



Supplement of

Recalibration of low-cost O₃ and PM_{2.5} sensors: linking practices to recent air sensor test protocols

Paul Gäbel and Elke Hertig

Correspondence to: Paul Gäbel (paul.gaebel@med.uni-augsburg.de) and Elke Hertig (elke.hertig@med.uni-augsburg.de)

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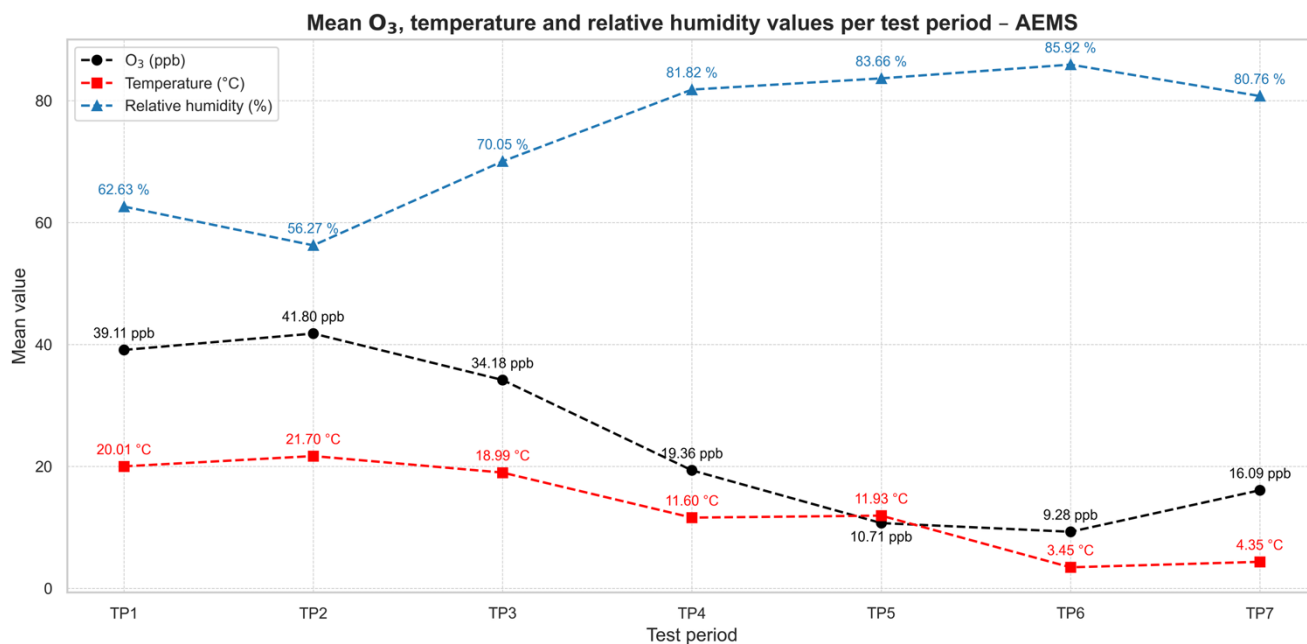


Figure S1. Test period (TP1–TP7) means of ambient temperature, relative humidity and O₃ given by the reference station AEMS (TP1 = 10 June – 10 July 2022, TP2 = 11 July – 11 August 2022, TP3 = 11 August – 10 September 2022, TP4 = 10 September – 11 October 2022, TP5 = 11 October – 12 November 2022, TP6 = 12 November – 12 December 2022, TP7 = 12 December 2022 – 11 January 2023).

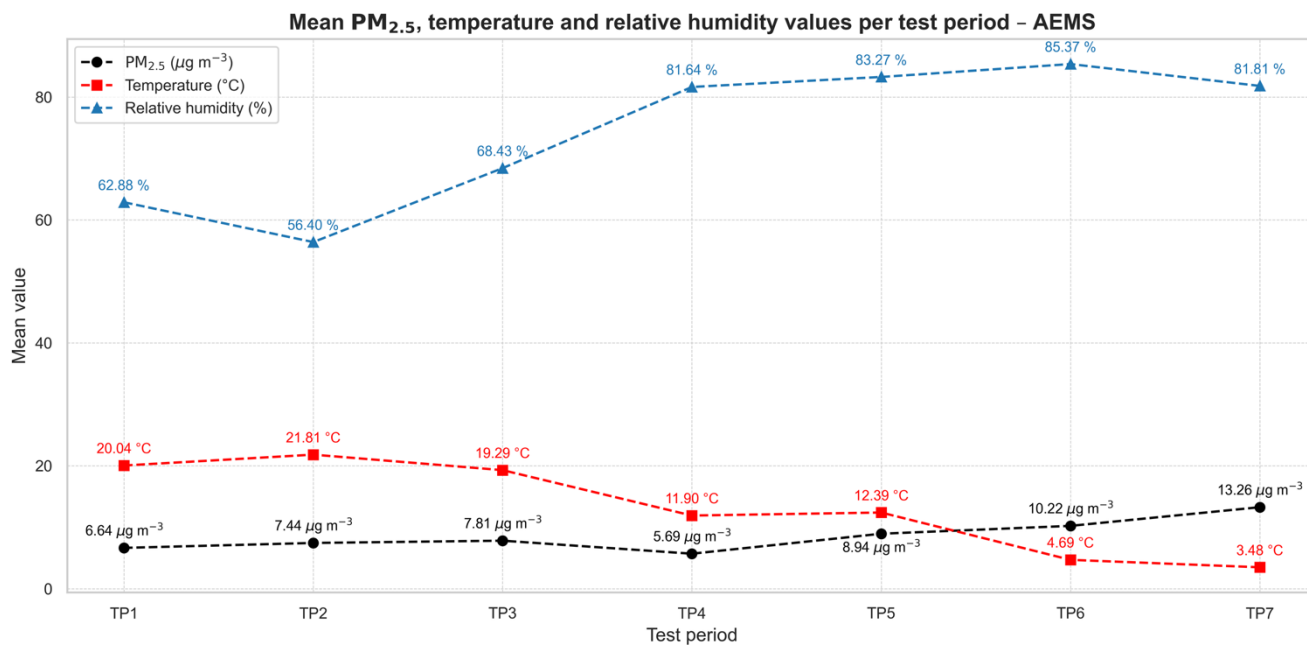


Figure S2. Test period (TP1–TP7) means of ambient temperature, relative humidity and PM_{2.5} given by the reference station AEMS (TP1 = 11 June – 10 July 2022, TP2 = 11 July – 9 August 2022, TP3 = 10 August – 8 September 2022, TP4 = 9 September – 8 October 2022, TP5 = 9 October – 7 November 2022, TP6 = 8 November – 7 December 2022, TP7 = 8 December 2022 – 6 January 2023).

