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Evaluating machine learning model performance in a two-step colocation process for TVOC and BTEX sensor calibration

Caroline Frischmon et al.

Correspondence to: Caroline Frischmon (caroline.frischmon@colorado.edu)

Table S1. Correlation coefficients before harmonization correction (left column) and after harmonization correction (right column) between the colocation HAQ-Pod and other HAQ-Pods during harmonization

	HAQ-Pod 1		HAQ-Pod 2		HAQ-Pod 3	
Sensor	**Uncorrected**	**Corrected**	**Uncorrected**	**Corrected**	**Uncorrected**	**Corrected**
Figaro 2600	0.96	1	0.93	1	0.99	1
Figaro 2602	0.97	0.98	0.93	0.98	0.99	0.99
Figaro 2611	0.94	0.99	0.87	0.98	0.98	0.99
Alphasense NO2 B-4	0.95	0.96	0.99	0.99	0.95	0.96
Temperature	0.99	0.99	1	1	0.99	0.99
Humidity	1	1	1	1	0.99	0.99

Table S2. Coefficients (β) for TGS 2600 linear correction developed during harmonization

HAQ-Pod	**β_0 (intercept)**	**β_1 (TGS 2600)**	**β_2 (time elapsed)**
1	32.44	1.10	-3.15E-06
2	18.89	1.15	-3.92E-06
3	-22.90	0.98	1.07E-06

Table S3. Coefficients (β) for TGS 2602 linear correction developed during harmonization

HAQ-Pod	**β_0 (intercept)**	**β_1 (TGS 2602)**	**β_2 (time elapsed)**
1	30.53	0.87	-7.97E-07
2	24.11	1.02	-2.00E-06
3	29.84	0.77	2.61E-07

Table S4. Coefficients (β) for TGS 2611 linear correction developed during harmonization

HAQ-Pod	**β_0 (intercept)**	**β_1 (TGS 2611)**	**β_2 (time elapsed)**
1	-6.82	1.12	2.10E-06
2	-13.25	1.11	3.11E-06
3	-10.04	1.11	9.40E-07

Table S5. Coefficients (β) for NO_2 B-4 linear correction developed during harmonization

HAQ-Pod	**β_0 (intercept)**	**β_1 (NO_2 B-4)**	**β_2 (time elapsed)**
1	-9.84	0.72	2.71E-07
2	1.51	0.92	2.69E-08
3	-4.03	0.72	1.52E-07

Table S6. Coefficients (β) for Temperature linear correction developed during harmonization

HAQ-Pod	β_0 (intercept)	β_1 (temperature)	β_2 (time elapsed)
1	-11.92	1.05	2.67E-08
2	7.55	0.98	6.12E-10
3	2.91	0.99	4.58E-08

Table S7. Coefficients (β) for Humidity linear correction developed during harmonization

HAQ-Pod	β_0 (intercept)	β_1 (humidity)	β_2 (time elapsed)
1	-2.50	0.91	-3.62E-08
2	1.06	0.97	-5.96E-10
3	2.87	0.93	-1.78E-07

