</i> = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.5	29.6	-0.8	-0.10
roadside (<i>n</i> = 25)	0.36	0.55 (0.29, 0.81)	-0.18	4.0	37.5	-2.5	-0.26
urban traffic (<i>n</i> = 11)	0.74	0.81 (0.51, 1.10)	0.64	2.4	29.0	-1.2	-0.15
urban background (<i>n</i> = 87)	0.69	0.80 (0.71, 0.90)	0.66	1.9	23.8	-0.3	-0.04
urban traffic + urban background (<i>n</i> = 98)	0.69	0.80 (0.71, 0.89)	0.66	2.0	24.5	-0.4	-0.06
<i>Column model</i>							
overall (<i>n</i> = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
roadside (<i>n</i> = 25)	0.29	0.47 (0.21, 0.74)	-0.13	4.0	36.7	-2.1	-0.21
urban traffic (<i>n</i> = 11)	0.72	0.77 (0.47, 1.06)	0.69	2.2	27.1	-0.6	-0.08
urban background (<i>n</i> = 87)	0.65	0.73 (0.63, 0.83)	0.64	2.0	24.5	-0.1	-0.01
urban traffic + urban background (<i>n</i> = 98)	0.66	0.73 (0.65, 0.82)	0.65	2.0	24.8	-0.2	-0.02
Urban traffic ≤50 m + major road definition changed^{d,e}							
	R ²	β (95% CI)	MSE-R ²	RMSE (ppb)	RMSE (%)	Bias (ppb)	FB (-)

Surface model

overall (<i>n</i> = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
roadside (<i>n</i> = 25)	0.36	0.55 (0.29, 0.81)	-0.18	4.1	37.5	-2.5	-0.26
urban traffic (<i>n</i> = 10)	0.74	0.81 (0.49, 1.12)	0.64	2.5	29.9	-1.2	-0.16
urban background (<i>n</i> = 88)	0.69	0.80 (0.71, 0.90)	0.66	1.9	23.7	-0.3	-0.04
urban traffic + urban background (<i>n</i> = 98)	0.69	0.80 (0.71, 0.89)	0.66	2.0	24.5	-0.4	-0.06

Column model

overall (<i>n</i> = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
roadside (<i>n</i> = 25)	0.29	0.47 (0.21, 0.74)	-0.13	4.0	36.7	-2.1	-0.21
urban traffic (<i>n</i> = 10)	0.72	0.76 (0.45, 1.08)	0.69	2.3	27.9	-0.6	-0.08
urban background (<i>n</i> = 88)	0.65	0.73 (0.64, 0.83)	0.64	2.0	24.4	-0.1	-0.01
urban traffic + urban background (<i>n</i> = 98)	0.66	0.73 (0.65, 0.82)	0.65	2.0	24.8	-0.2	-0.02

Urban traffic ≤200 m^c*Surface model*

overall (<i>n</i> = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
roadside (<i>n</i> = 25)	0.36	0.55 (0.29, 0.81)	-0.18	4.1	37.5	-2.5	-0.26
urban traffic (<i>n</i> = 33)	0.75	0.94 (0.77, 1.10)	0.70	1.9	21.4	-0.2	-0.02
urban background (<i>n</i> = 65)	0.66	0.71 (0.60, 0.82)	0.62	2.0	26.2	-0.6	-0.08
urban traffic + urban background (<i>n</i> = 98)	0.69	0.80 (0.71, 0.89)	0.66	2.0	24.5	-0.4	-0.06

Column model

overall (<i>n</i> = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
roadside (<i>n</i> = 25)	0.29	0.47 (0.21, 0.74)	-0.13	4.0	36.7	-2.1	-0.21
urban traffic (<i>n</i> = 33)	0.73	0.86 (0.71, 1.02)	0.71	1.8	21.1	0.2	0.02
urban background (<i>n</i> = 65)	0.61	0.64 (0.53, 0.74)	0.60	2.1	26.9	-0.3	-0.04
urban traffic + urban background (<i>n</i> = 98)	0.66	0.73 (0.65, 0.82)	0.65	2.0	24.8	-0.2	-0.02