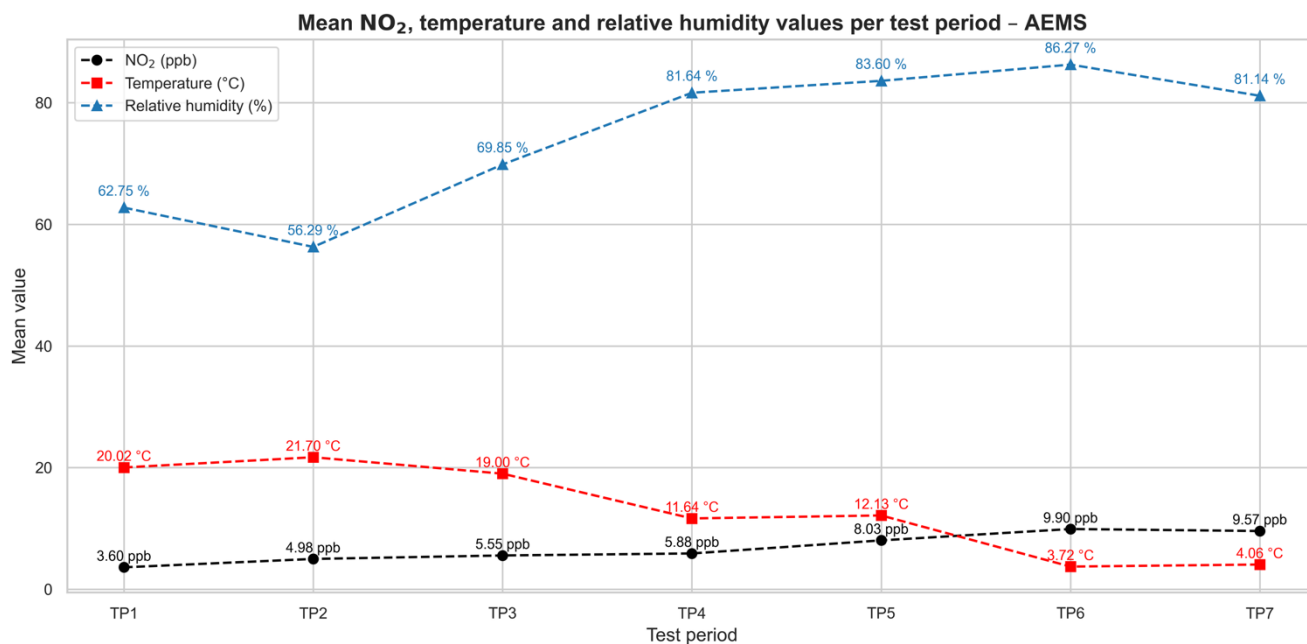


Figure S3. Test period (TP1–TP7) means of ambient temperature, relative humidity and NO₂ given by the reference station AEMS (TP1 = 10 June – 10 July 2022, TP2 = 10 July – 10 August 2022, TP3 = 11 August – 10 September 2022, TP4 = 10 September – 10 October 2022, TP5 = 10 October – 11 November 2022, TP6 = 11 November – 11 December 2022, TP7 = 11 December 2022 – 10 January 2023).

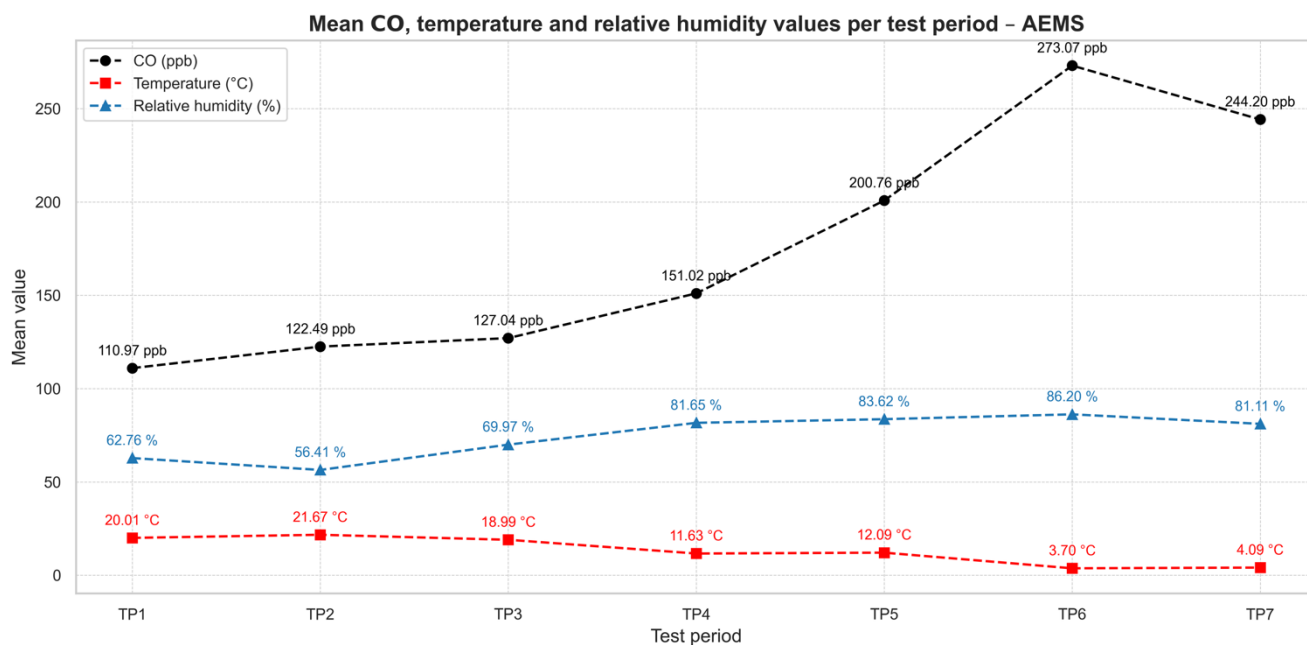


Figure S4. Test period (TP1–TP7) means of ambient temperature, relative humidity and CO given by the reference station AEMS (TP1 = 10 June – 10 July 2022, TP2 = 10 July – 11 August 2022, TP3 = 11 August – 10 September 2022, TP4 = 10 September – 10 October 2022, TP5 = 10 October – 11 November 2022, TP6 = 11 November – 11 December 2022, TP7 = 11 December 2022 – 10 January 2023).

Table S1. DQOs for indicative measurements and objective estimation set in the AQD 2008/50/EC and in CEN/TS 17660-1:2021 and class 3 set in CEN/TS 17660-1:2021.

Pollutant	Averaging Period	LV	DQO of Class 1 sensor system	DQO of Class 2 sensor system	DQO of Class 3 sensor system
	h	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$ (% of LV)	$\mu\text{g m}^{-3}$ (% of LV)	$\mu\text{g m}^{-3}$ (% of LV)
NO₂	1	200	50 (25 %)	150 (75 %)	400 (200 %)
O₃	8 ^a	120	36 (30 %)	90 (75 %)	240 (200 %)
CO	8 ^b	10 ^c	2.5 ^c (25 %)	7.5 ^c (75 %)	20 ^c (200 %)

^a For O₃, an averaging period of 1 h instead of 8 h shall be used for the evaluation of the sensor system at the limit value (LV) to do the classification.

^b For CO, an averaging period of 1 h instead of 8 h shall be used for the evaluation of the sensor system at the limit value (LV) to do the classification.

^c In mg m^{-3} .

Table S2. DQOs for indicative measurements and objective estimation set in the AQD 2008/50/EC and in CEN/TS 17660-2:2024 and class 3 set in CEN/TS 17660-2:2024.

Pollutant	Averaging Period	LV	DQO of Class 1 sensor system	DQO of Class 2 sensor system	DQO of Class 3 sensor system
	h	$\mu\text{g m}^{-3}$	$\mu\text{g m}^{-3}$ (% of LV)	$\mu\text{g m}^{-3}$ (% of LV)	$\mu\text{g m}^{-3}$ (% of LV)
PM_{2.5}	24	30 ^a	15 (50 %)	30 (100 %)	60 (200 %)

^a For PM_{2.5} a concentration of 30 $\mu\text{g m}^{-3}$ shall be used as a substitute value for the daily limit value (LV).

Table S3. Description of the employed calibration models.

Calibration Model	Description	Tuned Hyperparameters	R package	Reference
Extreme Gradient Boosting	- Decision tree-based ensemble machine learning method - employs the gradient boosting framework - Boosting is the concept of producing a strong learner from weak learners - predictions are created from weak learners that continuously develop over the mistakes of the former learners	nrounds eta max_depth lambda alpha	xgboost	Mienye, I. D., & Sun, Y. (2022). A Survey of Ensemble Learning: Concepts, Algorithms, Applications, and Prospects. IEEE Access, 10, 99129–99149. https://doi.org/10.1109/access.2022.3207287 Zounemat-Kermani, M., Batelaan, O., Fadaee, M., & Hinkelmann, R. (2021). Ensemble machine learning paradigms in hydrology: A review. Journal of Hydrology, 598, 126266. https://doi.org/10.1016/j.jhydrol.2021.126266
Random Forest	- tree-based ensemble machine learning method that uses decision trees as base-learners - employs the bagging technique to build multiple decision trees using bootstrapped samples - the bagging technique generates random samples with replacements from the input data and trains the decision trees from the samples - predictions are created from the trained decision trees	mtry sample.fraction min.node.size num.trees	ranger	Mienye, I. D., & Sun, Y. (2022). A Survey of Ensemble Learning: Concepts, Algorithms, Applications, and Prospects. IEEE Access, 10, 99129–99149. https://doi.org/10.1109/access.2022.3207287 Zounemat-Kermani, M., Batelaan, O., Fadaee, M., & Hinkelmann, R. (2021). Ensemble machine learning paradigms in hydrology: A review. Journal of Hydrology, 598, 126266. https://doi.org/10.1016/j.jhydrol.2021.126266
Multiple Linear Regression	- regression method, which models linear relationships using least squares estimation - linear combination of features (also called independent or explanatory variables), which are weighted by coefficients, to predict the target or dependent variable - Assumptions: - linear relationship between features and target - residuals are normally distributed and independent - constant variance of residuals (Homoscedastic) - no outlier - no or a lack of multicollinearity	—	stats	Uyanik, G. K., & Güler, N. (2013). A Study on Multiple Linear Regression Analysis. Procedia - Social and Behavioral Sciences, 106, 234–240. https://doi.org/10.1016/j.sbspro.2013.12.027 Wilks, D. S. (2011). Statistical methods in the atmospheric sciences (Vol. 100). Academic press.

