Supplementary Information

Design and evaluation of short-term monitoring campaigns for long-term air pollution exposure assessment

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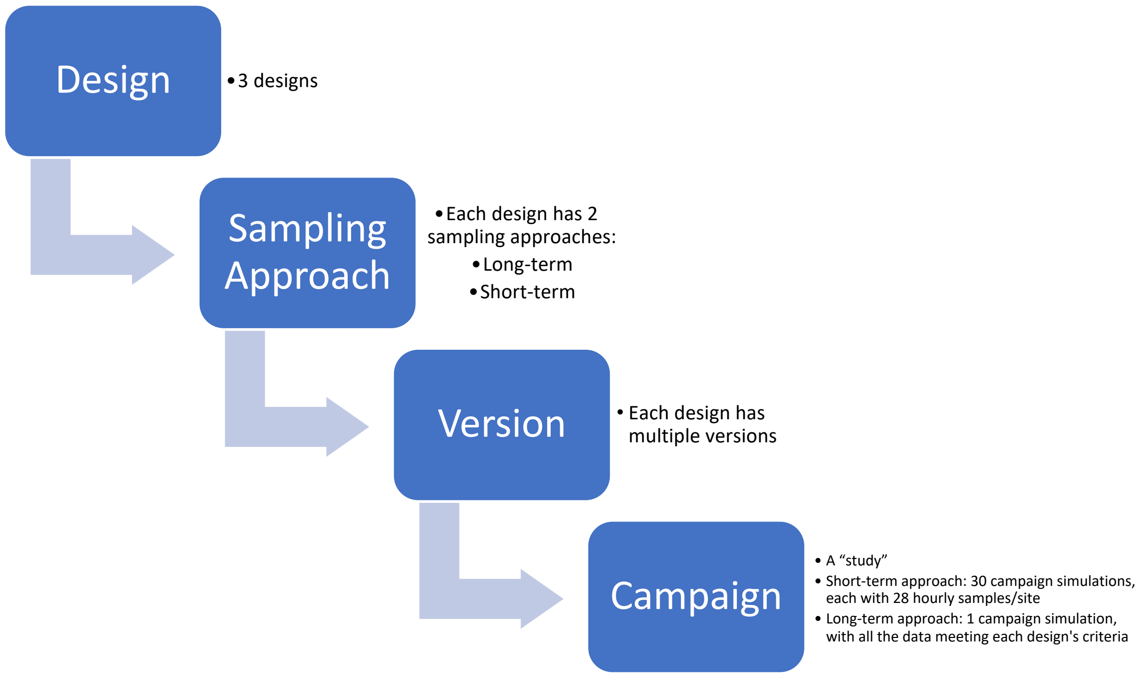
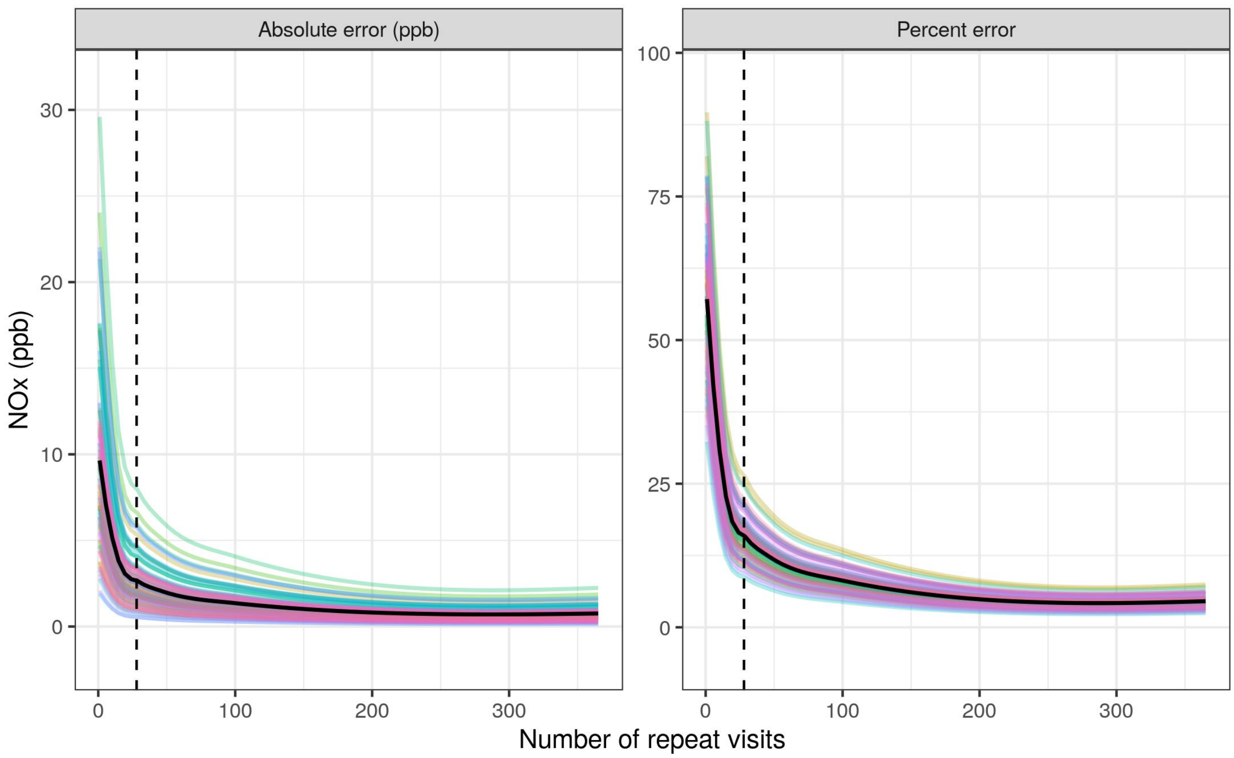


Figure S1. Hierarchical structure of simulations.



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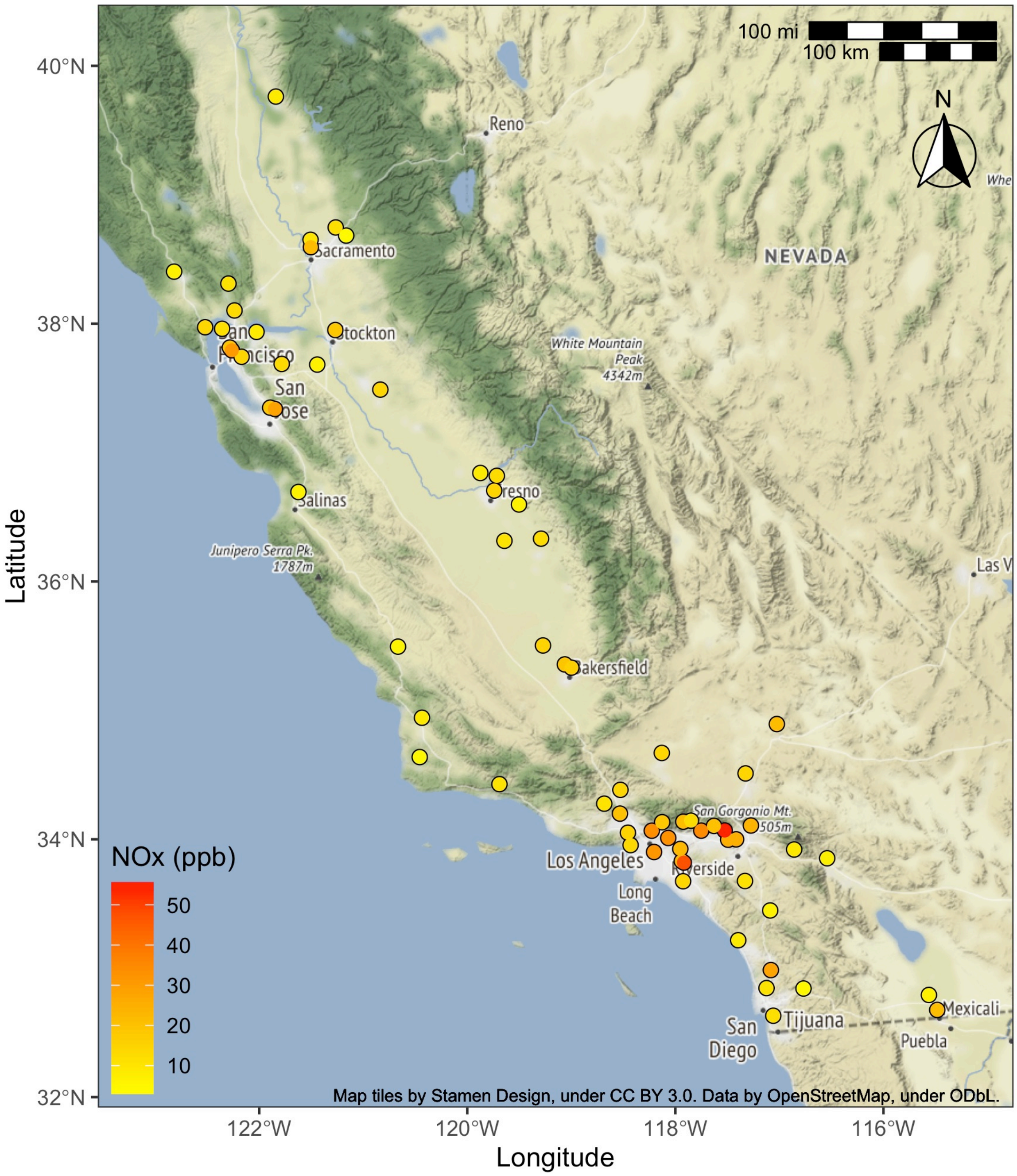

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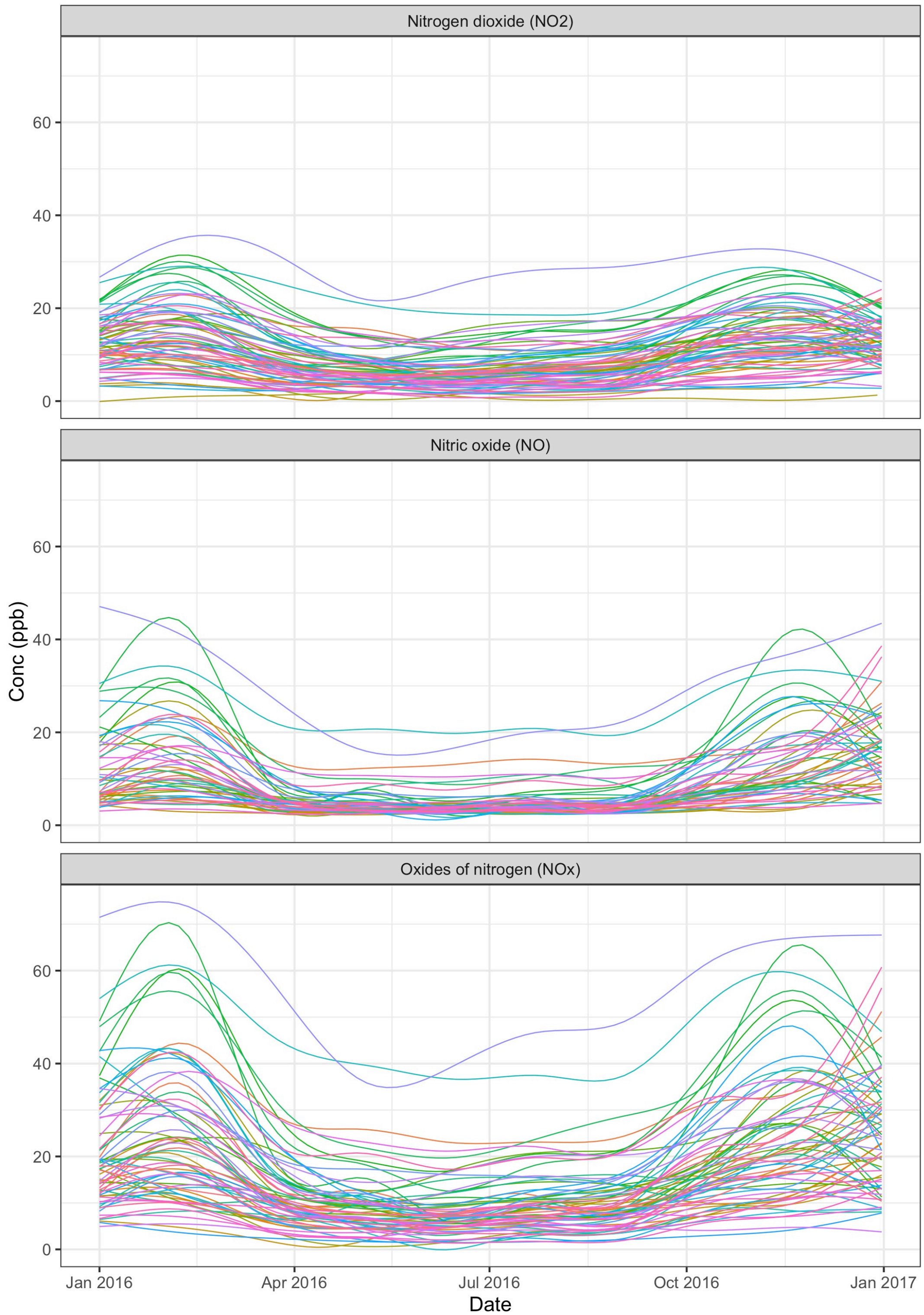