Urban traffic ≤ 200 m + major road definition changed^{d,e}	R²	β (95% CI)	MSE-R²	RMSE (ppb)	RMSE (%)	Bias (ppb)	FB (-)
<i>Surface model</i>							
overall (n = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
roadside (n = 25)	0.36	0.55 (0.29, 0.81)	-0.18	4.1	37.5	-2.5	-0.26
urban traffic (n = 32)	0.75	0.93 (0.77, 1.10)	0.70	1.9	21.5	-0.1	-0.02
urban background (n = 66)	0.66	0.71 (0.60, 0.81)	0.62	2.0	26.1	-0.6	-0.08
urban traffic + urban background (n = 98)	0.69	0.80 (0.71, 0.89)	0.66	2.0	24.5	-0.4	-0.06
<i>Column model</i>							
overall (n = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
roadside (n = 25)	0.29	0.47 (0.21, 0.74)	-0.13	4.0	36.7	-2.1	-0.21
urban traffic (n = 32)	0.73	0.86 (0.70, 1.02)	0.71	1.9	21.2	0.2	0.02
urban background (n = 66)	0.61	0.64 (0.53, 0.74)	0.60	2.1	26.8	-0.3	-0.04
urban traffic + urban background (n = 98)	0.66	0.73 (0.65, 0.82)	0.65	2.0	24.8	-0.2	-0.02

^a the effect of changing the definition of roadside while keeping other definitions constant (i.e., urban traffic are non-roadside sites ≤ 100 m from major road; urban background sites are > 100 m from a major road). ^b the effect of changing the definition of a major road while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 100 m from major road; urban background sites are > 100 m from a major road). ^c the effect of changing the definition of urban traffic sites while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 50 or ≤ 200 m from major road; urban background sites are > 50 or > 200 m from a major road). ^d the effect of changing both the definition of urban traffic sites and the definition of a major road while keeping other definitions constant (i.e., roadside ≤ 15 m; urban traffic are non-roadside sites ≤ 50 or ≤ 200 m from major road; urban background sites are > 50 or > 200 m from a major road).

^e major roads were originally defined as national/state highways, arterial roads (which are major connector roads for national and state highways) and sub-arterial roads (which are connectors between highways and/or arterial roads, or serve as an alternative for arterial roads).⁶ The definition change we assessed here was restricting major roads to only as national/state highways and arterial roads (i.e., dropping sub-arterial roads from the definition). The positional accuracy of roads data was ± 2 m in urban areas and ± 10 m in rural and remote areas. The attribute accuracy was 99.09% for key attributes (name and unique identifier).⁶

Table S10. Results of spatial correlation assessment on the residuals for each validation analysis.

Surface model	Moran's I	z-score	p-value
overall ($n = 123$)	0.28	0.30	0.77
roadside ($n = 25$)	-0.18	-0.31	0.75
urban traffic ($n = 18$)	0.57	1.46	0.14
urban background ($n = 80$)	0.38	0.41	0.68
urban traffic + urban background ($n = 98$)	0.23	0.24	0.81
Column model			
overall ($n = 123$)	0.34	0.36	0.72
roadside ($n = 25$)	-0.16	-0.27	0.79
urban traffic ($n = 18$)	0.53	1.37	0.17
urban background ($n = 80$)	0.55	0.58	0.56
urban traffic + urban background ($n = 98$)	0.33	0.35	0.73

Table S11. Model performance by measurement campaign used for validation and overall.