Calibration Model	Description	Tuned Hyperparameters	R package	Reference
Ridge Regression	- linear least squares regression method augmented by L2 regularization to address the bias-variance trade-off - can be viewed as penalized regression - Multiple linear regression is the simple non-regularized case of ridge regression	s	glmnet	Wanishsakpong, W., & Notodiputro, K. A. (2024). Comparing the performance of Ridge Regression and Lasso techniques for modelling daily maximum temperatures in Utraradit Province of Thailand. <i>Modeling Earth Systems and Environment</i> , 10(4), 5703–5716. https://doi.org/10.1007/s40808-024-02087-z
				Nowack, P., Konstantinovskiy, L., Gardiner, H., & Cant, J. (2021). Machine learning calibration of low-cost NO2 and PM10 sensors: non-linear algorithms and their impact on site transferability. <i>Atmospheric Measurement Techniques</i> , 14(8), 5637–5655. https://doi.org/10.5194/amt-14-5637-2021
				Asilevi, P. J., Dzidzorm, E. N., Boakye, P., & Quansah, E. (2025). Nitrogen dioxide (NO2) Meteorology and predictability for air quality management using TROPOMI. <i>Npj Clean Air</i> , 1(1). https://doi.org/10.1038/s44407-024-00003-4

Table S4. Performances of LCS calibration models for NO₂ and CO for each AELCM box using hourly means. Results were observed on the NO₂ training dataset (11 January, 19:00:00–10 June 2022, 18:00:00) and NO₂ test dataset (10 June 2022, 19:00:00–10 January 2023, 13:00:00) as well as on the CO training dataset (11 January, 19:00:00–10 June 2022, 19:00:00) and CO test dataset (10 June 2022, 20:00:00–10 January 2023, 16:00:00).

Model target	Training R ²	Training MAE (ppb)	Training RMSE (ppb)	Test R ²	Test MAE (ppb)	Test RMSE (ppb)
NO ₂ (MLR, 009)	0.86	1.88	2.56	0.70	2.37	3.20
NO ₂ (MLR, 010)	0.86	1.99	2.62	0.71	2.84	3.63
NO ₂ (RR, 009)	0.79	2.84	3.76	0.64	2.57	3.32
NO ₂ (RR, 010)	0.78	2.82	3.71	0.63	2.83	3.55
NO ₂ (XGB, 009)	0.94	1.23	1.74	0.78	2.09	3.09
NO ₂ (XGB, 010)	0.91	1.69	2.51	0.76	2.01	2.84
NO ₂ (RF, 009)	0.99	0.57	0.82	0.79	1.89	2.70
NO ₂ (RF, 010)	0.92	1.42	2.02	0.75	2.33	3.09
CO (MLR, 009)	0.97	11.08	14.59	0.97	12.11	18.18
CO (MLR, 010)	0.97	12.56	15.93	0.96	14.80	21.85
CO (RR, 009)	0.94	14.80	22.04	0.93	18.81	28.62
CO (RR, 010)	0.93	16.30	23.52	0.89	23.04	35.16
CO (XGB, 009)	0.98	18.06	22.84	0.97	16.37	21.47
CO (XGB, 010)	0.99	24.73	28.52	0.96	25.66	33.72
CO (RF, 009)	1.00	3.62	5.36	0.96	16.01	25.17
CO (RF, 010)	0.99	4.48	6.50	0.97	13.94	19.88

Performance Metrics NO₂

Table S5. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.76/0.77		0.80/0.83		0.81/0.86		0.95/0.95	0.85/0.88
R ²	0.47/0.52		0.62/0.66		0.66/0.78		0.91/0.92	0.79/0.84
RMSE [ppb]	2.01/1.85		3.05/2.67		2.87/2.42		2.79/2.43	2.71/2.36
MAE [ppb]	1.30/1.29		2.06/1.83		2.19/1.82		2.20/1.77	1.94/1.68
Slope	0.53/0.62		0.58/0.62		0.81/0.72		0.90/0.83	0.89/0.80
Delta Slope	0.47/0.38		0.42/0.38		0.19/0.28		0.10/0.17	0.11/0.20
Intercept	1.10/1.31		0.83/1.24		1.40/1.28		2.52/2.05	0.54/0.93
Intercept	1.10/1.31		0.83/1.24		1.40/1.28		2.52/2.05	0.54/0.93
AELCM009								
Rs		0.77/0.81		0.87/0.88		0.86/0.92		0.87/0.89
R ²		0.54/0.60		0.81/0.84		0.79/0.86		0.76/0.80
RMSE [ppb]		3.67/3.00		2.36/2.07		2.89/2.36		3.02/2.51
MAE [ppb]		2.37/1.87		1.52/1.52		2.30/1.77		2.06/1.72
Slope		0.39/0.51		0.77/0.88		0.69/0.81		0.70/0.77
Delta Slope		0.61/0.49		0.23/0.12		0.31/0.19		0.30/0.23
Intercept		0.98/1.23		0.63/0.89		1.34/0.43		0.60/0.76
Intercept		0.98/1.23		0.63/0.89		1.34/0.43		0.60/0.76

Table S6. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.69/0.76		0.77/0.81		0.82/0.85		0.94/0.95	0.83/0.87
R ²	0.48/0.54		0.60/0.67		0.67/0.76		0.90/0.90	0.78/0.82
RMSE [ppb]	2.00/1.88		2.75/2.50		2.99/2.35		3.72/2.99	2.93/2.46
MAE [ppb]	1.45/1.38		1.88/1.74		2.32/1.84		3.14/2.44	2.20/1.85
Slope	0.64/0.66		0.67/0.66		0.86/0.78		0.87/0.82	0.91/0.84
Delta Slope	0.36/0.34		0.33/0.34		0.14/0.22		0.13/0.18	0.09/0.16
Intercept	1.66/1.66		1.72/1.70		1.70/1.59		3.93/3.23	1.51/1.50
Intercept	1.66/1.66		1.72/1.70		1.70/1.59		3.93/3.23	1.51/1.50
AELCM009								
Rs		0.71/0.79		0.86/0.88		0.87/0.91		0.86/0.89
R ²		0.46/0.55		0.81/0.85		0.79/0.85		0.75/0.79
RMSE [ppb]		3.32/2.94		2.24/2.03		2.47/2.27		2.72/2.44
MAE [ppb]		2.10/1.79		1.65/1.56		1.90/1.75		1.88/1.70
Slope		0.43/0.53		0.74/0.82		0.70/0.79		0.70/0.75
Delta Slope		0.57/0.47		0.26/0.18		0.30/0.21		0.30/0.25
Intercept		1.77/1.69		1.35/1.39		2.26/1.01		1.39/1.28
Intercept		1.77/1.69		1.35/1.39		2.26/1.01		1.39/1.28