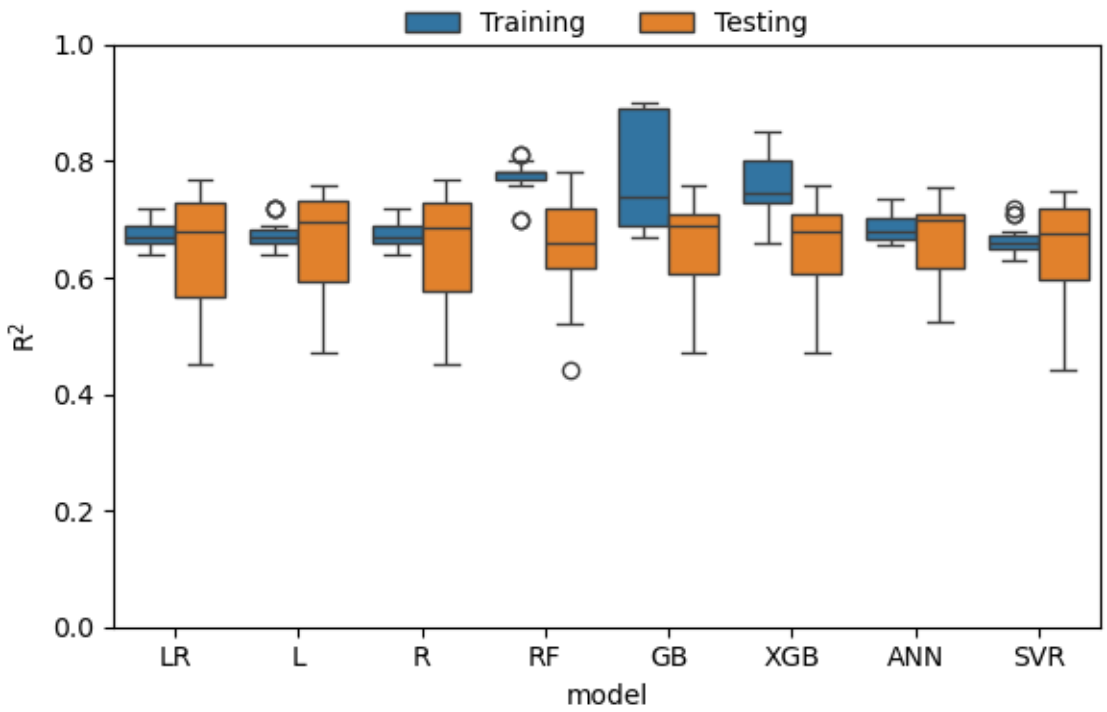


Figure S1. R^2 for the TVOC calibration models

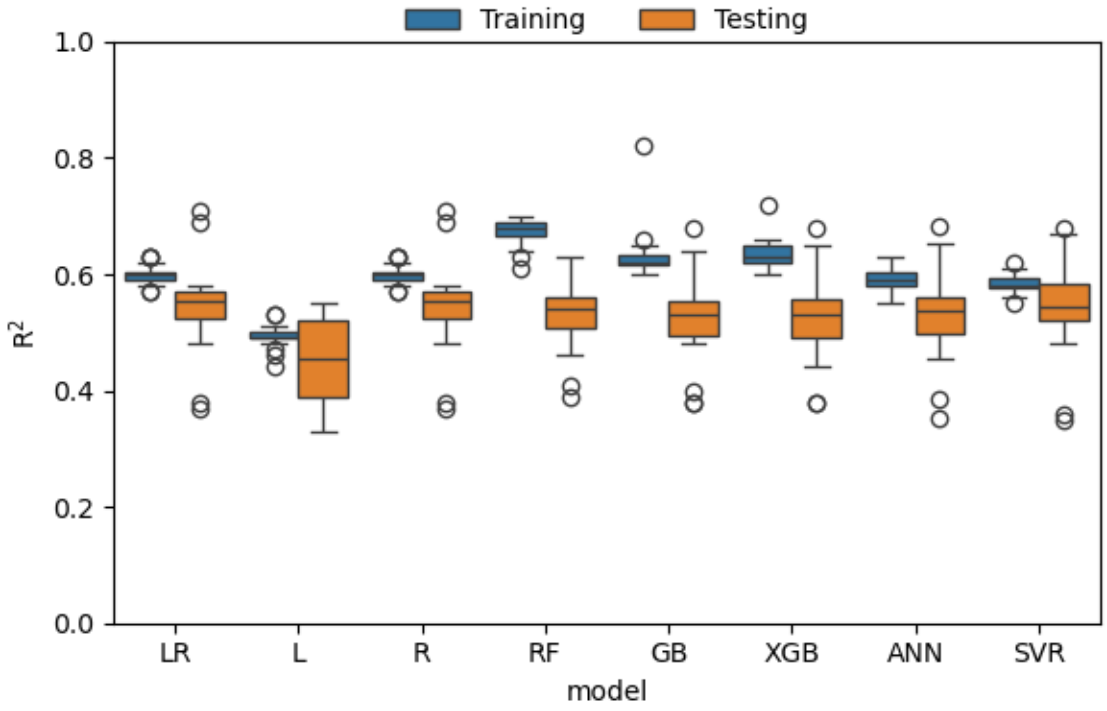


Figure S2. R^2 for the BTEX calibration models

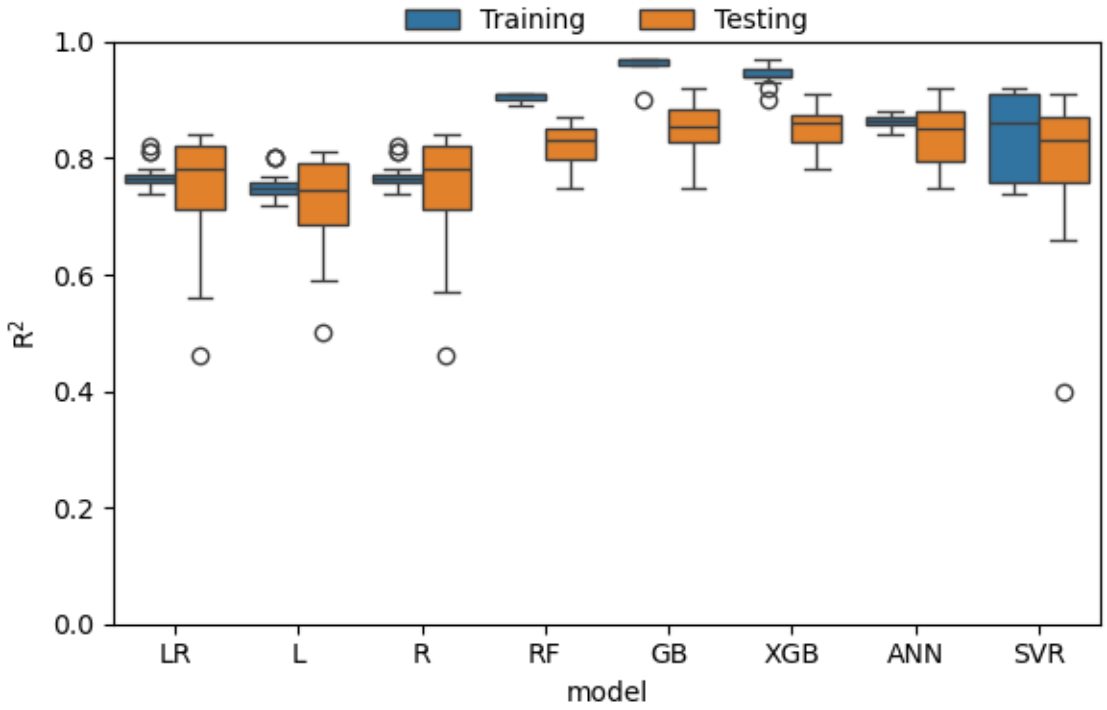


Figure S3. R^2 for the NO_2 calibration models