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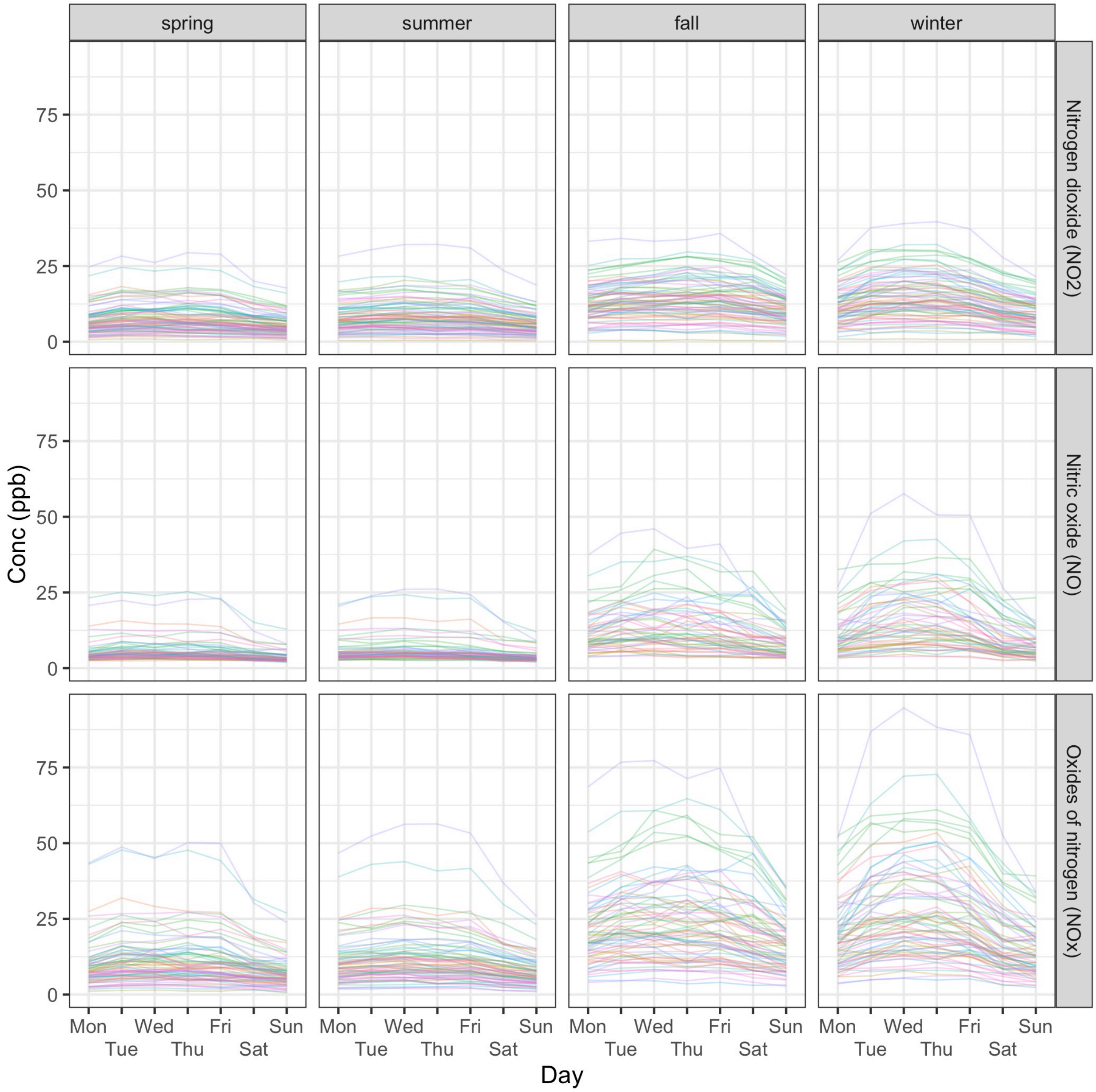

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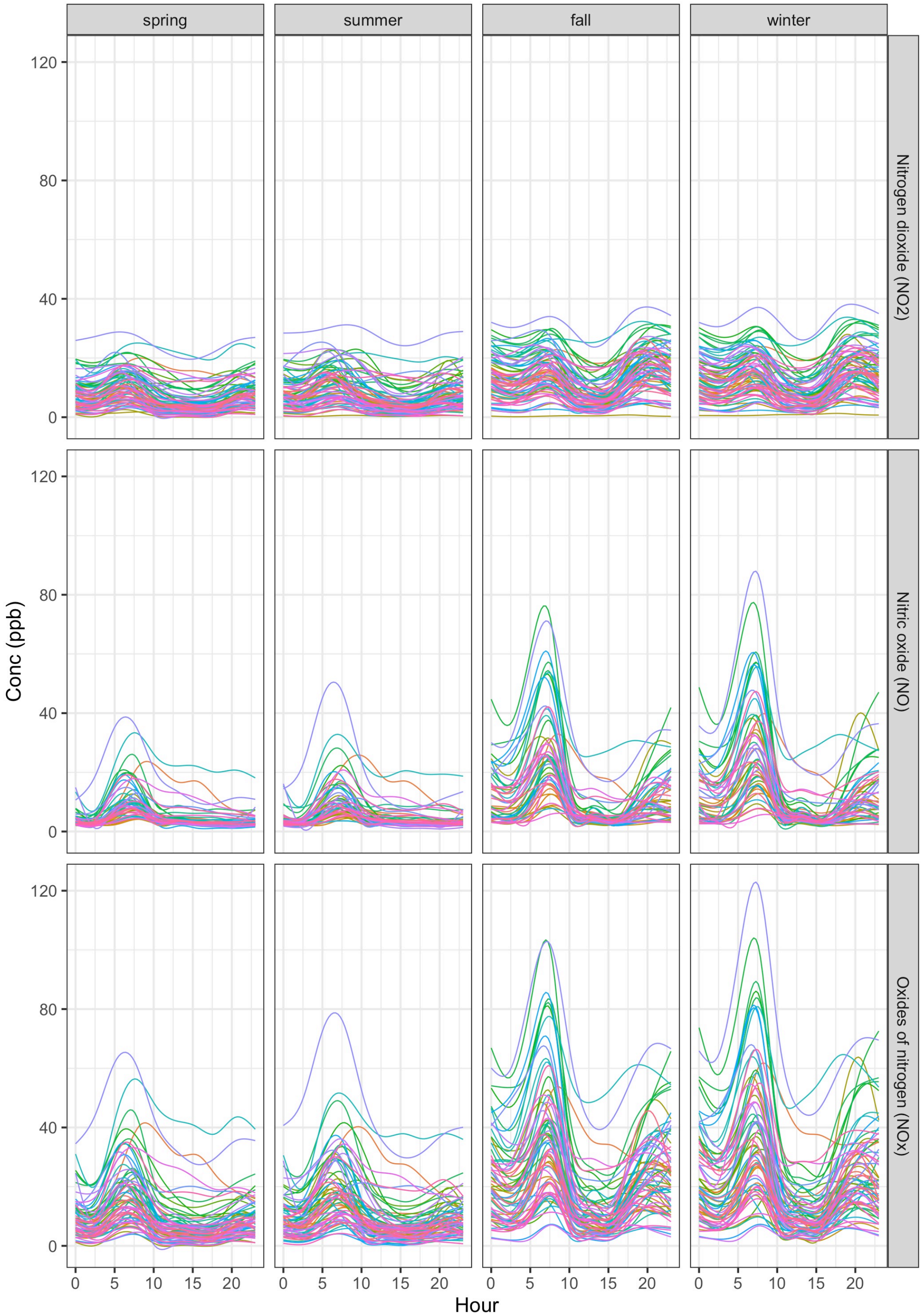