Table S7. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.72/0.73		0.78/0.78		0.79/0.79		0.93/0.93	0.82/0.82
R ²	0.43/0.44		0.50/0.50		0.56/0.55		0.82/0.83	0.67/0.67
RMSE [ppb]	3.02/2.50		3.17/3.05		3.41/3.18		3.95/4.45	3.41/3.37
MAE [ppb]	2.43/2.01		2.41/2.30		2.56/2.45		3.37/3.74	2.69/2.63
Slope	1.01/0.78		0.64/0.49		0.69/0.52		0.64/0.49	0.76/0.58
Delta Slope	0.01/0.22		0.36/0.51		0.31/0.48		0.36/0.51	0.24/0.42
Intercept	0.20/1.54		1.89/2.86		3.45/4.17		4.84/5.30	2.22/3.16
Intercept	0.20/1.54		1.89/2.86		3.45/4.17		4.84/5.30	2.22/3.16
AELCM009								
Rs		0.72/0.74		0.83/0.81		0.81/0.81		0.84/0.84
R ²		0.36/0.37		0.71/0.69		0.62/0.62		0.59/0.58
RMSE [ppb]		4.16/3.66		2.95/3.39		3.09/3.23		3.44/3.43
MAE [ppb]		3.18/2.73		2.42/2.87		2.37/2.49		2.66/2.70
Slope		0.67/0.55		0.54/0.41		0.63/0.47		0.69/0.55
Delta Slope		0.33/0.45		0.46/0.59		0.37/0.53		0.31/0.45
Intercept		0.81/1.85		3.17/4.28		3.87/5.05		2.07/3.19
Intercept		0.81/1.85		3.17/4.28		3.87/5.05		2.07/3.19

Table S8. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.45/0.49		0.69/0.69		0.82/0.82		0.93/0.93	0.77/0.76
R ²	0.25/0.29		0.52/0.51		0.64/0.65		0.91/0.91	0.75/0.74
RMSE [ppb]	3.16/2.80		3.02/3.11		3.23/2.95		4.60/3.67	3.56/3.15
MAE [ppb]	2.46/2.23		2.28/2.39		2.35/2.18		3.97/3.08	2.77/2.47
Slope	0.61/0.64		0.59/0.58		0.88/0.79		1.02/0.92	0.98/0.90
Delta Slope	0.39/0.36		0.41/0.42		0.12/0.21		0.02/0.08	0.02/0.10
Intercept	2.44/1.53		2.47/1.84		1.48/1.19		3.57/3.57	1.56/1.15
Intercept	2.44/1.53		2.47/1.84		1.48/1.19		3.57/3.57	1.56/1.15
AELCM009								
Rs		0.43/0.55		0.84/0.81		0.87/0.88		0.78/0.81
R ²		0.20/0.30		0.77/0.76		0.73/0.75		0.63/0.68
RMSE [ppb]		4.09/3.66		2.67/2.53		3.05/2.61		3.32/2.98
MAE [ppb]		3.02/2.65		1.96/1.94		2.29/1.93		2.42/2.17
Slope		0.35/0.40		0.74/0.70		0.95/0.84		0.74/0.71
Delta Slope		0.65/0.60		0.26/0.30		0.05/0.16		0.26/0.29
Intercept		3.50/3.22		0.44/1.64		-0.29/1.19		1.26/1.92
Intercept		3.50/3.22		0.44/1.64		0.29/1.19		1.26/1.92

Table S9. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.76/0.76	0.76/0.77			0.81/0.84	0.88/0.84		0.86/0.87
R ²	0.47/0.50	0.46/0.55			0.66/0.73	0.76/0.74		0.70/0.74
RMSE [ppb]	2.01/1.91	3.55/3.07			2.87/2.55	3.04/2.57		2.92/2.56
MAE [ppb]	1.30/1.29	2.25/1.94			2.19/1.93	2.44/1.97		2.04/1.78
Slope	0.53/0.60	0.42/0.51			0.81/0.73	0.87/0.77		0.88/0.78
Delta Slope	0.47/0.40	0.58/0.49			0.19/0.27	0.13/0.23		0.12/0.22
Intercept	1.10/1.22	1.25/1.37			1.40/1.45	2.95/2.47		0.62/1.02
Intercept	1.10/1.22	1.25/1.37			1.40/1.45	2.95/2.47		0.62/1.02
AELCM009								
Rs			0.81/0.84	0.87/0.87			0.95/0.95	0.88/0.89
R ²			0.64/0.71	0.81/0.82			0.91/0.91	0.83/0.85
RMSE [ppb]			3.58/2.63	2.36/2.20			3.35/2.80	3.14/2.55
MAE [ppb]			2.47/1.79	1.52/1.65			2.36/2.10	2.12/1.85
Slope			0.43/0.57	0.77/0.84			0.70/0.75	0.70/0.76
Delta Slope			0.57/0.43	0.23/0.16			0.30/0.25	0.30/0.24
Intercept			0.96/1.38	0.63/1.25			1.17/1.74	0.58/1.25
Intercept			0.96/1.38	0.63/1.25			1.17/1.74	0.58/1.25

Table S10. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.69/0.72	0.69/0.73			0.82/0.84	0.85/0.85		0.84/0.86
R ²	0.48/0.50	0.43/0.47			0.67/0.72	0.73/0.74		0.70/0.72
RMSE [ppb]	2.00/2.00	3.30/3.15			2.99/2.54	3.95/2.89		3.14/2.68
MAE [ppb]	1.45/1.46	2.21/2.08			2.32/1.98	3.35/2.26		2.33/1.95
Slope	0.64/0.66	0.52/0.55			0.86/0.79	0.86/0.82		0.91/0.82
Delta Slope	0.36/0.34	0.48/0.45			0.14/0.21	0.14/0.18		0.09/0.18
Intercept	1.66/1.68	2.49/2.35			1.70/1.57	4.24/2.97		1.59/1.60
Intercept	1.66/1.68	2.49/2.35			1.70/1.57	4.24/2.97		1.59/1.60
AELCM009								
Rs			0.80/0.83	0.86/0.85			0.95/0.95	0.86/0.88
R ²			0.61/0.69	0.81/0.81			0.93/0.93	0.84/0.85
RMSE [ppb]			3.19/2.51	2.24/2.34			2.68/2.59	2.73/2.48
MAE [ppb]			2.15/1.75	1.65/1.87			1.96/1.98	1.92/1.87
Slope			0.49/0.60	0.74/0.79			0.74/0.75	0.73/0.75
Delta Slope			0.51/0.40	0.26/0.21			0.26/0.25	0.27/0.25
Intercept			1.24/1.60	1.35/2.02			1.78/2.24	1.07/1.73
Intercept			1.24/1.60	1.35/2.02			1.78/2.24	1.07/1.73

Table S11. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.72/0.73	0.72/0.73			0.79/0.78	0.79/0.79		0.83/0.84
R ²	0.43/0.44	0.37/0.37			0.56/0.55	0.59/0.59		0.59/0.59
RMSE [ppb]	3.02/2.67	4.25/3.91			3.41/3.20	3.63/3.35		3.60/3.31
MAE [ppb]	2.43/2.13	3.34/3.00			2.56/2.44	2.90/2.68		2.81/2.56
Slope	1.01/0.89	0.72/0.63			0.69/0.60	0.64/0.55		0.85/0.75
Delta Slope	0.01/0.11	0.28/0.37			0.31/0.40	0.36/0.45		0.15/0.25
Intercept	0.20/0.64	0.94/1.25			3.45/3.64	5.25/5.37		1.58/1.89
Intercept	0.20/0.64	0.94/1.25			3.45/3.64	5.25/5.37		1.58/1.89
AELCM009								
Rs			0.75/0.77	0.83/0.82			0.94/0.94	0.85/0.84
R ²			0.47/0.47	0.71/0.69			0.84/0.85	0.74/0.73
RMSE [ppb]			3.27/3.17	2.95/3.57			3.66/4.78	3.31/3.90
MAE [ppb]			2.52/2.41	2.42/3.01			2.89/3.87	2.61/3.10
Slope			0.57/0.40	0.54/0.36			0.63/0.43	0.63/0.44
Delta Slope			0.43/0.60	0.46/0.64			0.37/0.57	0.37/0.56
Intercept			1.76/3.38	3.17/4.65			3.31/4.83	2.45/4.05
Intercept			1.76/3.38	3.17/4.65			3.31/4.83	2.45/4.05