Surface model	R²	β (95% CI)	MSE-R²	RMSE (ppb)	RMSE (%)	Bias (ppb)	FB (-)
overall (<i>n</i> = 123)	0.58	0.69 (0.61, 0.78)	0.51	2.6	29.6	-0.8	-0.10
Perth 1 (<i>n</i> = 43)	0.37	0.45 (0.30, 0.60)	0.31	2.3	39.7	-0.6	-0.11
urban traffic + urban background (<i>n</i> = 31)	0.55	0.39 (0.28, 0.50)	0.50	1.6	34.0	-0.2	-0.04
Sydney 1 (<i>n</i> = 33)	0.26	0.44 (0.21, 0.67)	0.13	2.1	17.8	-0.2	-0.01
urban traffic + urban background (<i>n</i> = 28)	0.44	0.83 (0.51, 1.15)	0.01	1.6	14.5	0.3	0.03
Sydney 2 (<i>n</i> = 47)	0.32	0.42 (0.27, 0.58)	0.03	3.1	33.7	-1.6	-0.19
urban traffic + urban background (<i>n</i> = 39)	0.30	0.40 (0.23, 0.56)	0.06	2.4	28.8	-1.1	-0.15
Column model							
overall (<i>n</i> = 123)	0.55	0.64 (0.55, 0.72)	0.52	2.5	29.5	-0.6	-0.07
Perth 1 (<i>n</i> = 43)	0.37	0.45 (0.30, 0.60)	0.35	2.2	38.6	0.2	0.04
urban traffic + urban background (<i>n</i> = 31)	0.57	0.39 (0.28, 0.50)	0.44	1.7	35.8	0.6	0.12
Sydney 1 (<i>n</i> = 33)	0.26	0.44 (0.21, 0.67)	0.11	2.1	17.9	-0.1	-0.01
urban traffic + urban background (<i>n</i> = 28)	0.43	0.86 (0.53, 1.18)	0.02	1.7	14.6	0.4	0.03
Sydney 2 (<i>n</i> = 47)	0.31	0.42 (0.27, 0.58)	0.02	3.1	33.8	-1.6	-0.19
urban traffic + urban background (<i>n</i> = 39)	0.30	0.39 (0.23, 0.56)	0.06	2.4	28.8	-1.1	-0.15

Table S12. Model performance when 8 additional validation sites were included, bringing the total number of sites from 123 to 131. The 8 sites had values of one or more LUR predictors that were outside the range used to develop the models.

Surface model	R²	β (95% CI)	MSE-R²	RMSE (ppb)	RMSE (%)	bias (ppb)	fb (-)
overall (<i>n</i> = 131)	0.54	0.82 (0.71, 0.93)	0.38	2.9	32.7	-0.5	-0.06
roadside (<i>n</i> = 26) ^a	0.32	0.67 (0.33, 1.01)	-0.36	4.4	39.6	-2.1	-0.20
urban traffic (<i>n</i> = 22) ^a	0.69	1.21 (0.90, 1.52)	0.29	3.0	30.5	0.5	0.05
urban background (<i>n</i> = 83) ^a	0.62	0.81 (0.69, 0.93)	0.55	2.2	27.7	-0.3	-0.04
urban traffic + urban background (<i>n</i> = 105)	0.65	0.94 (0.82, 1.05)	0.52	2.4	28.7	-0.1	-0.01
Column model							
overall (<i>n</i> = 131)	0.51	0.76 (0.65, 0.87)	0.39	2.9	32.5	-0.2	-0.02
roadside (<i>n</i> = 26) ^a	0.27	0.59 (0.25, 0.92)	-0.30	4.3	38.8	-1.7	-0.16
urban traffic (<i>n</i> = 22) ^a	0.69	1.15 (0.85, 1.45)	0.33	3.0	29.6	0.8	0.08
urban background (<i>n</i> = 83) ^a	0.58	0.73 (0.62, 0.85)	0.53	2.2	28.2	0.0	-0.003
urban traffic + urban background (<i>n</i> = 105)	0.62	0.87 (0.76, 0.98)	0.52	2.4	28.8	0.2	0.02

^a roadside are ≤ 15 m from a major road; urban traffic are non-roadside sites ≤100 m from major road; urban background sites are >100 m from a major road).