Figure S4. Heatmap of correlation coefficients of TVOC field data predictions by model type

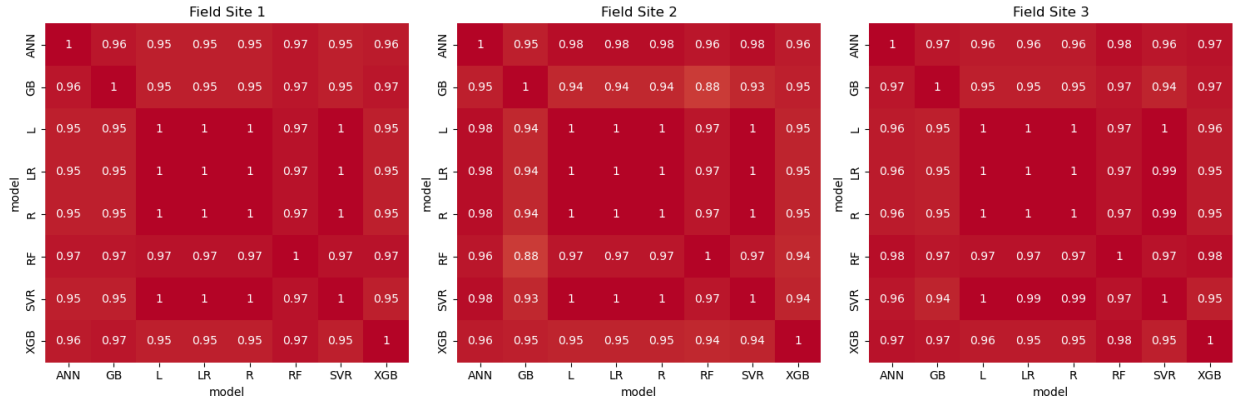


Figure S5. Heatmap of correlation coefficients of BTEX field data predictions by model type