Table S12. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.45/0.47	0.50/0.52			0.82/0.83	0.85/0.85		0.77/0.77
R ²	0.25/0.26	0.26/0.27			0.64/0.63	0.71/0.70		0.62/0.62
RMSE [ppb]	3.16/2.93	4.16/4.03			3.23/3.11	4.14/3.38		3.70/3.39
MAE [ppb]	2.46/2.30	3.25/3.11			2.35/2.24	3.40/2.61		2.87/2.57
Slope	0.61/0.62	0.46/0.46			0.88/0.83	0.89/0.84		0.87/0.82
Delta Slope	0.39/0.38	0.54/0.54			0.12/0.17	0.11/0.16		0.13/0.18
Intercept	2.44/1.94	3.79/3.24			1.48/1.10	4.05/3.39		2.26/1.85
Intercept	2.44/1.94	3.79/3.24			1.48/1.10	4.05/3.39		2.26/1.85
AELCM009								
Rs			0.64/0.73	0.84/0.80			0.94/0.94	0.84/0.85
R ²			0.48/0.54	0.77/0.75			0.91/0.92	0.81/0.82
RMSE [ppb]			3.33/3.02	2.67/2.55			2.64/2.29	2.90/2.64
MAE [ppb]			2.51/2.21	1.96/1.98			1.93/1.73	2.13/1.97
Slope			0.47/0.53	0.74/0.69			1.02/0.91	0.88/0.82
Delta Slope			0.53/0.47	0.26/0.31			0.02/0.09	0.12/0.18
Intercept			1.72/1.84	0.44/1.70			-0.66/0.95	-0.11/0.98
Intercept			1.72/1.84	0.44/1.70			0.66/0.95	0.11/0.98

Table S13. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.76/0.76	0.76/0.78	0.80/0.81				0.95/0.96	0.80/0.83
R ²	0.47/0.49	0.46/0.53	0.62/0.64				0.91/0.92	0.75/0.79
RMSE [ppb]	2.01/1.94	3.55/3.15	3.05/2.73				2.79/2.41	2.91/2.60
MAE [ppb]	1.30/1.30	2.25/2.00	2.06/1.87				2.20/1.77	1.95/1.74
Slope	0.53/0.61	0.42/0.53	0.58/0.66				0.90/0.83	0.85/0.81
Delta Slope	0.47/0.39	0.58/0.47	0.42/0.34				0.10/0.17	0.15/0.19
Intercept	1.10/1.14	1.25/1.23	0.83/0.99				2.52/2.10	0.35/0.69
Intercept	1.10/1.14	1.25/1.23	0.83/0.99				2.52/2.10	0.35/0.69
AELCM009								
Rs				0.87/0.88	0.78/0.85	0.86/0.89		0.88/0.90
R ²				0.81/0.83	0.61/0.73	0.79/0.81		0.76/0.81
RMSE [ppb]				2.36/2.11	3.30/2.44	2.89/2.32		2.88/2.30
MAE [ppb]				1.52/1.55	2.30/1.84	2.30/1.79		2.04/1.72
Slope				0.77/0.85	0.60/0.74	0.69/0.79		0.70/0.79
Delta Slope				0.23/0.15	0.40/0.26	0.31/0.21		0.30/0.21
Intercept				0.63/1.04	1.75/1.95	1.34/1.25		1.10/1.37
Intercept				0.63/1.04	1.75/1.95	1.34/1.25		1.10/1.37

Table S14. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.69/0.71	0.69/0.72	0.77/0.79				0.94/0.95	0.77/0.80
R ²	0.48/0.49	0.43/0.46	0.60/0.62				0.90/0.91	0.75/0.77
RMSE [ppb]	2.00/2.10	3.30/3.25	2.75/2.69				3.72/2.98	3.01/2.79
MAE [ppb]	1.45/1.54	2.21/2.20	1.88/1.89				3.14/2.46	2.17/2.02
Slope	0.64/0.69	0.52/0.58	0.67/0.70				0.87/0.83	0.87/0.82
Delta Slope	0.36/0.31	0.48/0.42	0.33/0.30				0.13/0.17	0.13/0.18
Intercept	1.66/1.74	2.49/2.51	1.72/1.75				3.93/3.24	1.54/1.73
Intercept	1.66/1.74	2.49/2.51	1.72/1.75				3.93/3.24	1.54/1.73
AELCM009								
Rs				0.86/0.88	0.81/0.86	0.87/0.89		0.89/0.90
R ²				0.81/0.83	0.68/0.75	0.79/0.81		0.78/0.81
RMSE [ppb]				2.24/2.14	2.78/2.38	2.47/2.23		2.51/2.25
MAE [ppb]				1.65/1.63	2.09/1.82	1.90/1.73		1.88/1.73
Slope				0.74/0.80	0.69/0.75	0.70/0.79		0.72/0.78
Delta Slope				0.26/0.20	0.31/0.25	0.30/0.21		0.28/0.22
Intercept				1.35/1.46	1.75/1.96	2.26/1.62		1.63/1.64
Intercept				1.35/1.46	1.75/1.96	2.26/1.62		1.63/1.64

Table S15. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.72/0.72	0.72/0.72	0.78/0.77				0.93/0.93	0.78/0.77
R ²	0.43/0.43	0.37/0.37	0.50/0.49				0.82/0.85	0.62/0.60
RMSE [ppb]	3.02/2.75	4.25/3.90	3.17/3.12				3.95/4.31	3.63/3.57
MAE [ppb]	2.43/2.21	3.34/3.01	2.41/2.35				3.37/3.65	2.89/2.80
Slope	1.01/0.90	0.72/0.63	0.64/0.56				0.64/0.50	0.77/0.65
Delta Slope	0.01/0.10	0.28/0.37	0.36/0.44				0.36/0.50	0.23/0.35
Intercept	0.20/0.60	0.94/1.29	1.89/2.28				4.84/5.34	1.65/2.12
Intercept	0.20/0.60	0.94/1.29	1.89/2.28				4.84/5.34	1.65/2.12
AELCM009								
Rs				0.83/0.83	0.80/0.78	0.81/0.79		0.86/0.85
R ²				0.71/0.69	0.59/0.56	0.62/0.59		0.66/0.63
RMSE [ppb]				2.95/3.45	3.09/3.17	3.09/3.29		3.04/3.30
MAE [ppb]				2.42/2.91	2.30/2.44	2.37/2.55		2.36/2.63
Slope				0.54/0.40	0.69/0.52	0.63/0.49		0.65/0.50
Delta Slope				0.46/0.60	0.31/0.48	0.37/0.51		0.35/0.50
Intercept				3.17/4.40	2.61/4.13	3.87/5.13		3.05/4.38
Intercept				3.17/4.40	2.61/4.13	3.87/5.13		3.05/4.38

Table S16. Performance metrics of the single NO₂ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.45/0.38	0.50/0.43	0.69/0.62				0.93/0.93	0.67/0.63
R ²	0.25/0.21	0.26/0.21	0.52/0.44				0.91/0.91	0.70/0.66
RMSE [ppb]	3.16/3.38	4.16/4.54	3.02/3.38				4.60/3.73	3.80/3.79
MAE [ppb]	2.46/2.70	3.25/3.65	2.28/2.62				3.97/3.16	2.99/3.03
Slope	0.61/0.58	0.46/0.42	0.59/0.57				1.02/0.91	0.93/0.84
Delta Slope	0.39/0.42	0.54/0.58	0.41/0.43				0.02/0.09	0.07/0.16
Intercept	2.44/2.64	3.79/4.31	2.47/2.88				3.57/3.75	1.93/2.45
Intercept	2.44/2.64	3.79/4.31	2.47/2.88				3.57/3.75	1.93/2.45
AELCM009								
Rs				0.84/0.82	0.83/0.82	0.87/0.87		0.88/0.87
R ²				0.77/0.75	0.65/0.65	0.73/0.73		0.73/0.73
RMSE [ppb]				2.67/2.55	3.45/3.10	3.05/2.71		3.07/2.80
MAE [ppb]				1.96/1.94	2.63/2.30	2.29/2.01		2.29/2.08
Slope				0.74/0.70	0.91/0.84	0.95/0.85		0.88/0.82
Delta Slope				0.26/0.30	0.09/0.16	0.05/0.15		0.12/0.18
Intercept				0.44/1.53	-0.56/0.58	-0.29/1.34		-0.13/1.10
Intercept				0.44/1.53	0.56/0.58	0.29/1.34		0.13/1.10