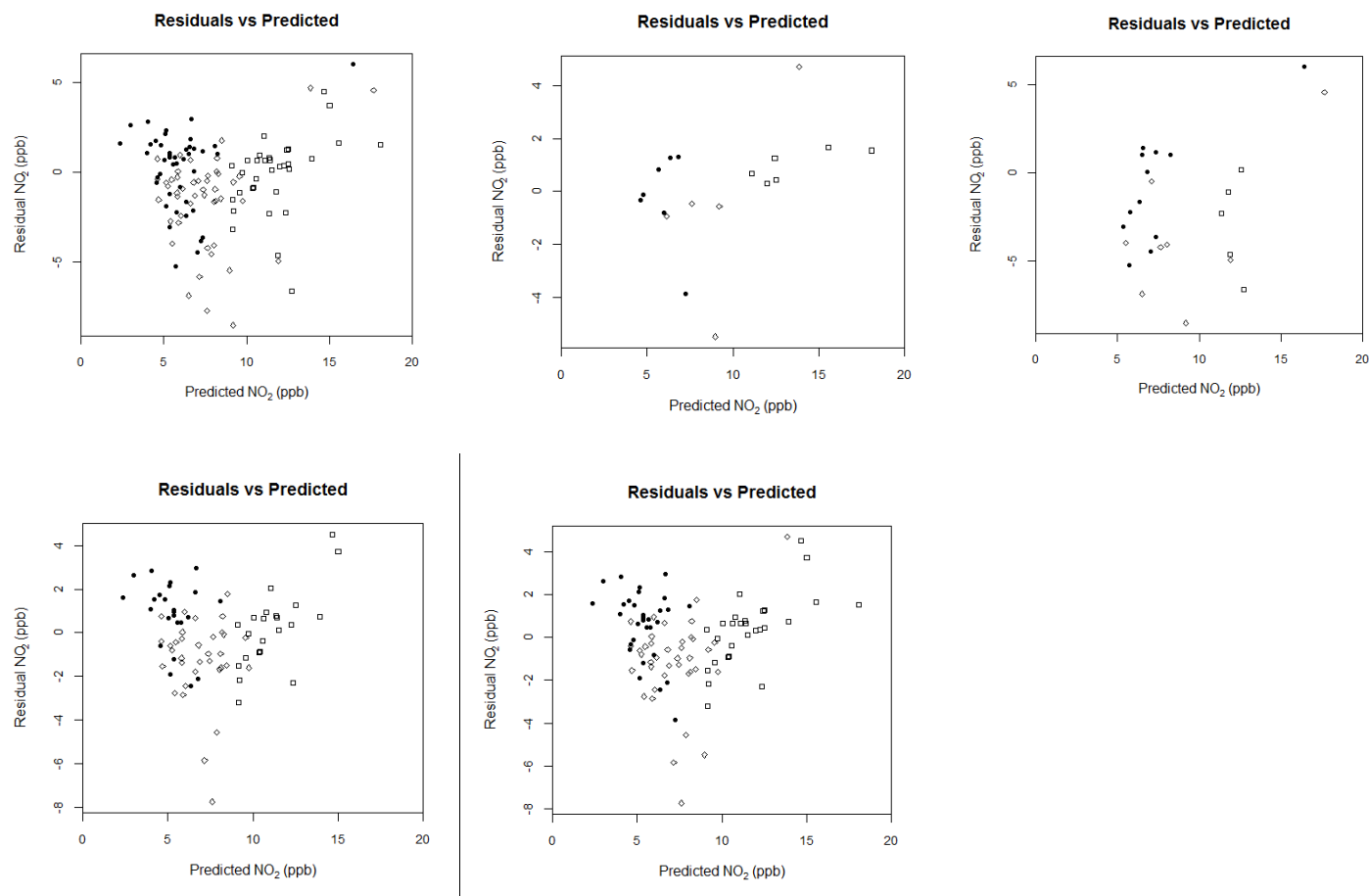


Figure S1. Residuals from regression of column model predictions on measured NO₂ plotted against predicted NO₂. Panels correspond to (from upper left to lower right) overall, roadside sites, urban traffic sites, urban background sites, urban traffic and urban background sites combined. Note: solid circles = Perth 1, hollow squares = Sydney 1, hollow diamonds = Sydney 2.