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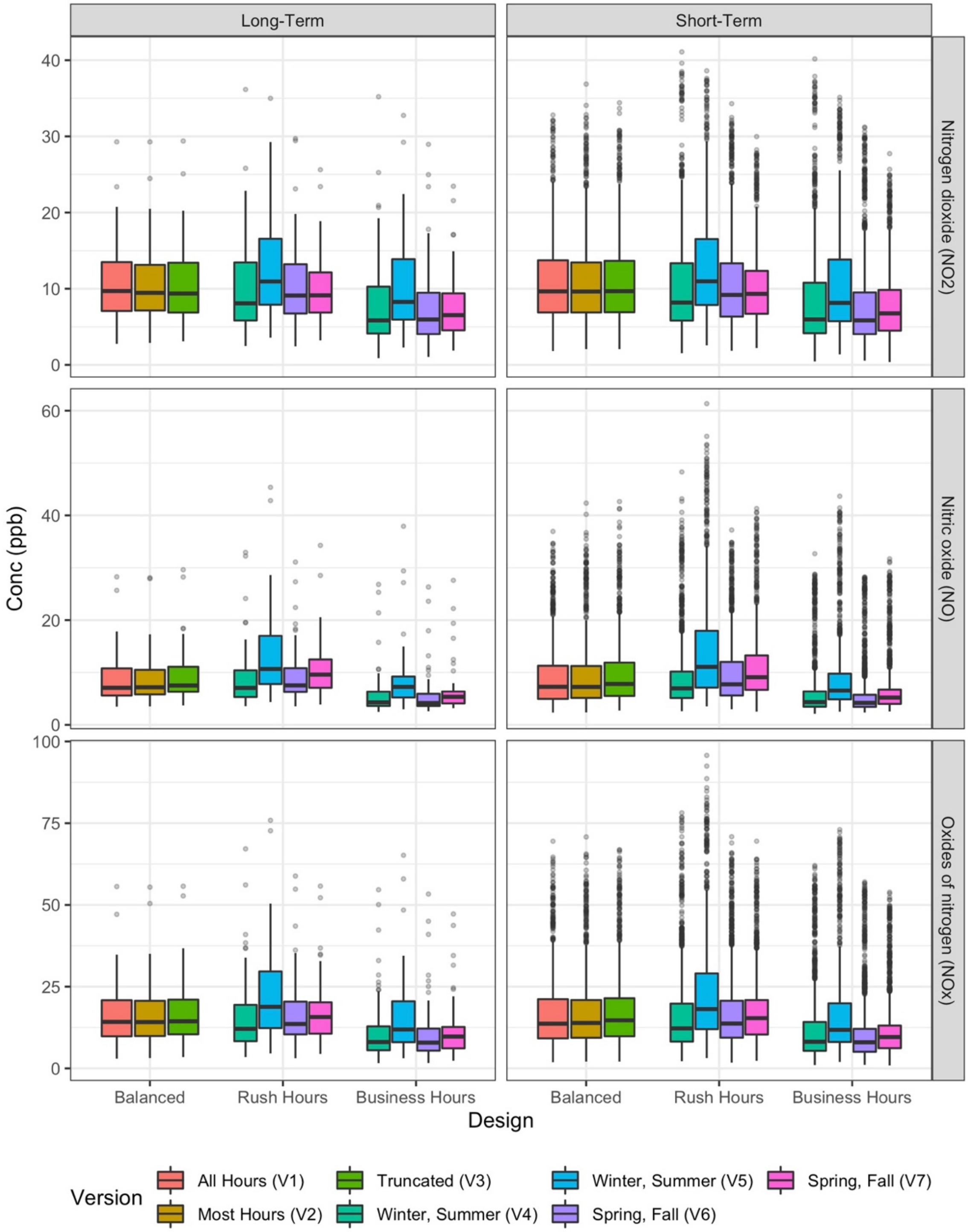
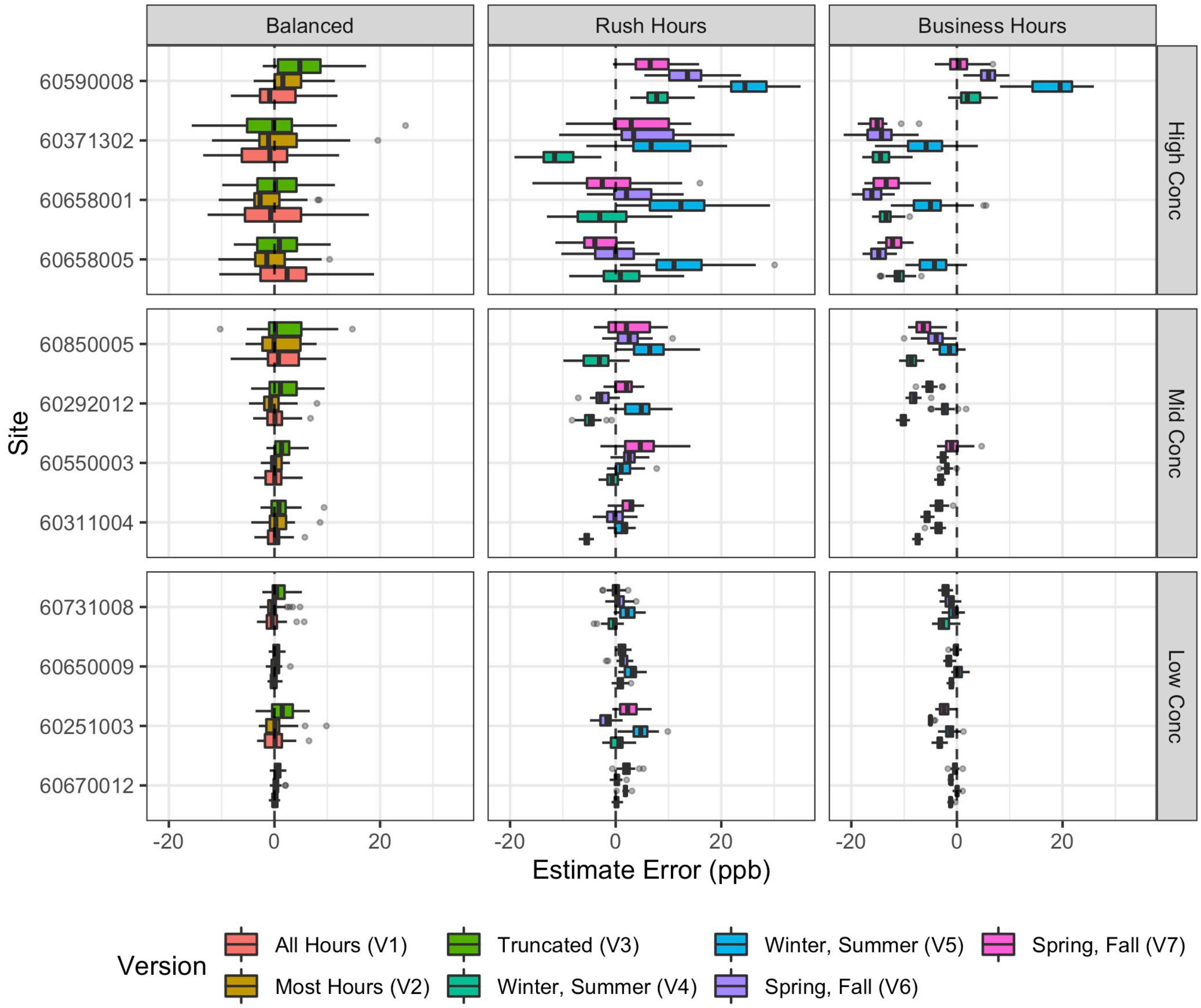


Figure S7. Annual average site concentration estimates for different pollutants and design versions. N=30 campaigns per design version x 69 sites for short-term approaches; N = 1 campaign per design version x 69 sites for long-term approaches. Short-term approaches appear to be more variable (less precise), in large part because all 30 campaigns are represented in the boxplots.



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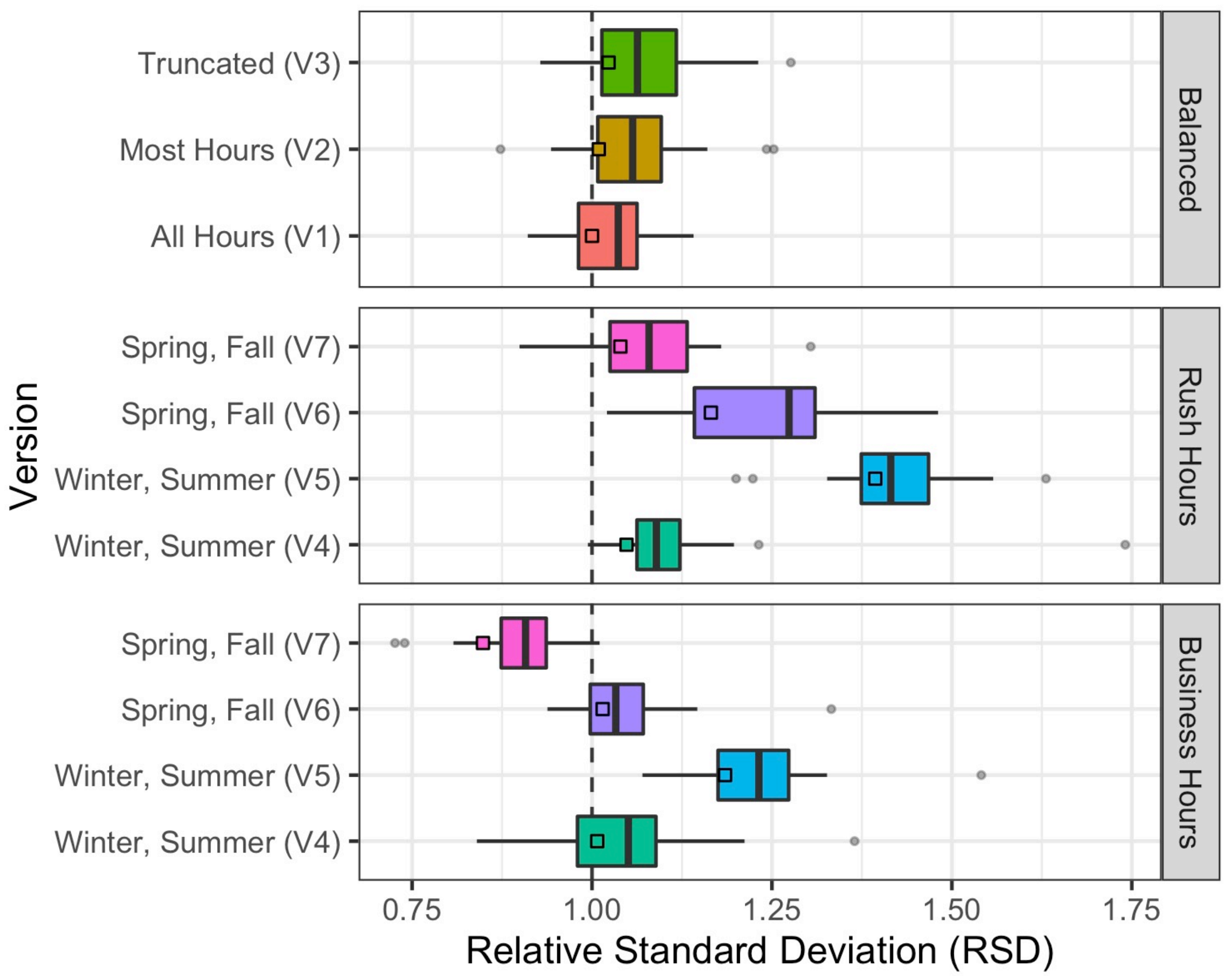
1.4 Model Predictions



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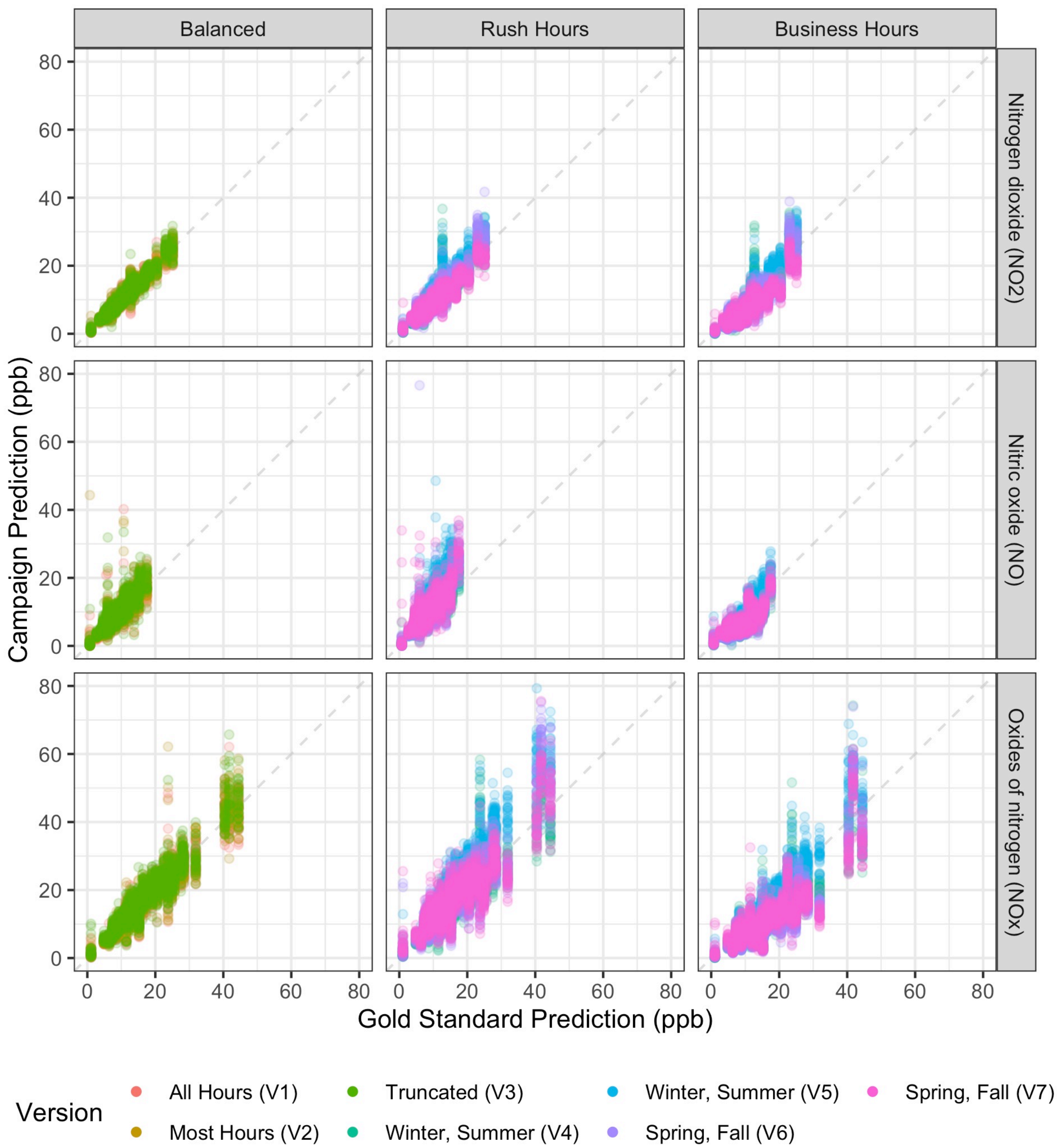


Figure S10. Scatterplot of cross-validated short-term predictions for 30 campaigns vs the gold standard predictions for NOx, NO, and NO2. Showing predictions below 80 ppb for clarity (see SI Figure S12 and Table S6 for predictions excluded).