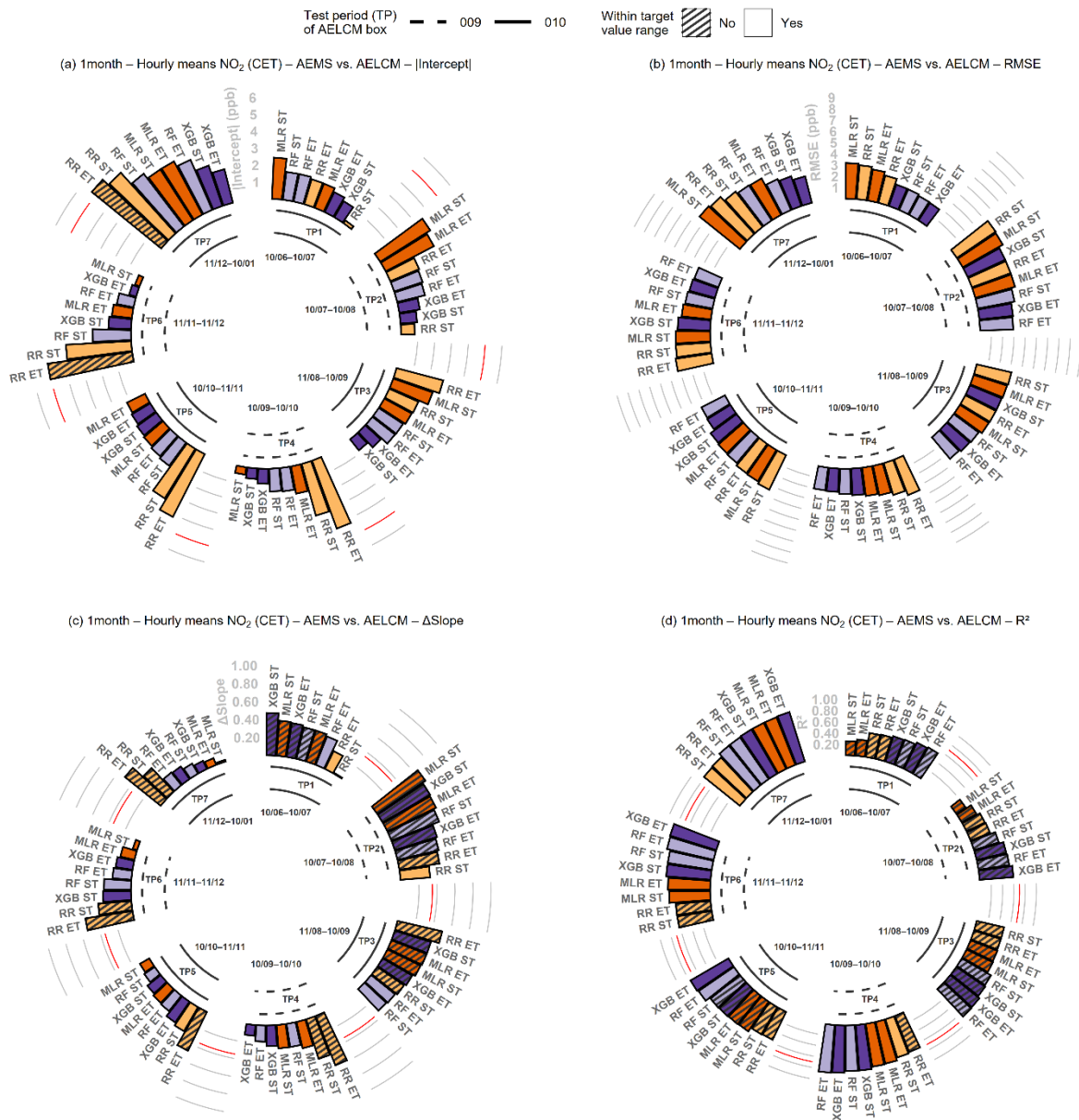


Figure S5. Performance metrics of the single NO₂ LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the one-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric (|Intercept| (a), RMSE (b), Δ Slope (c), R² (d)).

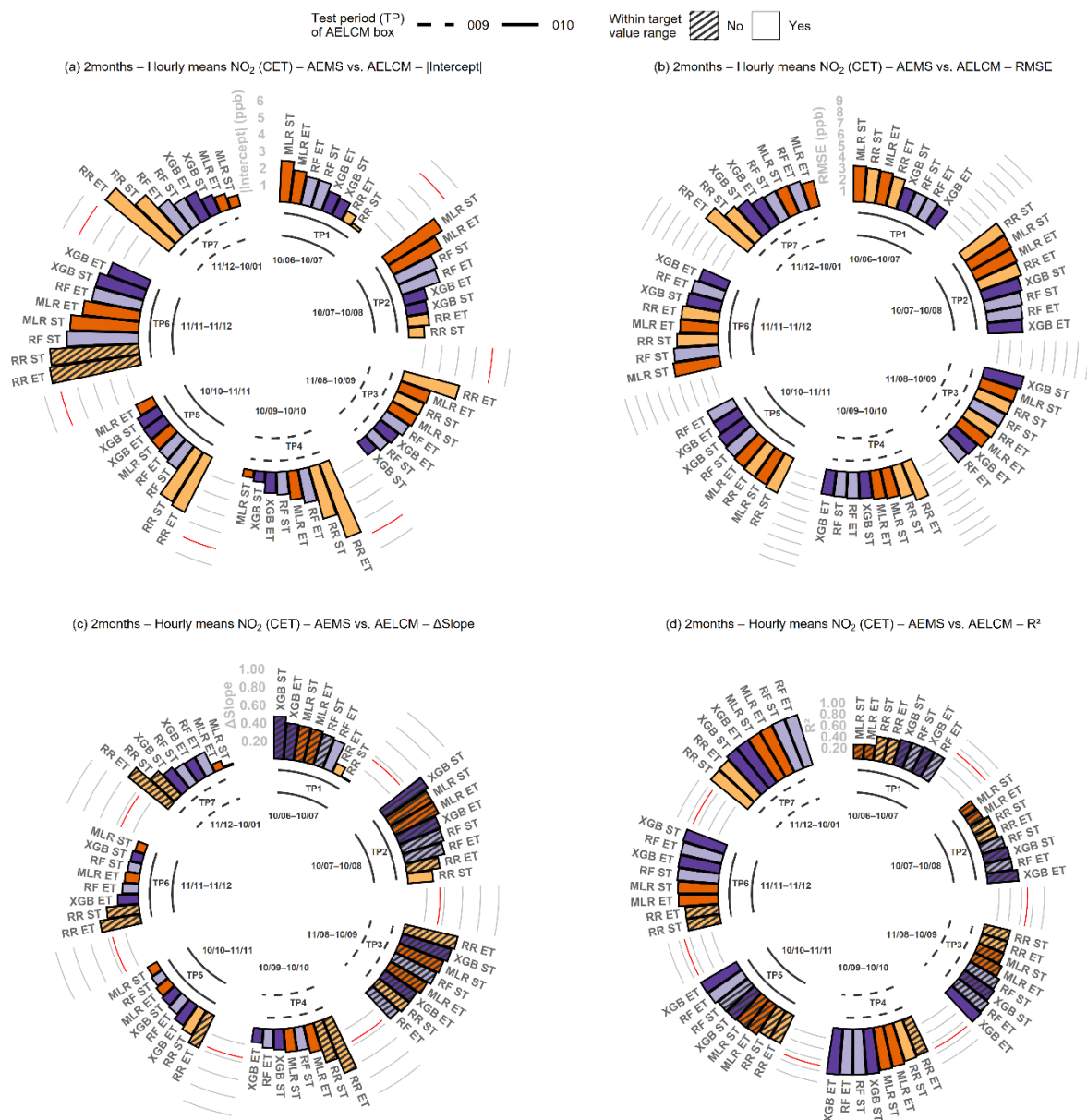


Figure S6. Performance metrics of the single NO₂ LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the two-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric (|Intercept| (a), RMSE (b), ΔSlope (c), R² (d)).