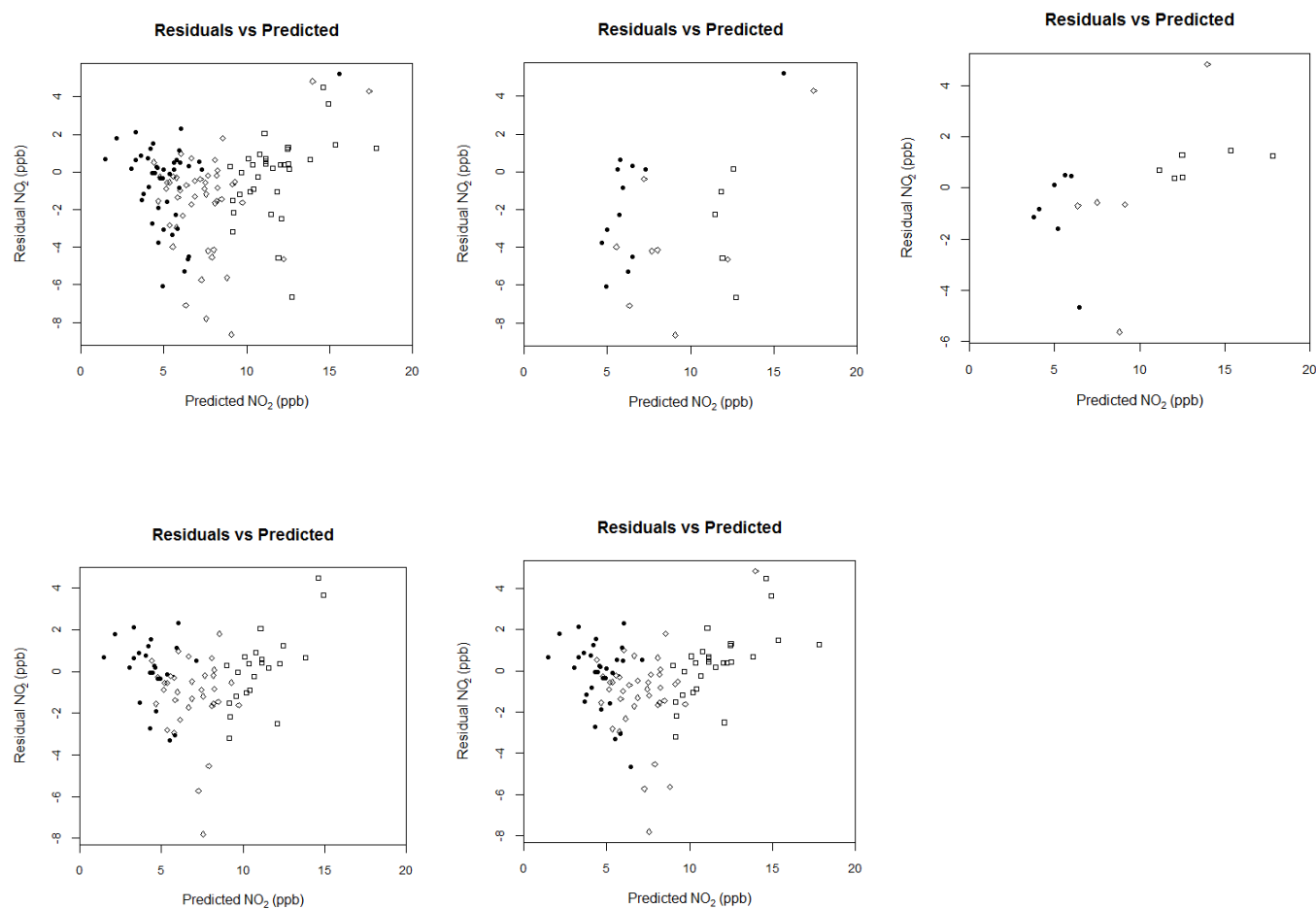


Figure S2. Residuals from regression of surface model predictions on measured NO₂ plotted against predicted NO₂. Panels correspond to (from upper left to lower right) overall, roadside sites, urban traffic sites, urban background sites, urban traffic and urban background sites combined. Note: solid circles = Perth 1, hollow squares = Sydney 1, hollow diamonds = Sydney combined.