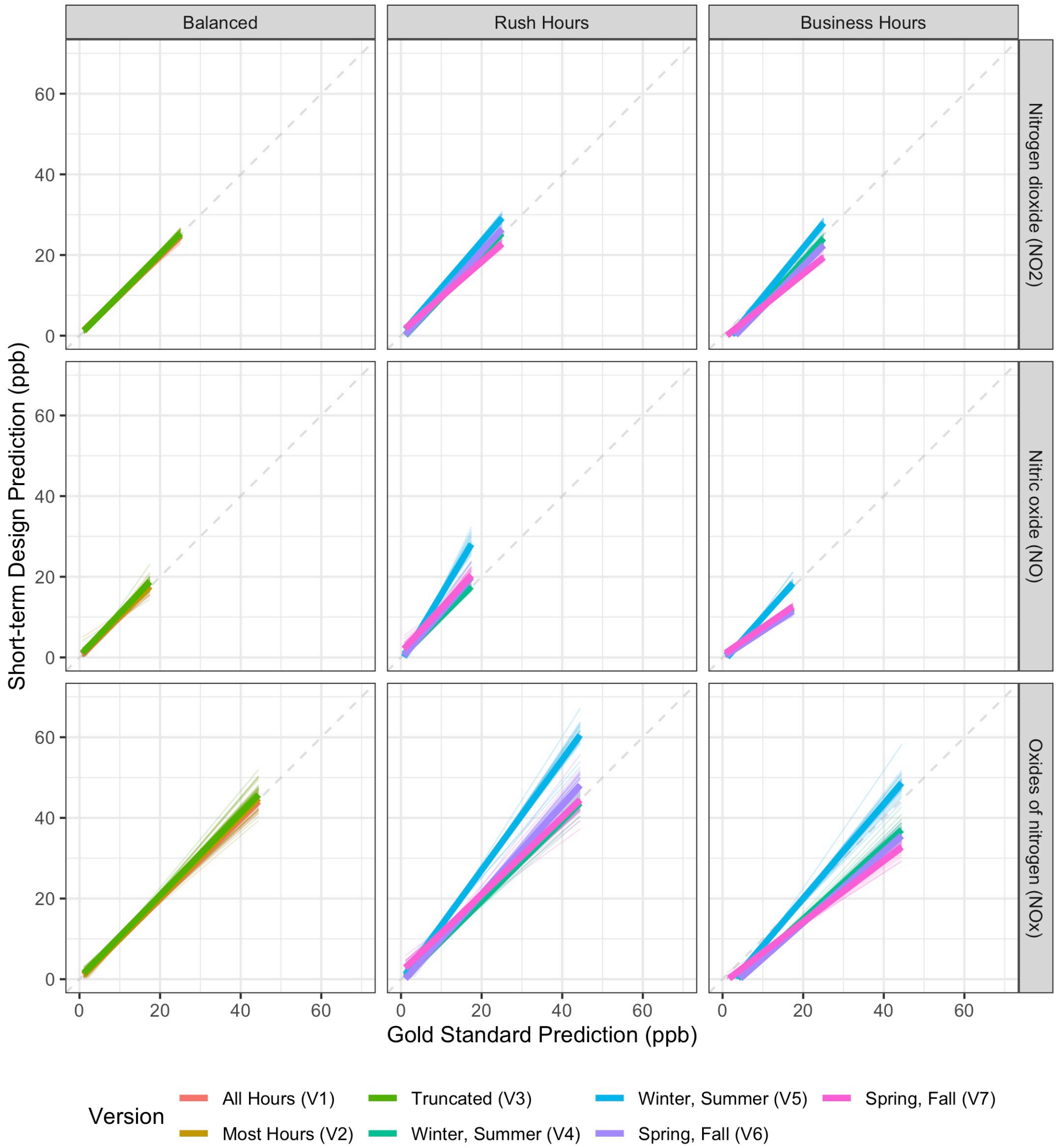


Figure S11. Best fit lines of cross-validated short-term predictions for 30 campaigns vs the gold standard predictions for NOx, NO, and NO2.

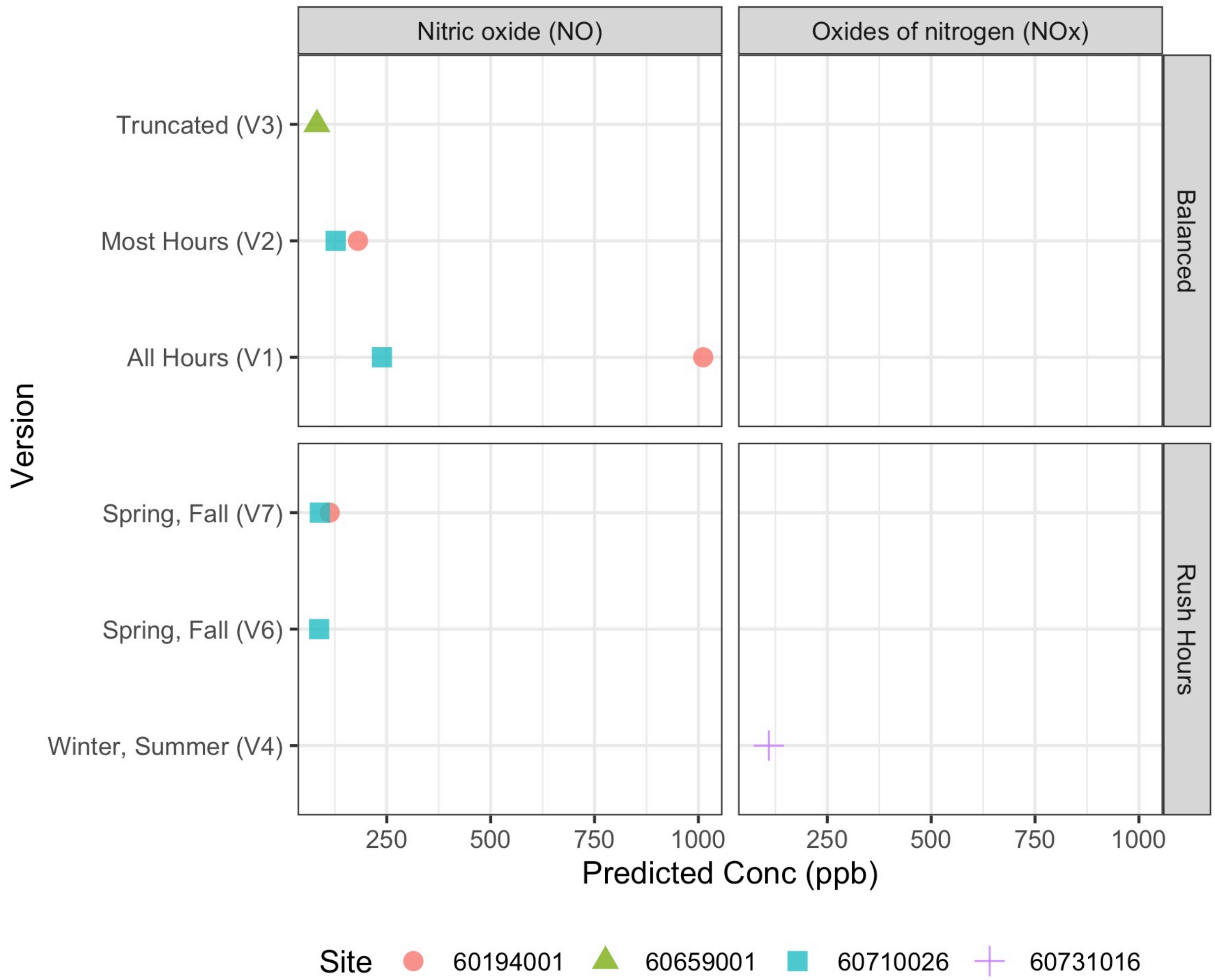


Figure S12. Predictions above 80 ppb excluded from prediction plots, if noted.

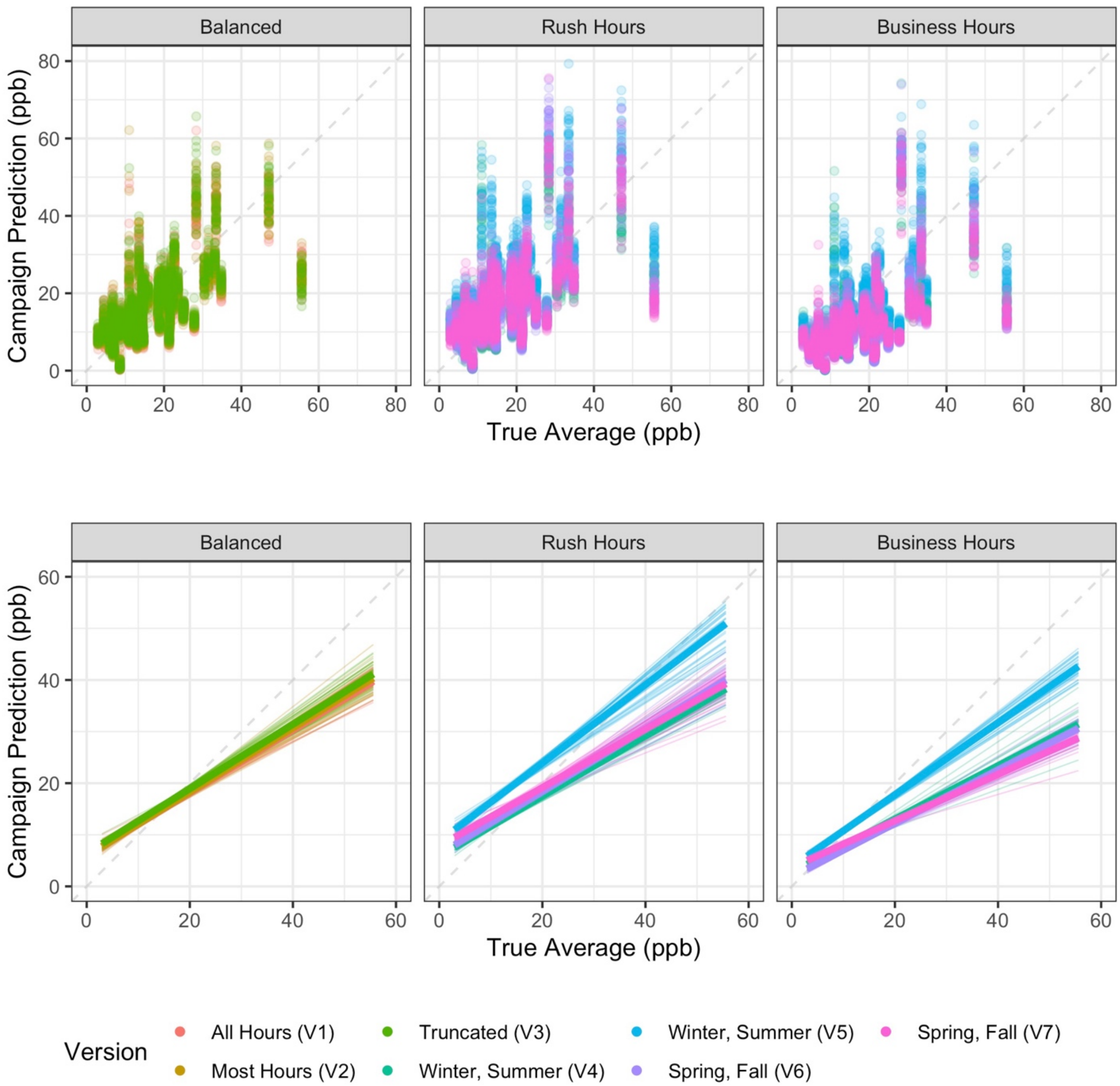


Figure S13. Scatterplots and best fit lines of cross-validated short-term predictions for 30 campaigns vs true average concentrations for NOx. Thin transparent lines are individual campaigns, colored by design version; thicker lines are the overall version trend. (One prediction is excluded for clarity from the Rush Hours Version 4 scatterplot at x=24 ppb, y=109 ppb [site 60731016] but is included in the line plots).

