Supplementary Material

Supplementary Material for the manuscript entitled “Assessing the impact of atmospheric CO_2 and NO_2 measurements from space on estimating city-scale fossil fuel CO_2 emissions in a data assimilation system” by Kaminski et al..

1 SUPPLEMENTARY TABLES AND FIGURES

1.1 Tables

Table S1. Fuel type, annual CO_2 emissions, and NO_2/XCO_2 emission ratio for the 10 power plants in the domain with highest CO_2 emissions.

Name	fuel type	CO2 emission [MtC/yr]	NO2/CO2 emission ratio
LEAG, Kraftwerk Jänschwalde	solid	6.48	0.0029
Kraftwerk Boxberg	solid	5.33	0.0025
LEAG, Kraftwerk Schwarze Pumpe	solid	3.36	0.0017
Uniper Kraftwerke GmbH (Schkopau)	solid	1.46	0.0024
PCK Raffinerie GmbH Schwedt	liquid	0.87	0.0025
ArcelorMittal Eisenhüttenstadt GmbH	gaseous	0.72	0.0018
Vattenfall Europe Wärme HKW Reuter-West	solid	0.59	0.0030
SKW Stickstoffwerke Piesteritz GmbH	solid	0.59	0.0008
VEO Vulkan-Energiewirtschaft - Oderbrücke GmbH	gaseous	0.46	0.0001
CEMEX Zement GmbH	solid	0.39	0.0036

Table S2. 1 sigma uncertainty range in the NO_2 to CO_2 emission ratio for each fuel type

fuel type	σ
solid	0.098
liquid	0.245
gaseous	0.924
average	0.422

Table S3. Mapping of parameters available in L2e files onto inputs required by the neural network.

Input NN	Available Variable	derivation
VZA	VZA	direct
SZA	SZA	direct
Albedo (NIR)	Albedo (858nm)	direct
Albedo (SWIR1)	Albedo (1640nm)	direct
Albedo (SWIR2)	Albedo (1640nm)	$0.75 \cdot \mathrm{alb\_1640}$
AOT (NIR)	AOT (765nm)	direct
AOT (SWIR1)	AOT (550nm), aerosol angstrom exponent (α)	$\mathrm{aot\_550} \cdot (1640/550)^{-\alpha}$
AOT (SWIR2)	AOT (550nm), aerosol angstrom exponent (α)	$\mathrm{aot\_550} \cdot (2050/550)^{-\alpha}$

Table S4. Prior and posterior uncertainties for the 10 power plants with the largest emissions in tC/day for winter period.

Exp. #	–	1	2	3	4	5	6	7
description	prior	EPFMAP	IUP	EPF	NO2 uniform	NO2 fueltype	NO2 plant	1/2 sigma
Jänschw.	3532.75	800.49	1106.05	2860.28	577.29	561.97	726.62	744.34
Boxberg	2905.43	944.55	1341.08	2397.57	529.48	518.84	794.25	823.03
Schw. Pumpe	1833.43	738.56	1011.30	1670.76	431.25	428.63	597.67	605.52
Uniper Schkopau	796.81	657.62	721.08	787.83	407.37	408.07	460.01	376.65
PCK Schwedt	472.25	447.06	459.63	470.83	374.90	400.78	400.62	232.78
Arcelor Mittal	390.58	347.30	366.66	388.97	298.17	324.85	341.92	189.08
Reuter-West	320.97	306.26	313.30	320.15	281.49	281.55	282.66	158.53
SKW Piesteritz	320.40	292.89	307.45	318.70	285.80	285.82	285.97	156.32
VEO Oderbr.	252.08	245.37	248.54	251.85	245.19	245.26	245.31	125.15
CEMEX Zement	210.37	200.95	205.92	209.94	160.04	160.12	163.88	103.94

Table S5. Prior and posterior uncertainties for other sector for different spatial scales: entire domain (row 3), city (rows 4-6), Berlin district (rows 7-9), 2 x 2 km^2, average over Berlin (row 10) in tC/day for winter period.

Exp. #	–	1	2	3	4	5	6	7
description	prior	EPFMAP	IUP	EPF	NO2 uniform	NO2 fueltype	NO2 plant	1/2 sigma
Domain	1851.14	1448.05	1593.69	1812.25	1291.06	1297.91	1299.34	1426.83
Berlin	1498.14	1083.58	1241.07	1460.02	745.16	763.99	777.42	1067.52
Potsdam	241.72	237.39	239.56	241.50	210.32	210.36	210.44	237.19
Cottbus	152.60	150.33	151.48	152.52	113.43	113.65	113.90	150.26
Bln Spandau	327.91	315.06	321.48	327.38	244.44	244.53	244.60	314.85
Bln Chbg.-Wilmd.	550.18	492.41	516.72	545.66	352.84	352.89	354.78	489.95
Bln Mitte	512.27	461.26	481.53	507.61	331.64	331.68	332.84	460.43
Berlin 2x2 km^2 avg	86.39	85.46	85.89	86.32	82.09	82.14	82.19	85.44

Table S6. Prior and posterior uncertainties for the 10 power plants with the largest emissions in tC/day for summer period.