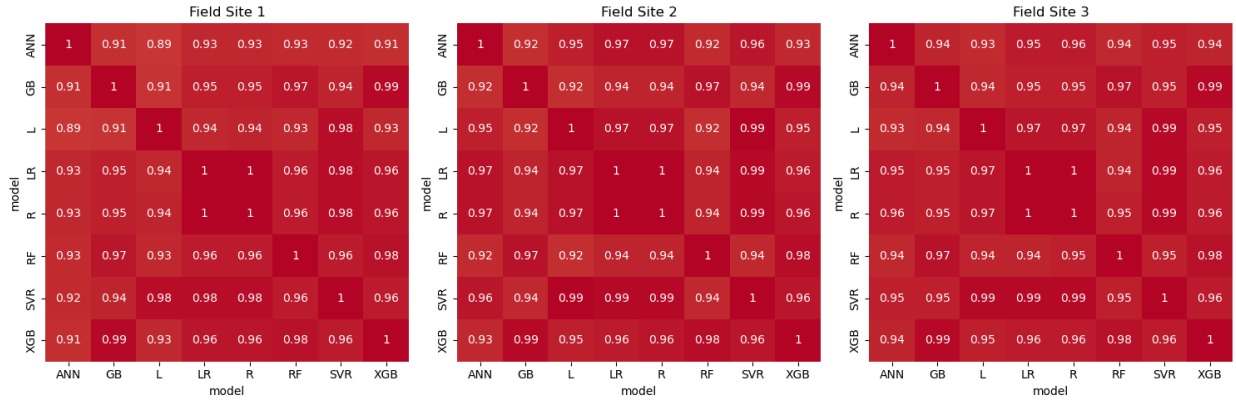
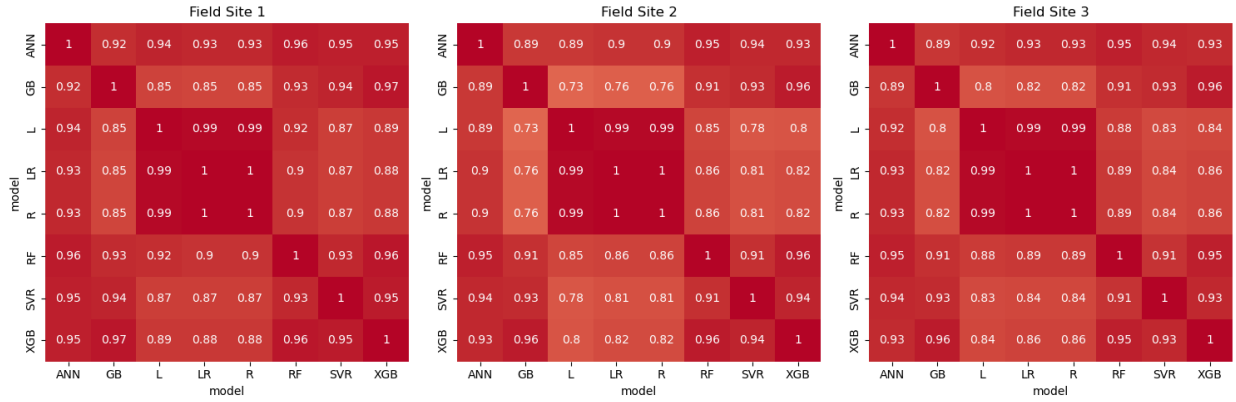


Figure S6. Heatmap of correlation coefficients of NO_2 field data predictions by model type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ANN 1 0.92 0.94 0.93 0.93 0.96 0.95 0.95
GB 0.92 1 0.85 0.85 0.85 0.93 0.94 0.97
L 0.94 0.85 1 0.99 0.99 0.92 0.87 0.89
LR 0.93 0.85 0.99 1 1 0.9 0.87 0.88
R 0.93 0.85 0.99 1 1 0.9 0.87 0.88
RF 0.96 0.93 0.92 0.9 0.9 1 0.93 0.96
SVR 0.95 0.94 0.87 0.87 0.87 0.93 1 0.95
XGB 0.95 0.97 0.89 0.88 0.88 0.96 0.95 1
model
ANN GB L LR R RF SVR XGB
model
Field Site 2
ANN 1 0.89 0.89 0.9 0.9 0.95 0.94 0.93
GB 0.89 1 0.73 0.76 0.76 0.91 0.93 0.96
L 0.89 0.73 1 0.99 0.99 0.85 0.78 0.8
LR 0.9 0.76 0.99 1 1 0.86 0.81 0.82
R 0.9 0.76 0.99 1 1 0.86 0.81 0.82
RF 0.95 0.91 0.85 0.86 0.86 1 0.91 0.96
SVR 0.94 0.93 0.78 0.81 0.81 0.91 1 0.94
XGB 0.93 0.96 0.8 0.82 0.82 0.96 0.94 1
model
ANN GB L LR R RF SVR XGB
model
Field Site 3
ANN 1 0.89 0.92 0.93 0.93 0.95 0.94 0.93
GB 0.89 1 0.8 0.82 0.82 0.91 0.93 0.96
L 0.92 0.8 1 0.99 0.99 0.88 0.83 0.84
LR 0.93 0.82 0.99 1 1 0.89 0.84 0.86
R 0.93 0.82 0.99 1 1 0.89 0.84 0.86
RF 0.95 0.91 0.88 0.89 0.89 1 0.91 0.95
SVR 0.94 0.93 0.83 0.84 0.84 0.91 1 0.93
XGB 0.93 0.96 0.84 0.86 0.86 0.95 0.93 1
model
ANN GB L LR R RF SVR XGB
model