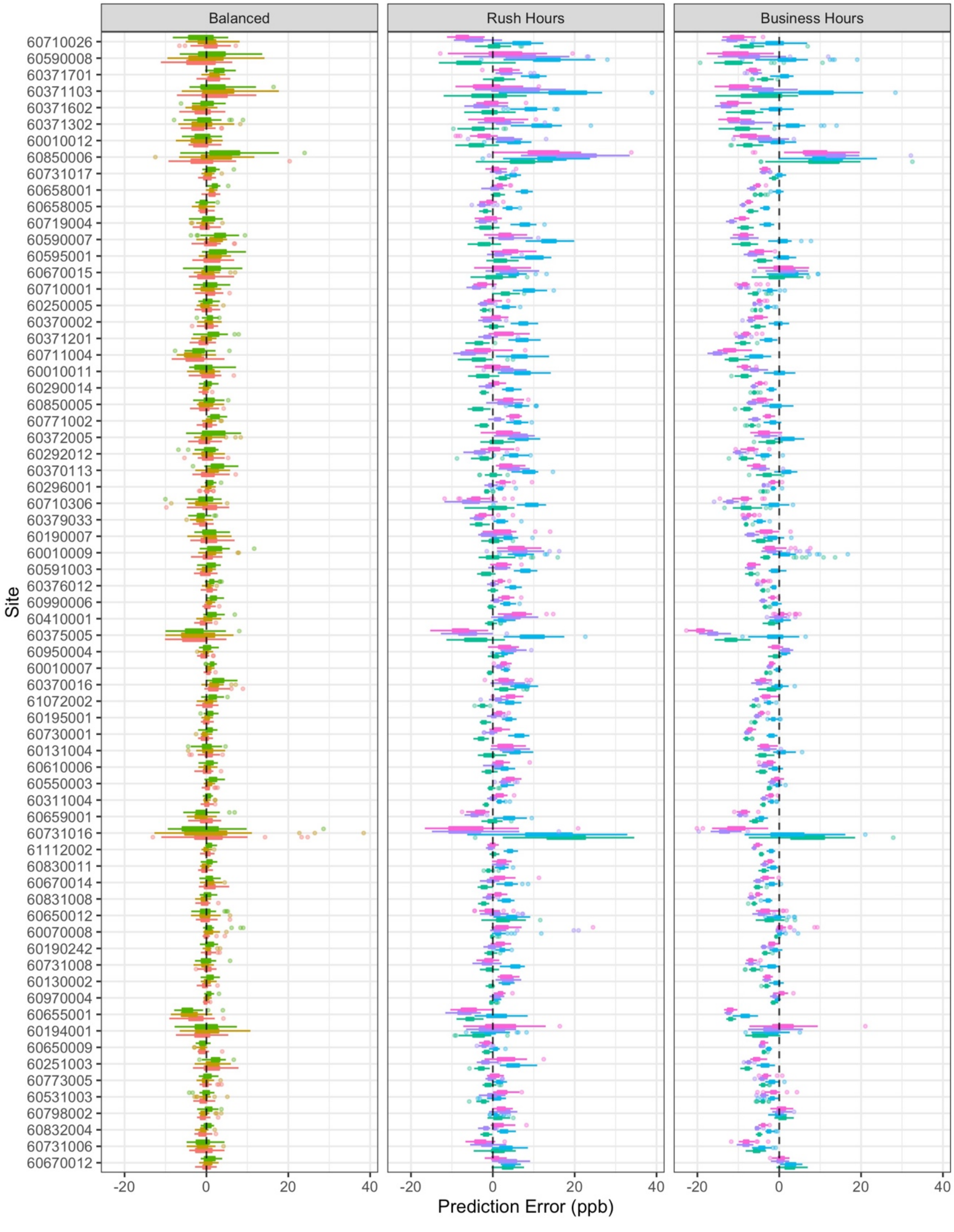
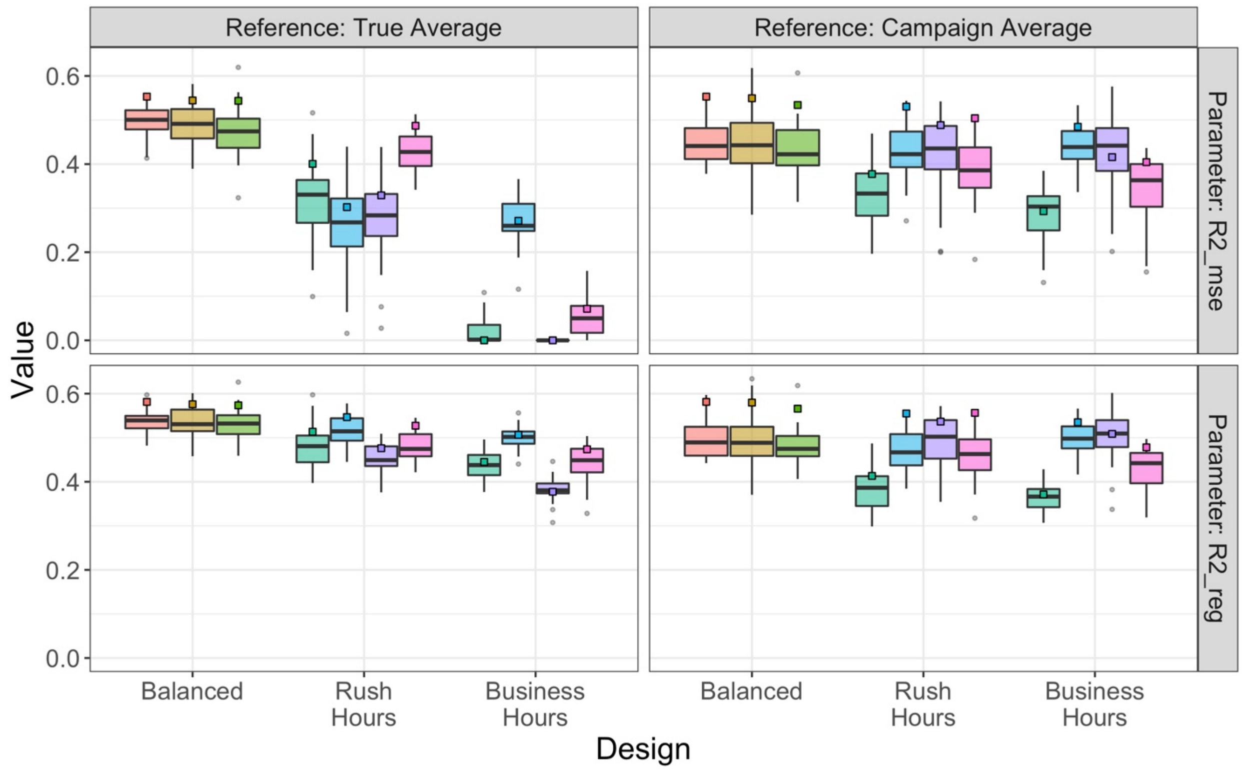


Figure S14. Site-specific NOx prediction biases for short-term designs (N = 30 campaigns) as compared to the gold standard (long-term Balanced Design Version 1) predictions for all sites. Sites are arranged by the true NOx measurement, with higher concentration sites higher up. One prediction bias for site 60731016 is excluded (86 ppb for Rush Hours Version 4) for clarity.

1.5 Model Assessment



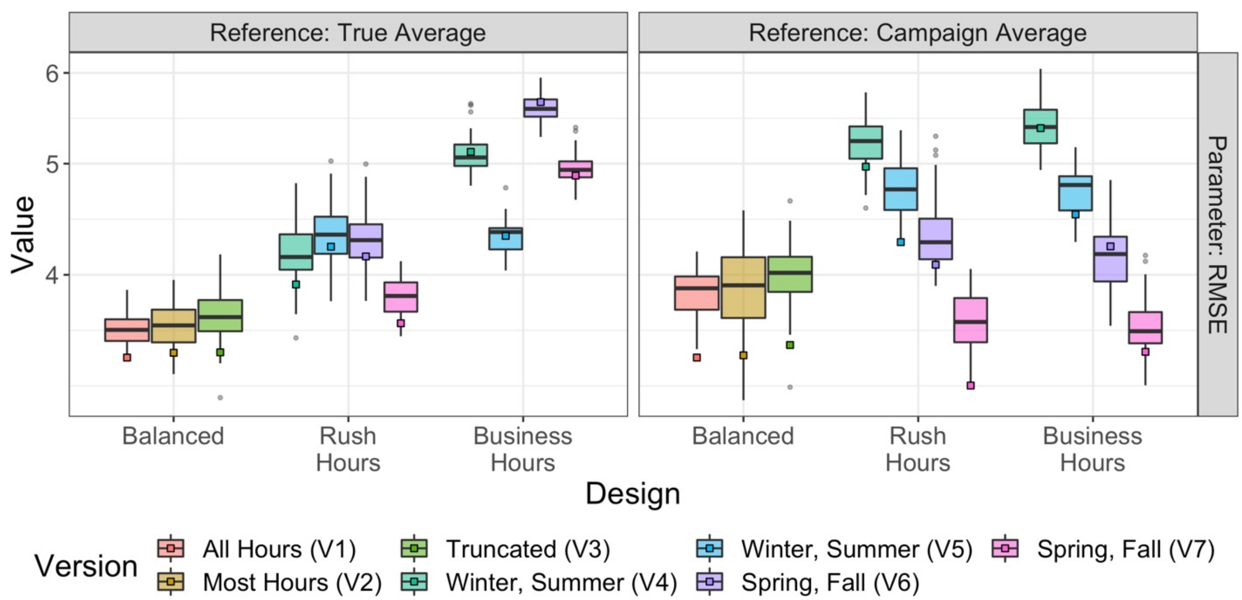


Figure S15. NO_2 Model performances (R^2_{MSE}, R^2_{reg}, and RMSE), as determined by each campaign's cross-validated predictions relative to: a) the true averages (long-term Balanced Version 1), and b) its campaign averages. Boxplots are for short-term approaches (30 campaigns), while squares are for long-term approaches (1 campaign).