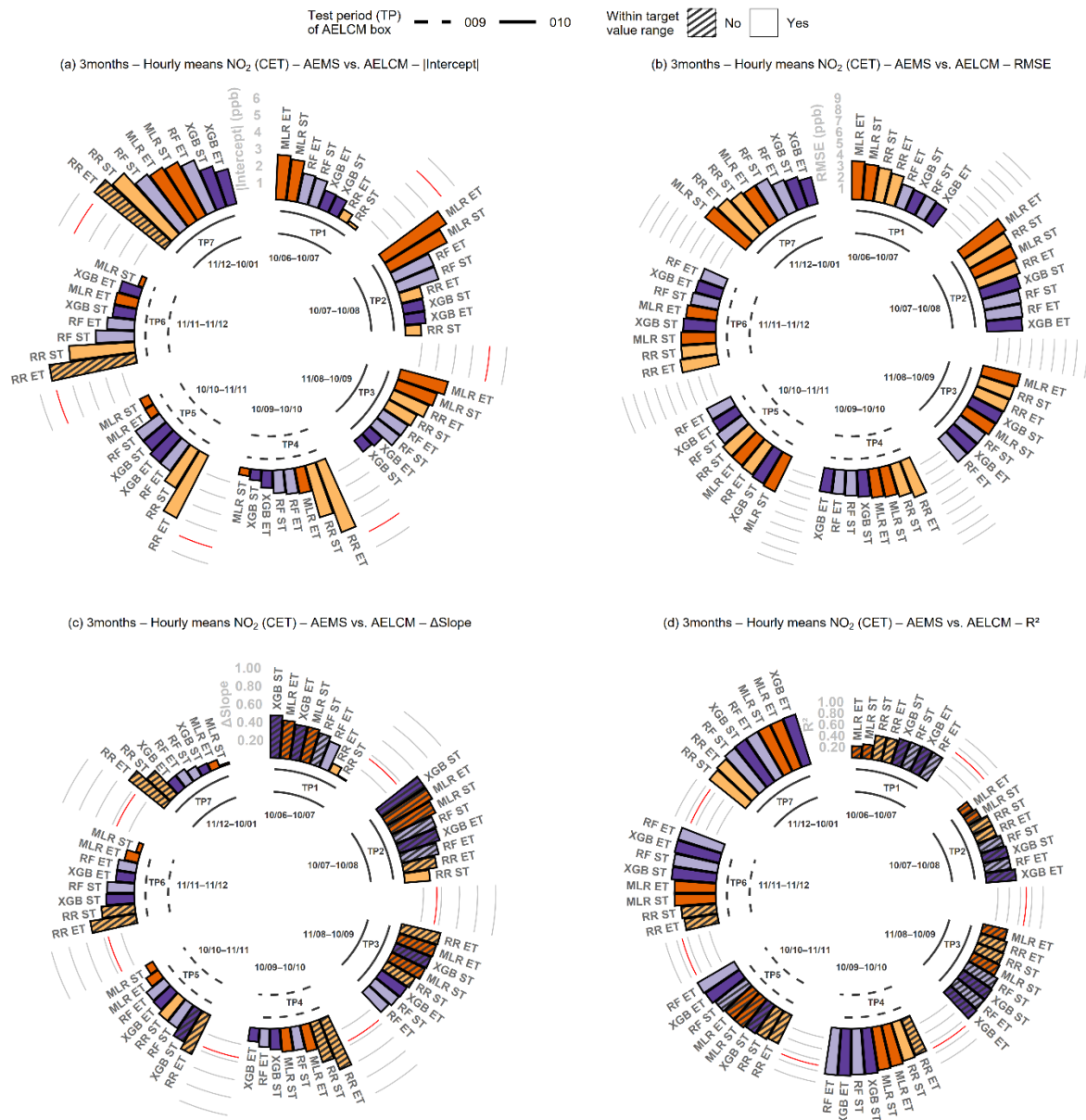


Figure S7. Performance metrics of the single NO₂ LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the three-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric (|Intercept| (a), RMSE (b), ΔSlope (c), R² (d)).

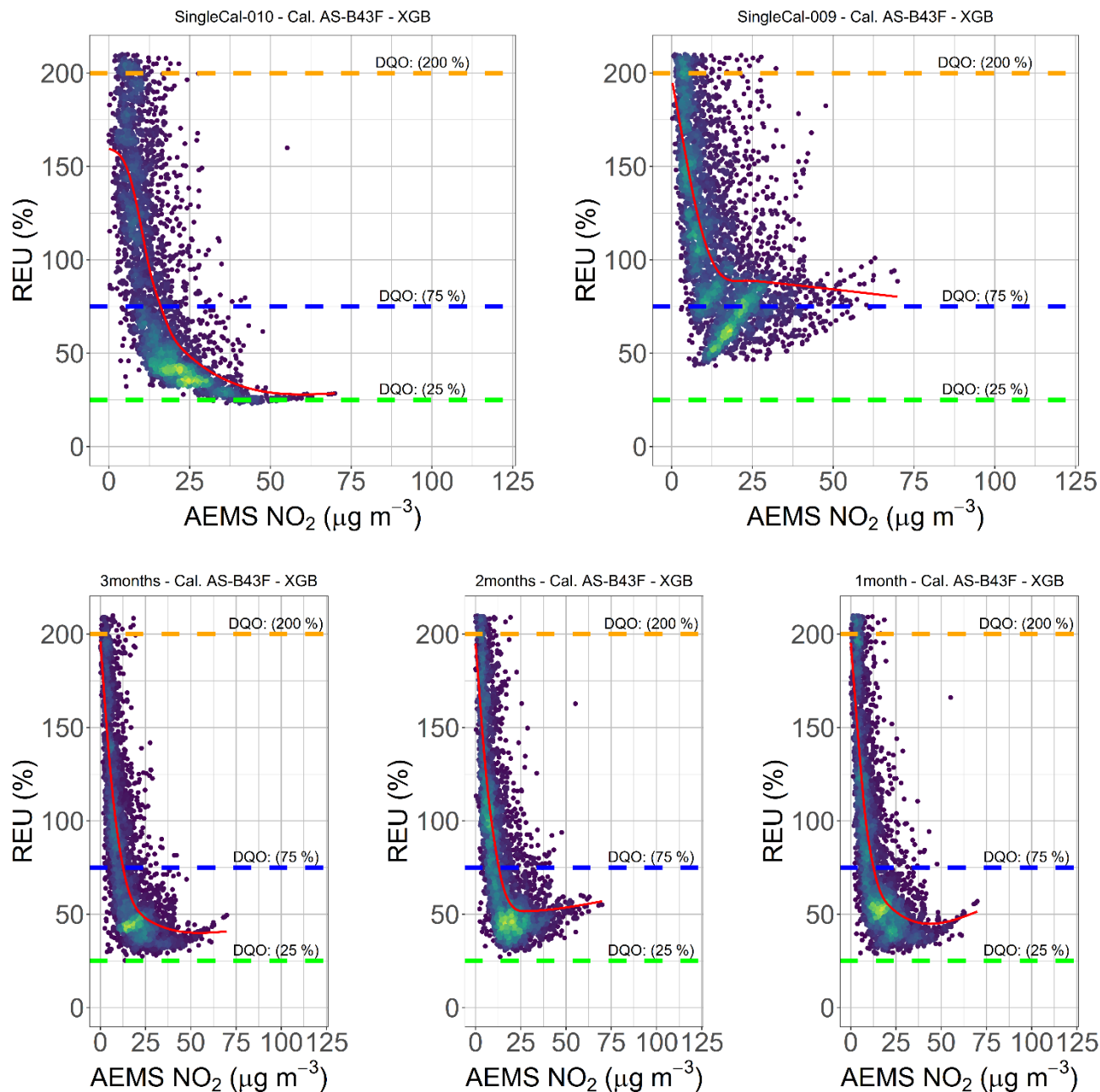


Figure S8. Calculated REU values for XGB calibrated NO₂ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (NO₂ Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