Exp. #	–	1	2	3	4	5	6	7
description	prior	EPFMAP	IUP	EPF	NO2 uniform	NO2 fueltype	NO2 plant	1/2 sigma
Jänschw.	3532.75	373.50	775.01	489.02	295.80	295.38	363.12	366.99
Boxberg	2905.43	390.08	803.37	476.66	270.88	270.74	372.08	376.10
Schw. Pumpe	1833.43	382.96	756.70	480.65	295.53	295.65	360.28	358.54
Uniper Schkopau	796.81	796.81	796.81	796.81	796.81	796.81	796.81	398.40
PCK Schwedt	472.25	399.73	453.86	412.09	326.82	361.25	361.35	225.24
Arcelor Mittal	390.58	305.21	355.73	334.26	280.86	288.32	297.31	179.02
Reuter-West	320.97	296.13	310.29	306.56	256.75	257.09	260.41	157.03
SKW Piesteritz	320.40	249.63	296.26	294.40	247.42	247.42	247.41	148.62
VEO Oderbr.	252.08	231.08	244.00	238.62	226.71	229.02	230.12	122.05
CEMEX Zement	210.37	189.58	203.81	196.61	163.09	163.27	165.57	102.20

Table S7. Prior and posterior uncertainties for other sector for different spatial scales: entire domain (row 3), city (rows 4-6), Berlin district (rows 7-9), 2 x 2 km^2, average over Berlin (row 10) in tC/day for summer period.

Exp. #	–	1	2	3	4	5	6	7
description	prior	EPFMAP	IUP	EPF	NO2 uniform	NO2 fueltype	NO2 plant	1/2 sigma
Domain	1851.14	1282.58	1495.50	1404.09	1180.74	1181.57	1185.73	1242.49
Berlin	1498.14	791.39	1072.89	953.14	584.85	596.74	620.71	736.52
Potsdam	241.72	226.45	237.29	234.74	167.51	167.66	168.30	226.42
Cottbus	152.60	143.43	150.32	146.77	101.69	101.83	101.91	143.33
Bln Spandau	327.91	309.88	319.92	316.51	222.71	223.15	224.55	309.10
Bln Chbg.-Wilmd.	550.18	466.06	504.09	488.38	288.90	289.37	291.32	462.86
Bln Mitte	512.27	420.56	465.09	446.22	269.15	273.79	292.94	415.58
Berlin 2x2 km^2 avg	86.39	85.01	85.77	85.39	80.71	80.76	80.88	84.97

Table S8. Physics parameterisations used in the WRF simulations to force the CMAQ simulations in this paper.

Scheme	Option	Reference(s)
Microphysics	Morrison 2-moment Scheme	Morrison et al. (2009)
Radiation	RRTMG Short- and Longwave Schemes	Iacono et al. (2008)
Surface layer	Eta Similarity Scheme	Janjić (1994); Janjic (1996)
Land surface	5-layer Thermal Diffusion Scheme	Dudhia (1996)
Cumulus parameterisation	Grell 3D Ensemble Scheme	Grell (1993); Grell and Dévényi (2002)
PBL Physics	Mellor-Yamada-Janjic Scheme	Janjić (1994)