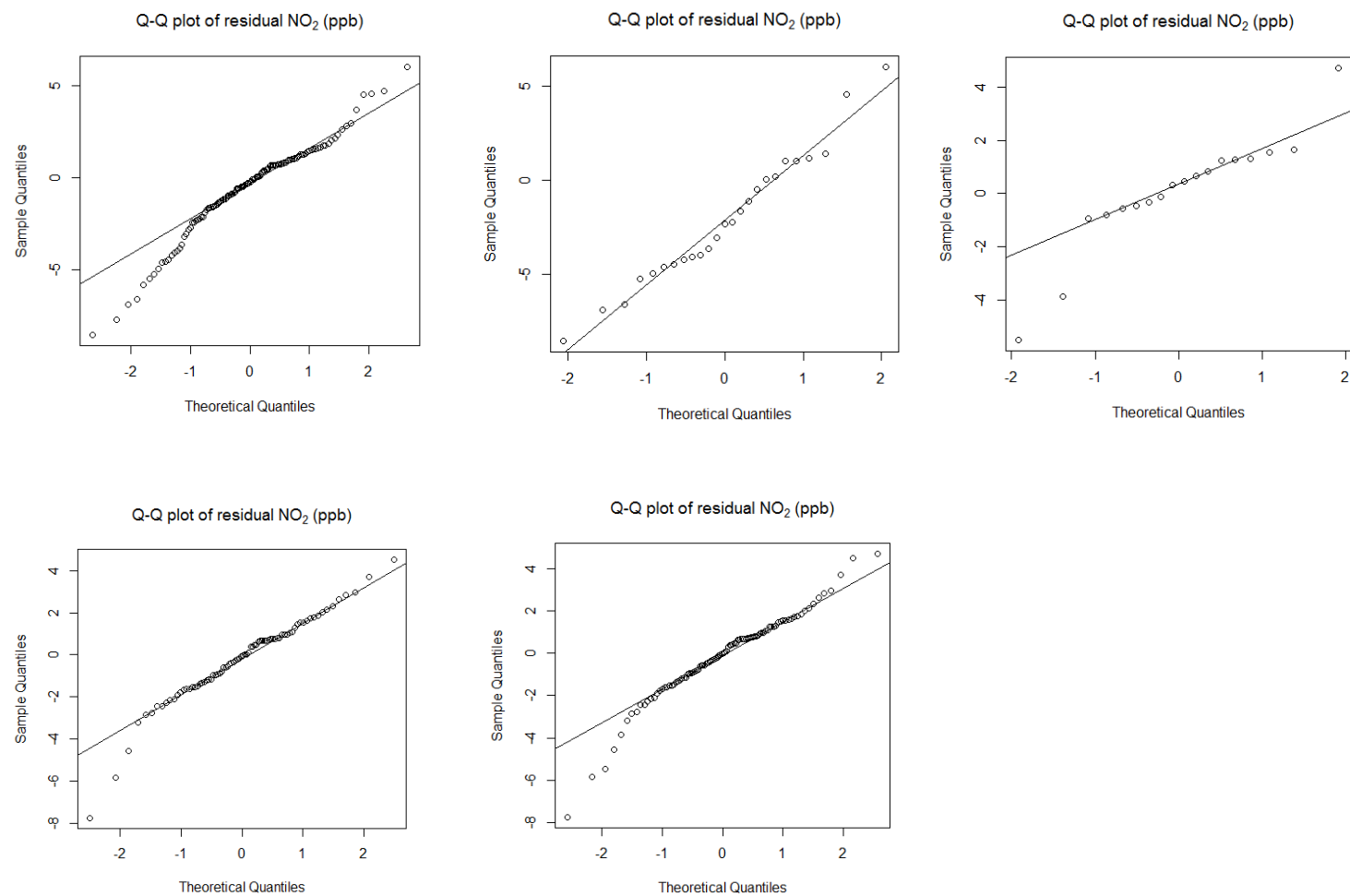


Figure S3. Q-Q plots of residuals from regression of column model predictions on measured NO₂. Panels correspond to (from upper left to lower right) overall, roadside sites, urban traffic sites, urban background sites, urban traffic and urban background sites combined.