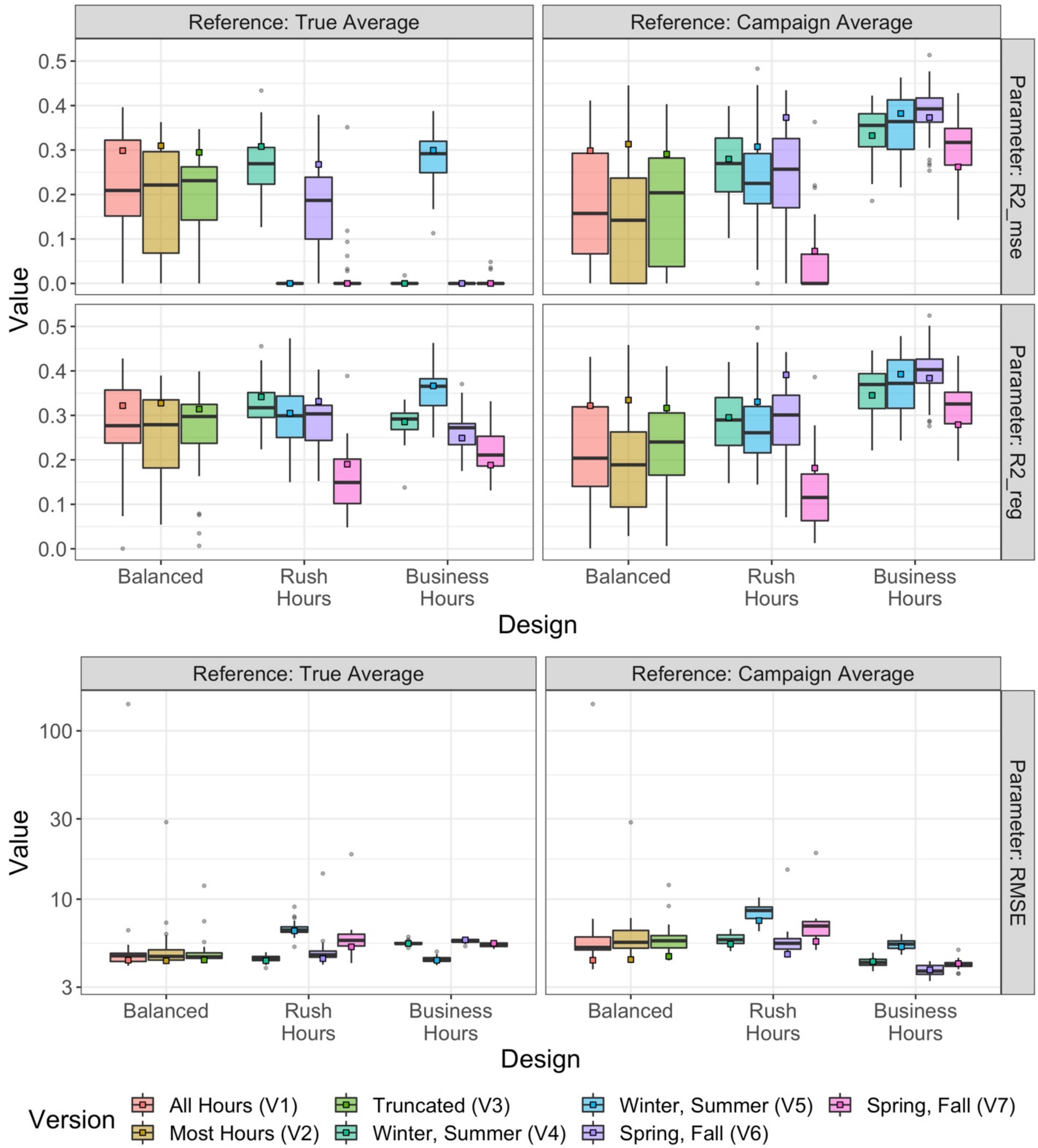


Figure S16. NO Model performances (R^2_{MSE}, R^2_{reg}, and RMSE), as determined by each campaign's cross-validated predictions relative to: a) the true averages (long-term Balanced Version 1), and b) its respective campaign averages. Boxplots are for short-term approaches (30 campaigns), while squares are for long-term approaches (1 campaign). A few influential outliers influenced these performance statistics more so than for NOx and NO_2.

1.6 Los Angeles-San Diego Sensitivity Analyses

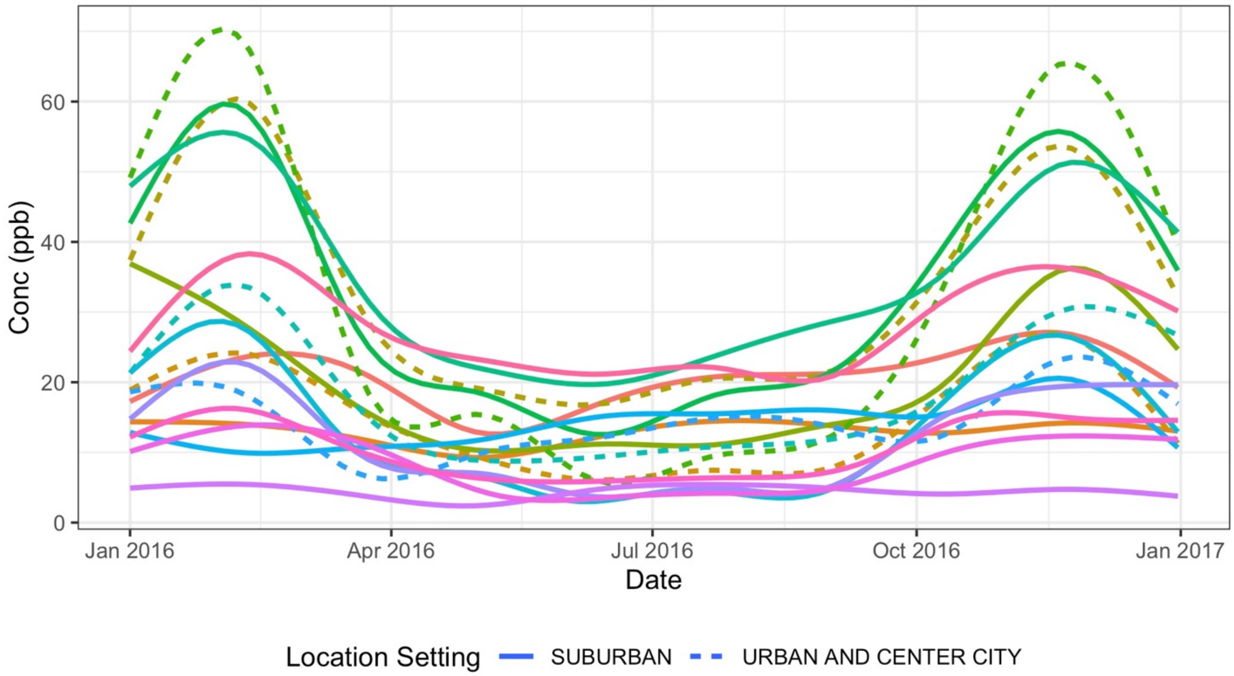


Figure S17. Concentration trends for NOx at AQS sites included in the Los Angeles-San Diego analysis (N=17). Colored smooth lines are individual sites.

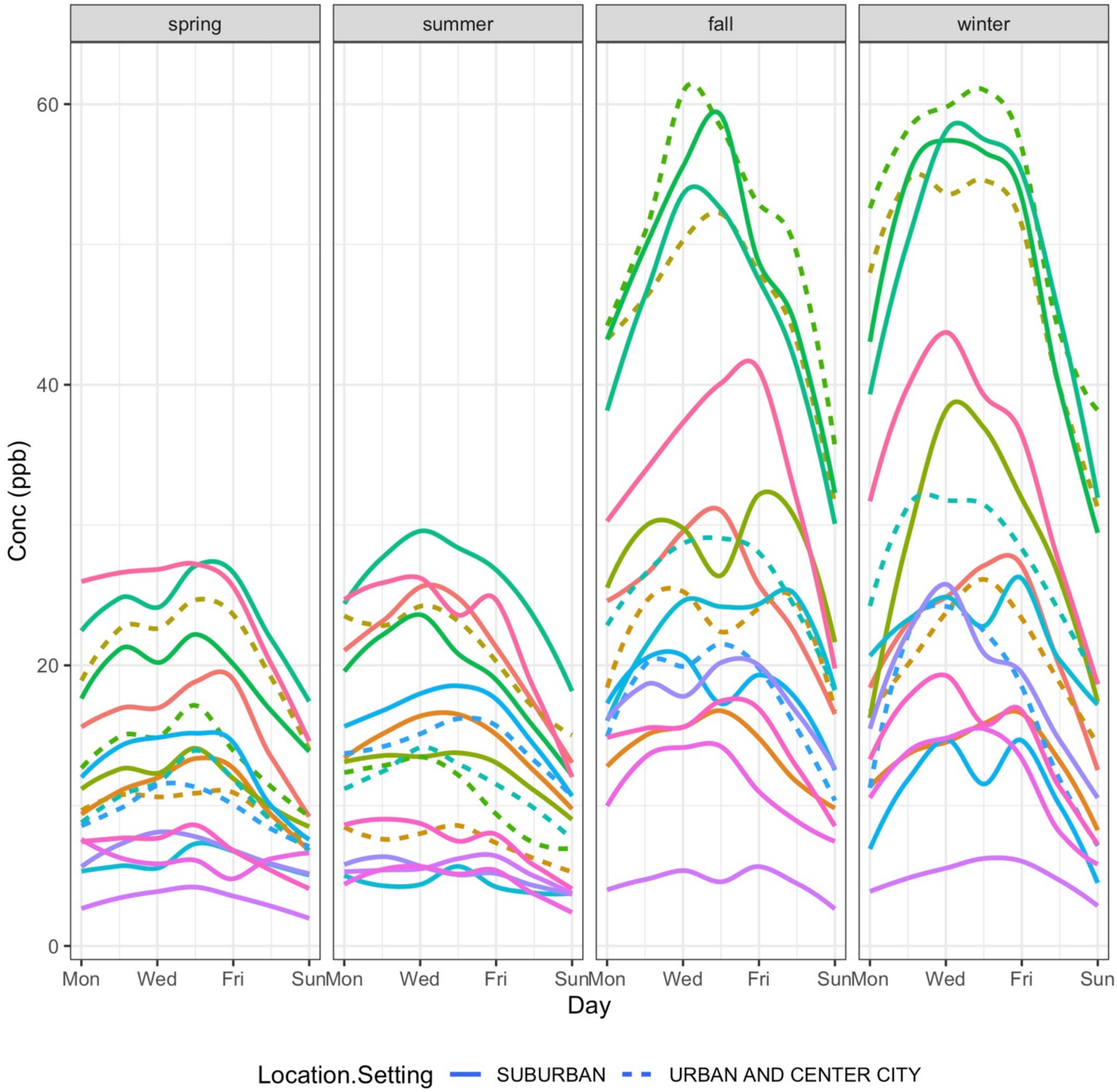


Figure S18. Concentration trends for NOx at AQS sites included in the Los Angeles-San Diego analysis (N=17) by day and season. Colored smooth lines are individual sites.