1.2 Figures

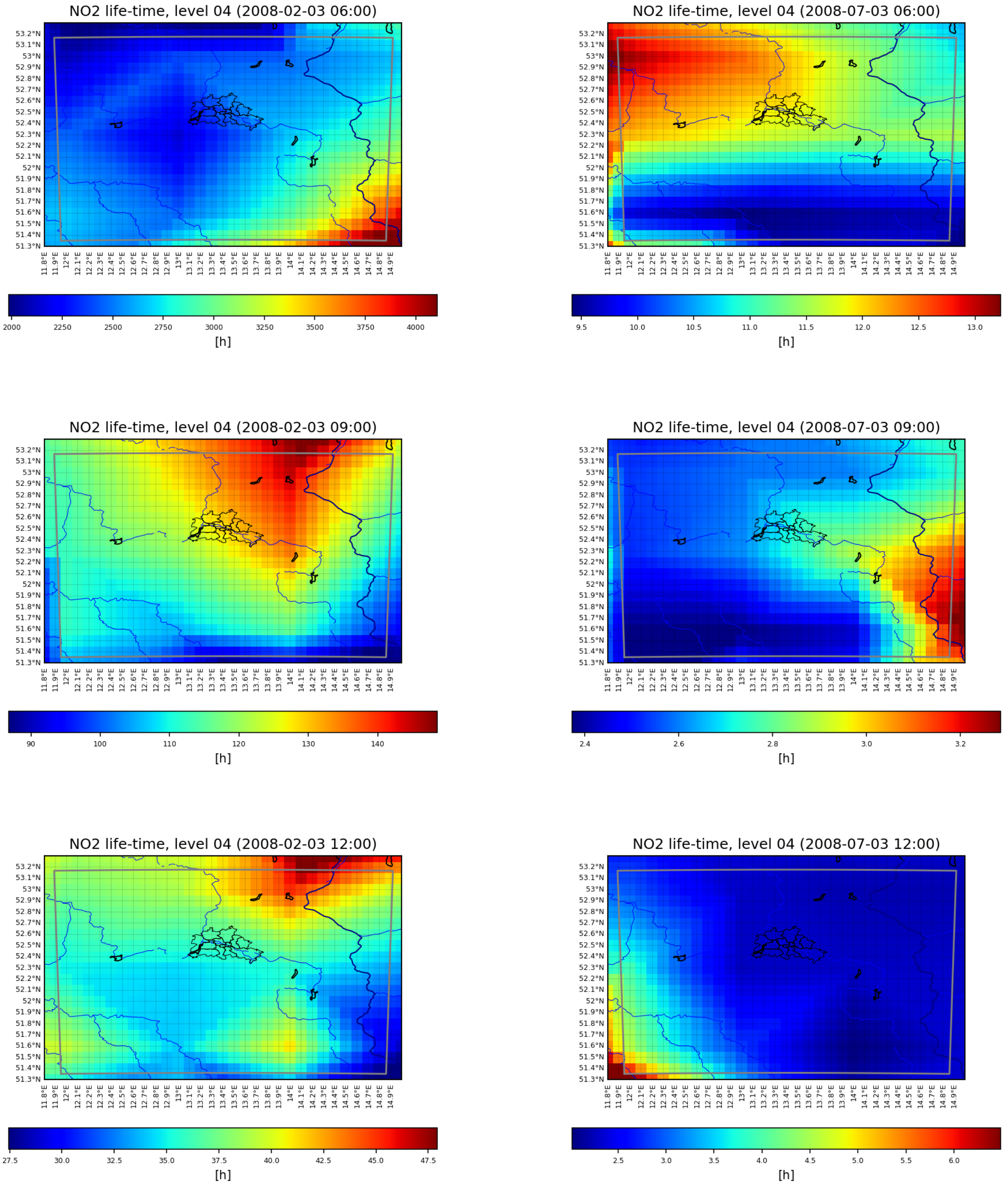

Figure S1. The lifetime of NO_2 over the study area in the planetary boundary layer for 3 February 2018 (left), and 3 July 2018 (right) at 6:00 UTC (top), 9:00 UTC (middle), and 12:00 UTC (bottom).