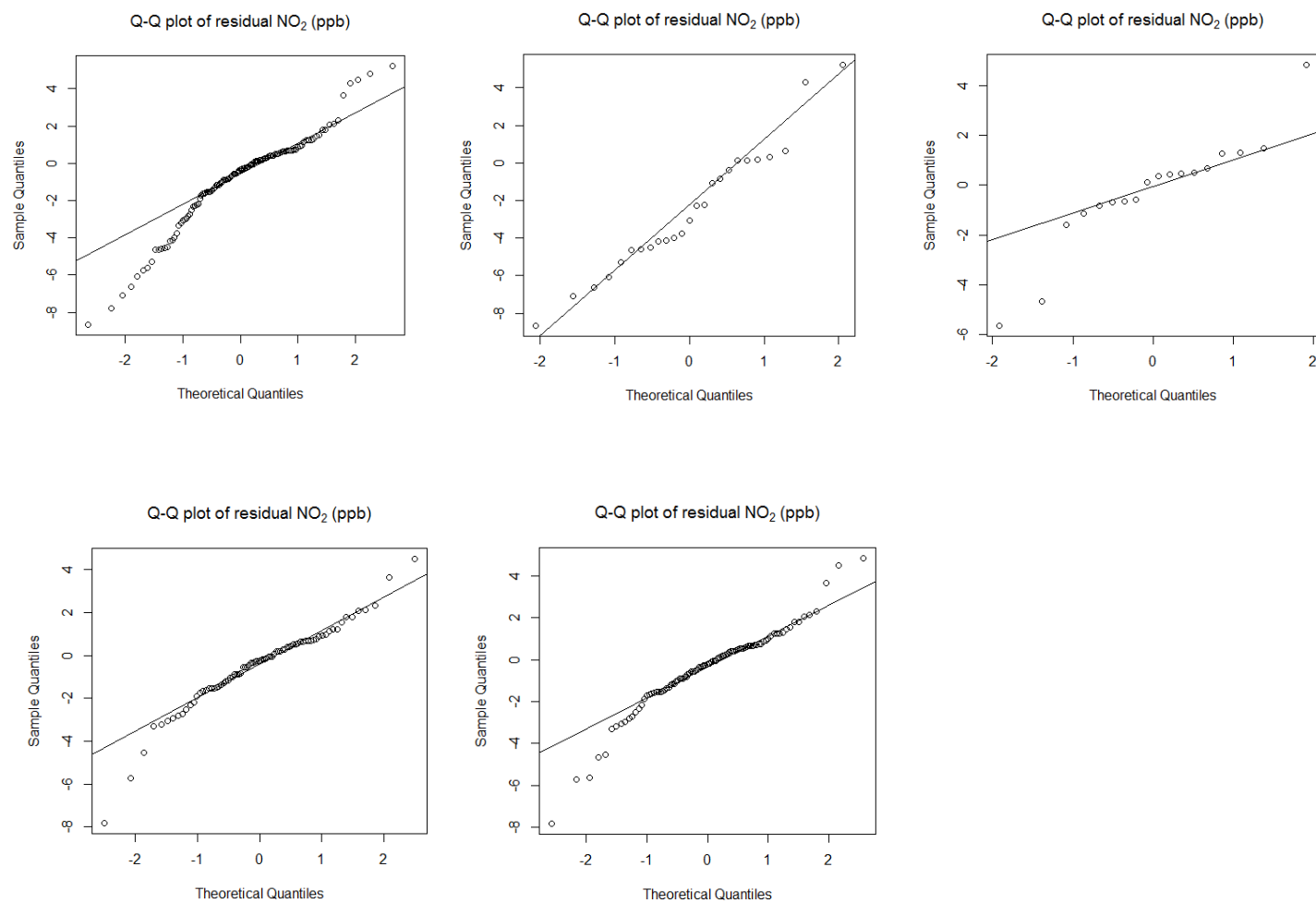


Figure S4. Q-Q plots of residuals from regression of surface model predictions on measured NO₂. Panels correspond to (from upper left to lower right) overall, roadside sites, urban traffic sites, urban background sites, urban traffic and urban background sites combined.