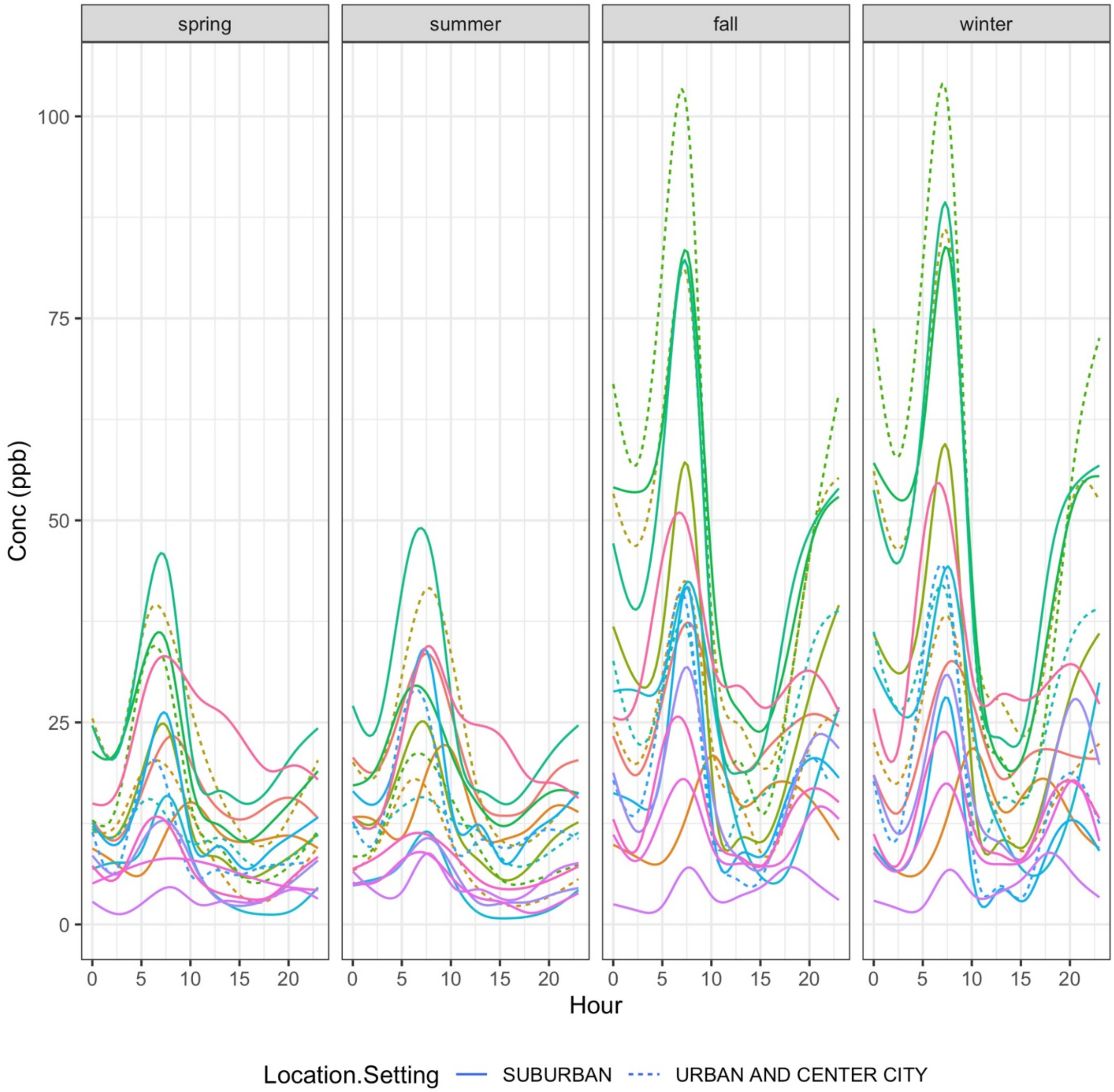
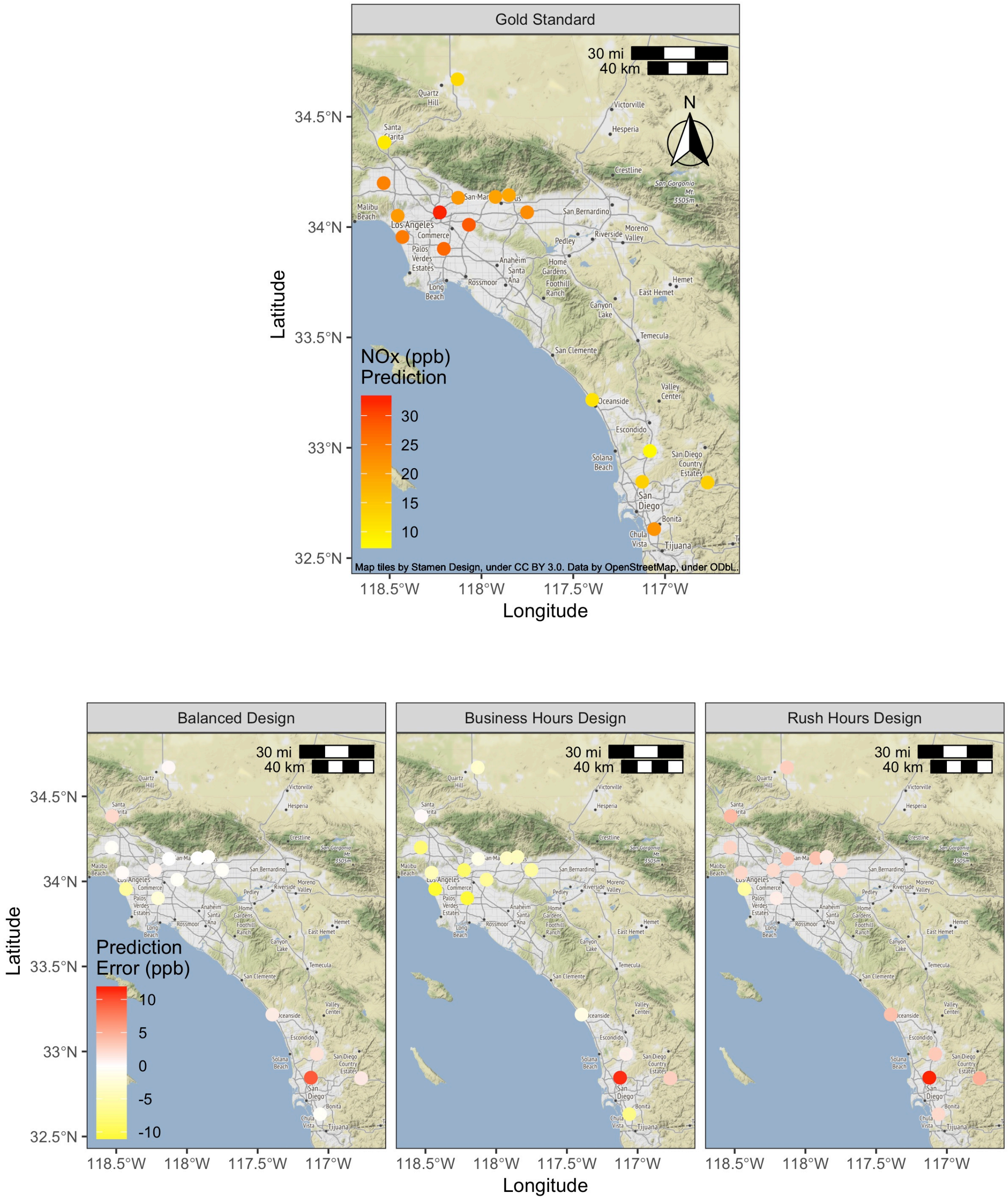


Figure S19. Concentration trends for NOx at AQS sites included in the Los Angeles-San Diego analysis (N=17) by hour and season. Colored smooth lines are individual sites.



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2 Tables

Table S1. Two-week sampling windows for the Rush Hours and Business Hours designs[a]

Version	Season	Start	End
4	summer	2016-06-20	2016-07-03
4	winter	2016-02-27	2016-03-11
5	summer	2016-08-07	2016-08-20
5	winter	2016-01-15	2016-01-28
6	spring	2016-04-15	2016-04-28
6	fall	2016-09-25	2016-10-08
7	spring	2016-05-15	2016-05-28
7	fall	2016-11-24	2016-12-07

[a] the same two-week periods for each version were used for all sites

Table S2. Geocovariates and buffers included in PLS regression (n = 321)

Kind	Covariate	Buffers	Description
airports	log_m_to_airp		log meters to closest airport
airports	log_m_to_l_airp		log meters to closest large airport
bus	log_m_to_bus		log meters to closest bus route
coast	log_m_to_coast		log meters to closest coastline
commercial and services	log_m_to_comm		log meters to closest commercial and services area
commercial and services	lu_comm_p	50, 100, 150, 300, 400, 500, 750, 1000, 1500, 3000, 5000, 10000, 15000	proportion of commercial land use
elevation	elev_above	1000, 5000	number of points (out of 24) more than 20 m and 50 m uphill of a location for a 1000 m and 5000 m buffer, respectively
elevation	elev_at_elev	1000, 5000	number of points (out of 24) within 20 m and 50 m of the location' elevation for a 1000 m and 5000 m buffer, respectively
elevation	elev_below	1000, 5000	number of points (out of 24) more than 20 m and 50 m downhill of a location for a 1000 m and 5000 m buffer, respectively
elevation	elev_elevation		elevation above sea level in meters
emissions/air pollutants	em_CO_s	3000, 15000, 30000	sum of major CO emissions from stacks
emissions/air pollutants	em_NOx_s	3000, 15000, 30000	sum of major NOx emissions from stacks

emissions/air pollutants	em_PM10_s	3000, 15000, 30000	sum of major PM10 emissions from stacks
emissions/air pollutants	em_PM25_s	3000, 15000, 30000	sum of major PM2.5 emissions from stacks
emissions/air pollutants	em_SO2_s	3000, 15000, 30000	sum of major SO2 emissions from stacks
emissions/air pollutants	no2_behr_2005		Columnar NO2 for 2005
emissions/air pollutants	no2_behr_2006		Columnar NO2 for 2006
emissions/air pollutants	no2_behr_2007		Columnar NO2 for 2007
imperviousness	imp_a	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	average imperviousness
land use	lu_bays_p	3000, 5000, 10000, 15000	proportion of land with bays and estuaries
land use	lu_crop_p	100, 150, 300, 400, 500, 750, 1000, 1500, 3000, 5000, 10000, 15000	proportion of cultivated crops such as orchards, vineyards, grains
land use	lu_green_p	750, 1000, 1500, 3000, 5000, 10000, 15000	proportion of evergreen forest land
land use	lu_grove_p	750, 1000, 1500, 3000, 5000, 10000, 15000	proportion of orchards, groves, vineyards, nurseries
land use	lu_herb_range_p	1000, 1500, 3000, 5000, 10000, 15000	proportion of herbaceous rangeland

land use	lu_industrial_p	150, 300, 400, 500, 750, 1000, 1500, 3000, 5000, 15000	proportion of industrial land use
land use	lu_mine_p	3000, 5000, 10000	proportion of land with strip mines, quarries, and gravel pits
land use	lu_mix_forest_p	10000, 15000	proportion of mixed forest land
land use	lu_mix_range_p	1500, 3000, 5000, 10000	proportion of mixed rangeland
land use	lu_mix_urban_p	150, 300, 400, 500, 750, 1000, 1500	proportion of mixed urban or built-up land
land use	lu_oth_urban_p	400, 500, 750, 1000, 1500, 5000	proportion of other urban or built-up land
land use	lu_reservior_p	5000	proportion of land with reservoirs
land use	lu_resi_p	50, 100, 150, 300, 400, 500, 750, 1000, 1500, 3000, 5000, 10000, 15000	Proportion of residential land use
land use	lu_shrub_p	400, 500, 750, 1000, 1500, 3000, 5000, 10000, 15000	proportion of shrubland
land use	lu_transition_p	750, 1000, 1500	proportion of transitional land use
land use	lu_unspec_p	10000, 15000	proportion of unspecified land use
land use	rlu_barren_p	3000, 5000	proportion of barren land
land use	rlu_crop_p	750, 1000, 3000, 5000	proportion of cropland and pastureland
land use	rlu_dev_hi_p	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	proportion of highly developed land (e.g., commercial and services; industrial; transportation, communication, and utilities)

land use	rlu_dev_lo_p	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	proportion of low developed land (e.g., residential)
land use	rlu_dev_med_p	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	proportion of medium developed land (e.g., residential)
land use	rlu_dev_open_p	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	proportion of developed open land
land use	rlu_grass_p	50, 100, 150, 300, 400, 500, 750, 1000, 3000, 5000	proportion of grasslands, herbaceous vegetation
land use	rlu_herb_wetland_p	5000	proportion of herb (nonforested) wetland
land use	rlu_mix_forest_p	3000, 5000	proportion of mixed forest
land use	rlu_pasture_p	1000, 3000, 5000	proportion of pasture, hay land
land use	rlu_shrub_p	400, 500, 750, 1000, 3000, 5000	proportion of shrubland
NDVI	ndvi_q25_a	250, 500, 1000, 2500, 5000, 7500, 10000	NDVI (25th quantile)
NDVI	ndvi_q50_a	250, 500, 1000, 2500, 5000, 7500, 10000	NDVI (50th quantile)
NDVI	ndvi_q75_a	250, 500, 1000, 2500, 5000, 7500, 10000	NDVI (75th quantile)
NDVI	ndvi_summer_a	250, 500, 1000, 2500, 5000, 7500, 10000	average summertime NDVI