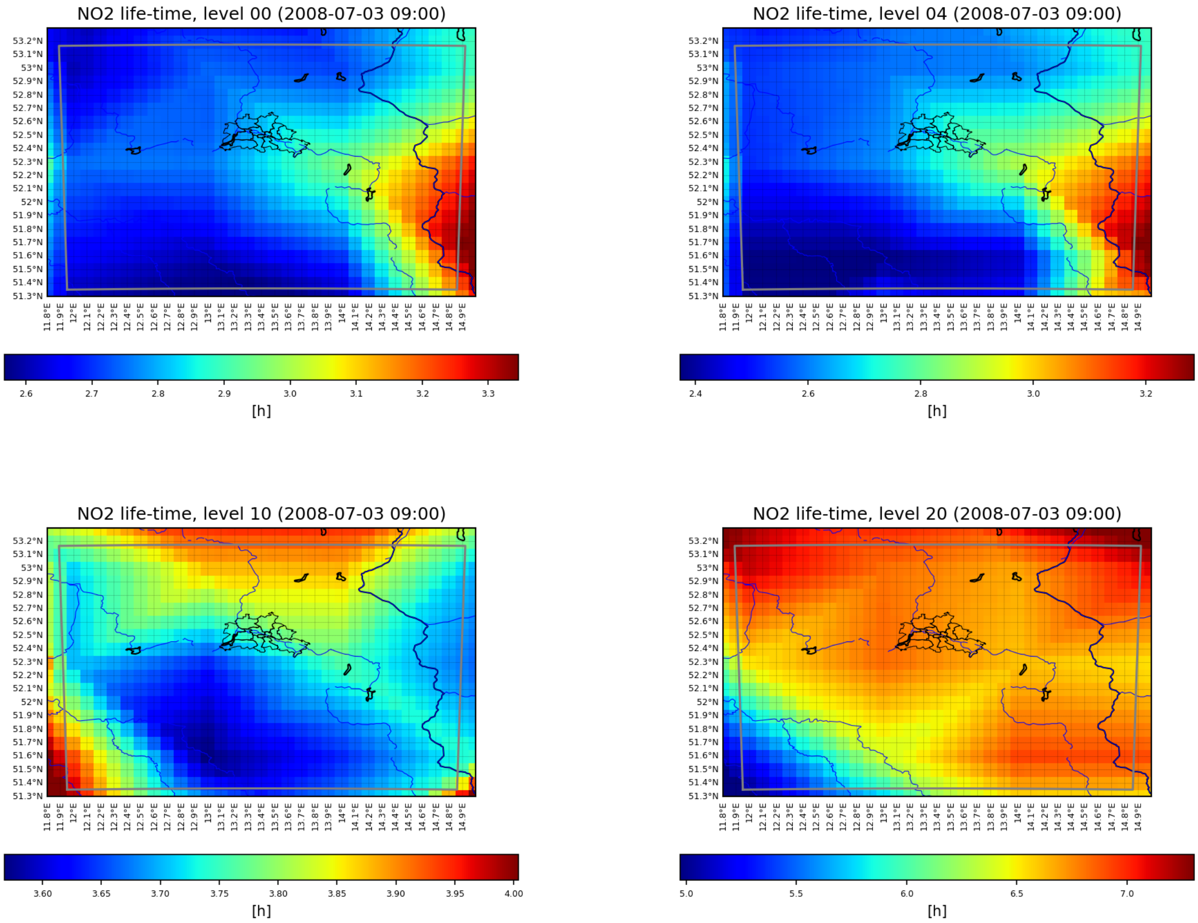

Figure S2. The lifetime of NO_2 over the study area at CAMS model levels 0 (surface, top left), 4 ($\approx$ 200 m, top right), 10 ($\approx$ 1500 m, bottom left), 20 ($\approx$ 5700 m, bottom right) for 3 July 2018 at 9:00 UTC.

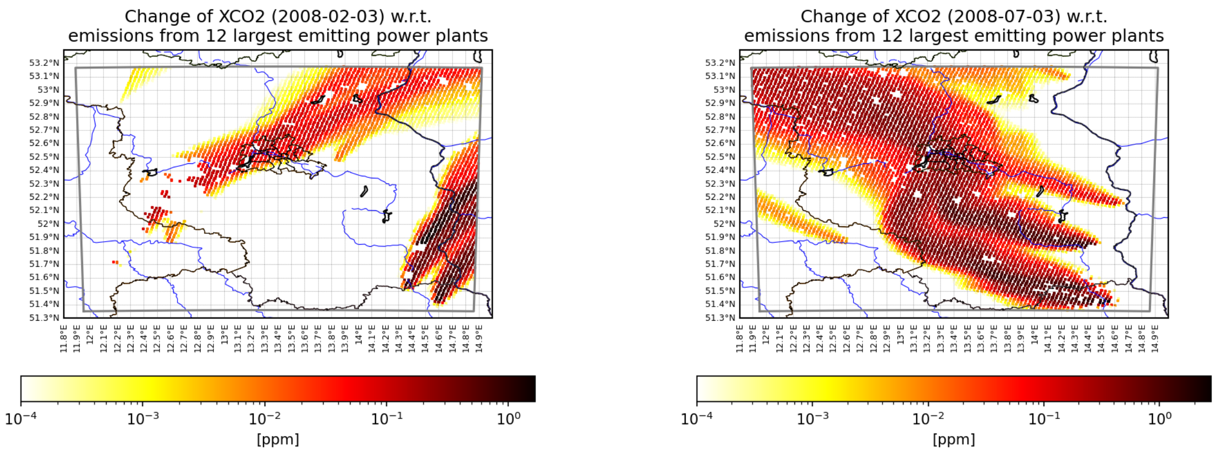

Figure S3. Simulated plumes for the 12 largest power plants in the domain (ppm) in winter (left) and summer (right).

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