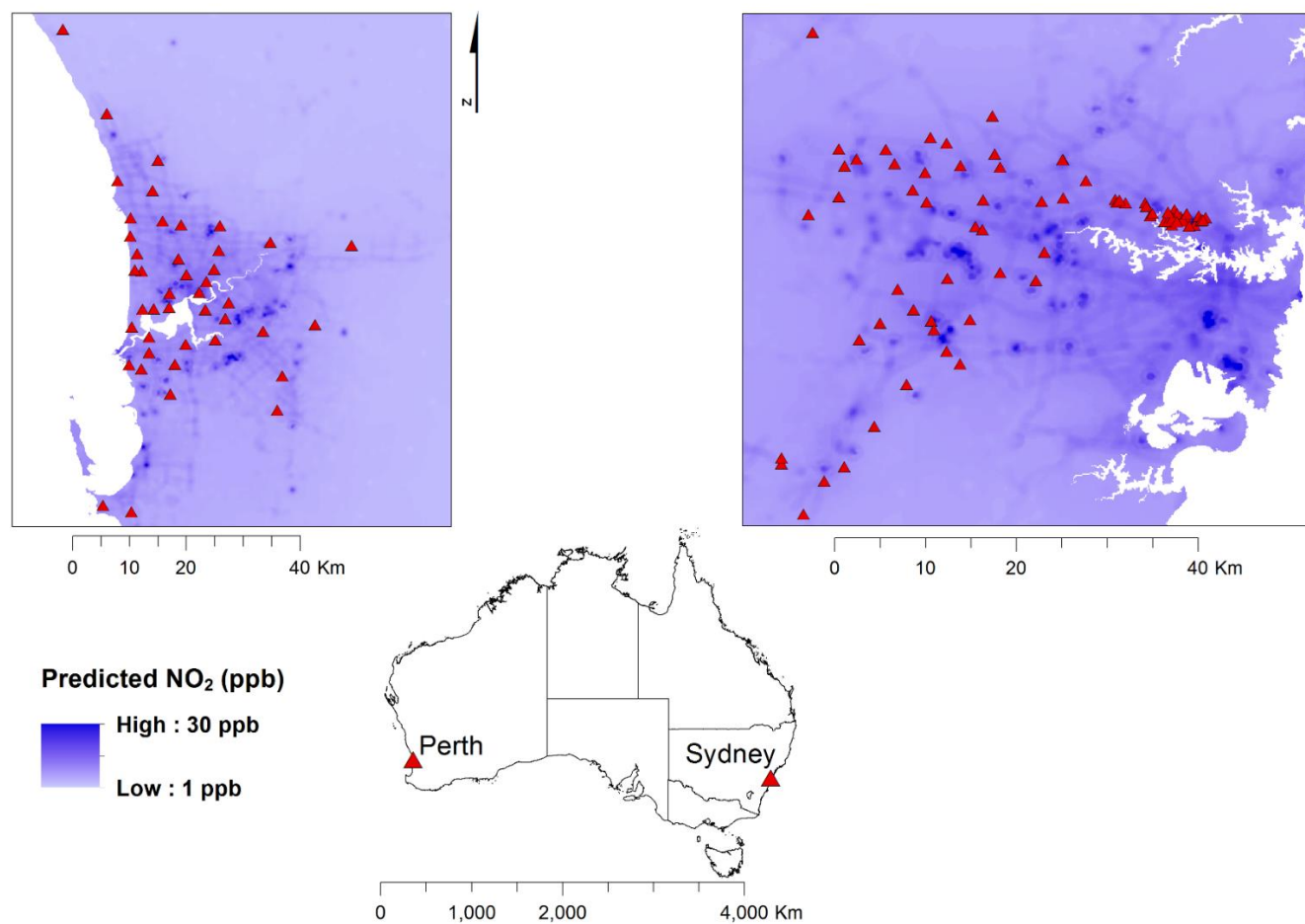


Figure S5. Annual mean NO₂ for 2008 predicted by the surface model. The outlines were created using census data published by the Australian Bureau of Statistics.⁷

References

1. Lewné, M.; Cyrys, J.; Meliefste, K.; Hoek, G.; Brauer, M.; Fischer, P.; Gehring, U.; Heinrich, J.; Brunekreef, B.; Bellander, T., Spatial variation in nitrogen dioxide in three European areas. *Sci. Total Environ.* **2004**, *332*, (1–3), 217-230.
2. Ayers, G. P.; Keywood, M. D.; Gillett, R.; Manins, P. C.; Malfroy, H.; Bardsley, T., Validation of passive diffusion samplers for SO₂ and NO₂. *Atmos. Environ.* **1998**, *32*, (20), 3587-3592.
3. Henderson, S. B.; Beckerman, B.; Jerrett, M.; Brauer, M., Application of Land Use Regression to Estimate Long-Term Concentrations of Traffic-Related Nitrogen Oxides and Fine Particulate Matter. *Environ. Sci. Technol.* **2007**, *41*, (7), 2422-2428.
4. Eeftens, M.; Beelen, R.; Fischer, P.; Brunekreef, B.; Meliefste, K.; Hoek, G., Stability of measured and modelled spatial contrasts in NO₂ over time. *Occup. Environ. Med.* **2011**, *68*, (10), 765-70.
5. Knibbs, L. D.; Hewson, M. G.; Bechle, M. J.; Marshall, J. D.; Barnett, A. G., A national satellite-based land-use regression model for air pollution exposure assessment in Australia. *Environ. Res.* **2014**, *135*, 204-211
6. Public Sector Mapping Agencies, Transport and topography product description, v3.6 2013; https://www.pasma.com.au/sites/default/files/transport_and_topography_product_description.pdf
7. Australian Bureau of Statistics, 2011, Digital Mesh Block Boundaries (Australia), viewed 05 May 2016, <<http://www.abs.gov.au/AUSSTATS/abs@.nsf/DetailsPage/1270.0.55.001July%202011>>