NDVI	ndvi_winter_a	250, 500, 1000, 2500, 5000, 7500, 10000	average wintertime NDVI
population	pop_s	500, 1000, 1500, 2000, 2500, 3000, 5000, 10000, 15000	2000 population density
port	log_m_to_s_port		log meters to closest small port
port	lu_transport_p	300, 400, 500, 750, 1000, 1500, 3000, 5000	proportion of transportation, communications, and utilities land
railroads, rail yards	log_m_to_rr		log meters to closest railroad
railroads, rail yards	log_m_to_ry		log meters to closest rail yard
roads	intersect_a1_a1_s	3000	intersect_a1_a1_s
roads	intersect_a1_a2_s	3000	intersect_a1_a2_s
roads	intersect_a1_a3_s	1000, 3000	number of a1-a3 road intersections
roads	intersect_a2_a2_s	3000	number of a2-a2 road intersections
roads	intersect_a2_a3_s	3000	number of a2-a3 road intersections
roads	intersect_a3_a3_s	500, 1000, 3000	number of a3-a3 road intersections
roads	ll_a1_s	500, 750, 1000, 1500, 3000, 5000	length of a1 roads
roads	ll_a2_s	1500, 3000, 5000	length of a2 roads
roads	ll_a3_s	50, 100, 150, 300, 400, 500, 750, 1000, 1500, 3000, 5000	length of a3 roads
roads	log_m_to_a1		log meters to closest a1 road
roads	log_m_to_a1_a1_intersect		log meters to closest a1-a1 road intersection
roads	log_m_to_a1_a2_intersect		log_m_to_a1_a2_intersect

roads	log_m_to_a1_a3_intersect		log meters to closest a1-a3 road intersection
roads	log_m_to_a2		log meters to closest a2 road
roads	log_m_to_a2_a2_intersect		log meters to closest a2-a2 road intersection
roads	log_m_to_a2_a3_intersect		log meters to closest a2-a3 road intersection
roads	log_m_to_a3		log meters to closest a3 road
roads	log_m_to_a3_a3_intersect		log meters to closest a3-a3 road intersection
truck routes	log_m_to_truck		log meters to closest truck route
truck routes	tl_s	750, 1000, 1500, 3000, 5000, 10000, 15000	length of truck routes
water	log_m_to_waterway		log meters to closest waterway
water	rlu_water_p	3000, 5000	proportion of water

Table S3. Distribution of the number of hourly and day equivalent (24 samples/day) observations per site[1]

Pollutant Name	Count	N	Min	Mean	SD	Median	IQR	Max
Oxides of nitrogen (NOx)	Day Equivalent	69	285	337	15	343	17	355
Oxides of nitrogen (NOx)	Hours	69	6,836	8,090	361	8,236	408	8,510
Nitric oxide (NO)	Day Equivalent	51	294	338	14	342	14	355
Nitric oxide (NO)	Hours	51	7,060	8,119	339	8,216	346	8,510
Nitrogen dioxide (NO2)	Day Equivalent	73	284	337	15	343	17	355
Nitrogen dioxide (NO2)	Hours	73	6,825	8,077	363	8,231	408	8,510

[1] N = number of sites.

2.1 Hourly Readings

Table S4. Distribution of hourly concentrations (ppb)[1]

Pollutant Name	N	Min	Mean	SD	Median	IQR	Max
Oxides of nitrogen (NOx)	558,207	-5	16	21	9	16	427
Nitric oxide (NO)	414,046	-5	9	16	4	5	381
Nitrogen dioxide (NO2)	589,625	-3	10	10	7	12	97

[1] N = total number of hourly readings.

2.2 Annual Average Estimates

Table S5. Distribution of annual average NOx estimates from various sampling approaches.[1]

Design	Version	Type	N	Min	Q25	Q50	Q75	Max	SD
Balanced	All Hours (V1)	Long-Term	69	3.0	9.8	14.2	20.8	55.6	9.8
Balanced	All Hours (V1)	Short-Term	2070	1.9	9.2	13.7	21.2	69.5	10.3
Balanced	Most Hours (V2)	Long-Term	69	3.2	9.9	14.1	20.7	55.4	9.9
Balanced	Most Hours (V2)	Short-Term	2070	2.1	9.4	13.9	20.9	70.8	10.3
Balanced	Truncated (V3)	Long-Term	69	3.4	10.4	14.4	21.0	55.7	10.1
Balanced	Truncated (V3)	Short-Term	2070	2.1	9.8	14.7	21.4	66.9	10.6
Rush Hours	Winter, Summer (V4)	Long-Term	69	3.5	8.3	12.1	19.4	67.1	12.0
Rush Hours	Winter, Summer (V4)	Short-Term	2070	2.2	8.2	12.2	19.8	78.2	12.0
Rush Hours	Winter, Summer (V5)	Long-Term	69	4.6	12.3	18.8	29.6	75.9	14.5
Rush Hours	Winter, Summer (V5)	Short-Term	2070	3.1	12.0	18.1	29.0	95.7	14.8
Rush Hours	Spring, Fall (V6)	Long-Term	69	3.1	10.4	13.6	20.4	58.8	11.3
Rush Hours	Spring, Fall (V6)	Short-Term	2070	1.7	9.4	13.7	20.7	70.8	11.7
Rush Hours	Spring, Fall (V7)	Long-Term	69	4.4	10.6	15.7	20.2	55.7	10.0
Rush Hours	Spring, Fall (V7)	Short-Term	2070	2.3	10.4	15.3	20.9	69.5	10.4
Business Hours	Winter, Summer (V4)	Long-Term	69	1.6	5.5	8.1	12.8	54.6	10.6

Business Hours	Winter, Summer (V4)	Short-Term	2070	1.0	5.4	8.1	14.2	62.1	10.7
Business Hours	Winter, Summer (V5)	Long-Term	69	3.1	8.0	11.9	20.5	65.2	12.0
Business Hours	Winter, Summer (V5)	Short-Term	2070	2.0	8.1	11.8	19.9	73.0	12.0
Business Hours	Spring, Fall (V6)	Long-Term	69	1.6	5.4	7.9	12.2	53.3	9.8
Business Hours	Spring, Fall (V6)	Short-Term	2070	1.1	5.1	8.0	12.1	57.1	9.8
Business Hours	Spring, Fall (V7)	Long-Term	69	2.3	6.1	9.7	12.7	47.2	8.7
Business Hours	Spring, Fall (V7)	Short-Term	2070	0.9	6.2	9.6	13.1	53.9	8.7

[1] N = Total number of sites x number of campaigns.

2.3 Model Predictions

Table S6. Predictions above 80 ppb excluded from prediction plots, if noted[1]

Pollutant Name	**Design**	**Version**	**N**	**Prediction (ppb)**
Oxides of nitrogen (NOx)	Rush Hours	Winter, Summer (V4)	1	109
Nitric oxide (NO)	Balanced	All Hours (V1)	2	238, 1012
Nitric oxide (NO)	Balanced	Most Hours (V2)	2	127, 181
Nitric oxide (NO)	Balanced	Truncated (V3)	1	82
Nitric oxide (NO)	Rush Hours	Spring, Fall (V6)	1	87
Nitric oxide (NO)	Rush Hours	Spring, Fall (V7)	2	89, 113

[1] N is the number of predictions.

Table S7. Distribution of prediction bias for short-term approaches relative to the gold standard predictions[1]

Pollutant Name	Design	N	Min	Q01	Median	IQR	Q99	Max
Oxides of nitrogen (NOx)	Balanced	6,210	-13.1	-6.9	0.2	2.4	7.9	38
Oxides of nitrogen (NOx)	Rush Hours	8,280	-16.6	-8.9	1.2	5.2	18.4	86
Oxides of nitrogen (NOx)	Business Hours	8,280	-22.7	-15.2	-3.8	5.3	12.8	33
Nitric oxide (NO)	Balanced	4,590	-10.5	-3.8	0.1	1.7	7.2	1,006[2]
Nitric oxide (NO)	Rush Hours	6,120	-7.9	-3.8	1.3	3.4	13.1	107
Nitric oxide (NO)	Business Hours	6,120	-10.6	-7	-1.8	3	4.2	10
Nitrogen dioxide (NO2)	Balanced	6,300	-6.9	-3	0.1	1.1	3.5	11
Nitrogen dioxide (NO2)	Rush Hours	8,400	-8.2	-4.7	0.1	2.3	6.6	24
Nitrogen dioxide (NO2)	Business Hours	8,400	-11.5	-7.5	-2.2	2.7	6.4	19

[1] N = the number of sites x 30 campaign repetitions x the number of versions per design
[2] This maximum is the result of a very large outlier prediction

Table S8. Site prediction error by design relative to the gold standard campaign predictions for the southern California sensitivity analysis (No. Predictions = 17 sites x 30 simulations/version x 3-4 versions/design).

Design	No. Predictions	Absolute Error (ppb)		Percent Error (%)	
		Median	IQR	Median	IQR
Balanced	1530	0.0	4.6	13.2	17.2
Rush Hours	2040	2.1	6.8	20.4	28.7

Business Hours	2040	-4.0	7.6	27.5	26.0

3 Equations

3.1 Methods

$$MSE_{ref} = \frac{1}{n}\sum_{i=1}^{n}\left(y_{i,ref} - \hat{y}_{i,campaign}\right)^2$$

Equation S1. Mean squared error (MSE) definition. Where $\hat{y}_{i,campaign}$ is the prediction from a campaign for a given design version; $y_{i,ref}$ is the reference value, either the true annual average or the estimated annual average from the same campaign (the typical approach in practice); and n is the total number of sites.

$$RMSE_{ref} = \sqrt{MSE_{ref}}$$

Equation S2. Root mean squared error (RMSE) definition

$$R^2_{MSE} = \max\left(0, 1 - \frac{MSE_{ref}}{\frac{1}{n}\sum_{i=1}^{n}\left(y_{i,ref} - \bar{y}_{campaign}\right)^2}\right)$$

Equation S3. MSE-based R^2 (R^2_{MSE}) definition. Where $\bar{y}_{campaign}$ is the average across all n sites for a given campaign.

4 Note

4.1 Methods

Note S1. Computing

All analyses were conducted in R (v 3.6.2, using RStudio v 1.2.5033)[1] using the following packages: dplyr (1.0.6),[2] forcats (0.5.0),[3] ggmap (3.0.0),[4] ggplot2 (3.3.3),[5] ggpubr (0.2.5),[6] ggrepel (0.8.1),[7] ggspatial (1.1.4),[8] glmnet (3.0-2),[9] kableExtra (1.1.0),[10] lubridate (1.7.10),[11] magrittr (1.5),[12] Matrix (1.2-18),[13] modelr (0.1.6),[14] pls (2.7-2),[15] purrr (0.3.3),[16] readr (1.3.1),[17] sf (0.9-5),[18] stringr (1.4.0),[19] tibble (3.1.2),[20] tidyr (1.0.2),[21] tidyverse (1.3.0),[22] and VCA (1.4.2).[23] All maps were created with map tiles by Stamen Design[24] under CC BY 3.0,[25] using data by OpenStreetMap under ODbL.[26]

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