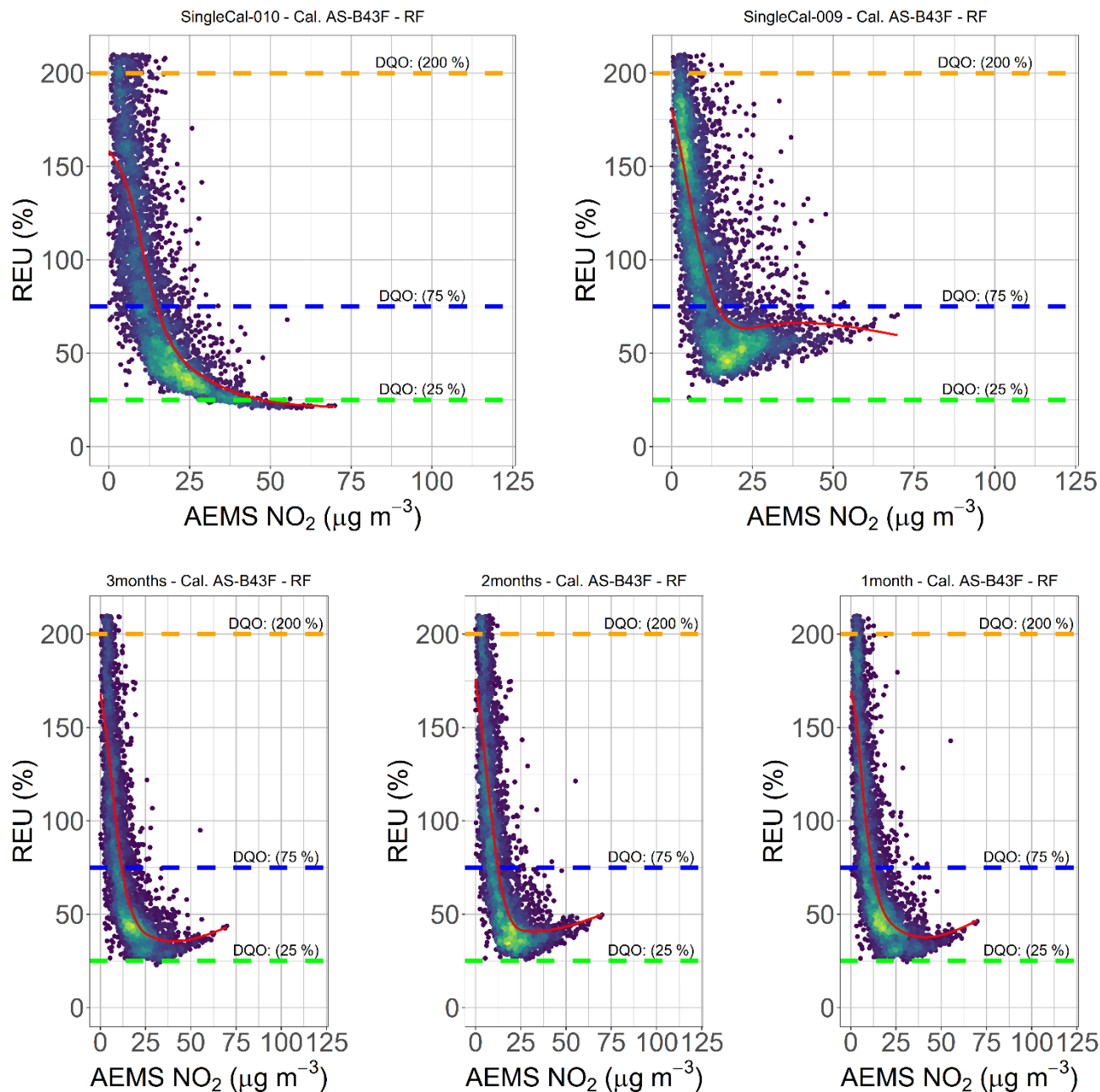


Figure S9. Calculated REU values for RF calibrated NO₂ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (NO₂ Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

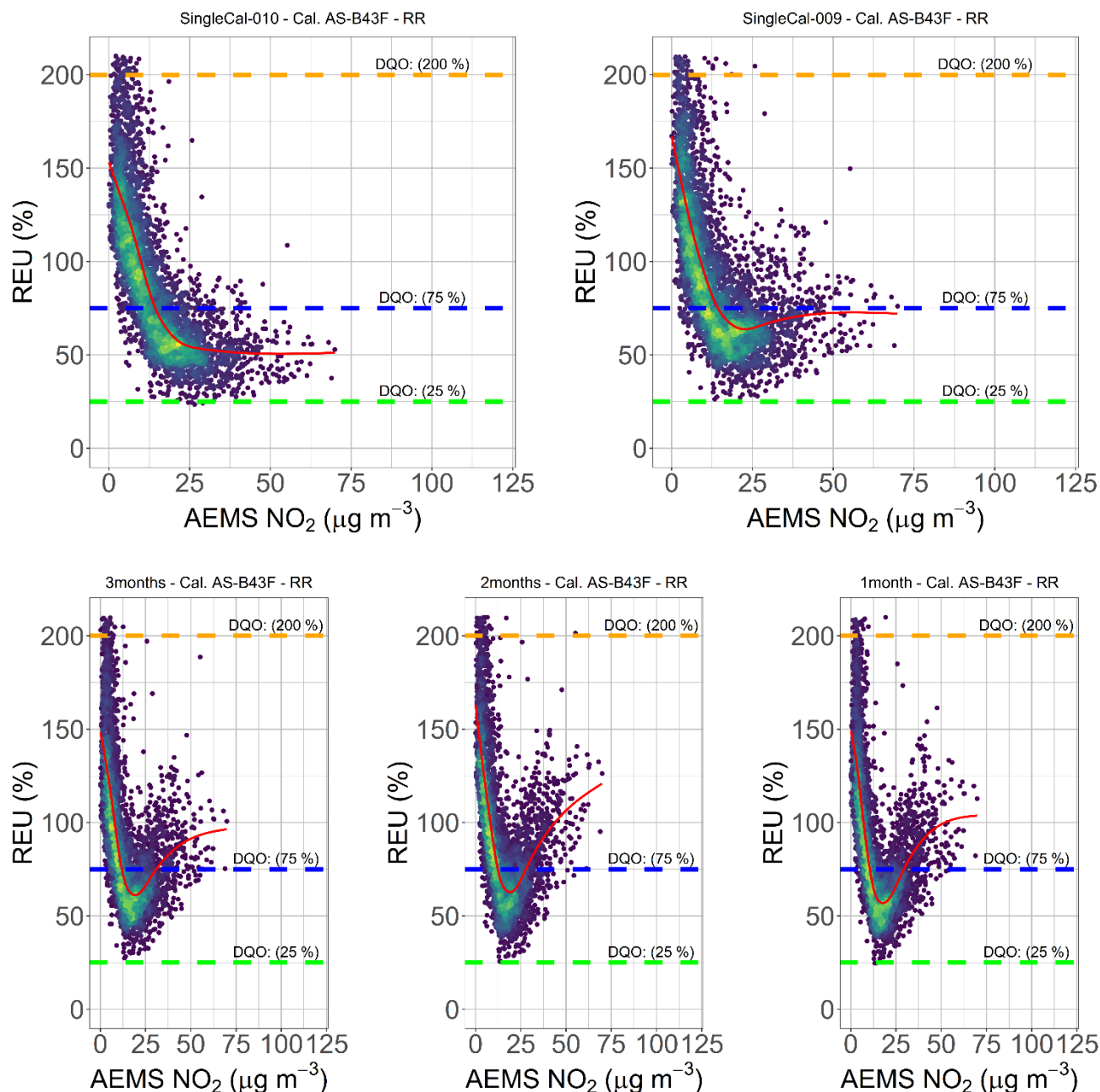


Figure S10. Calculated REU values for RR calibrated NO₂ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (NO₂ Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

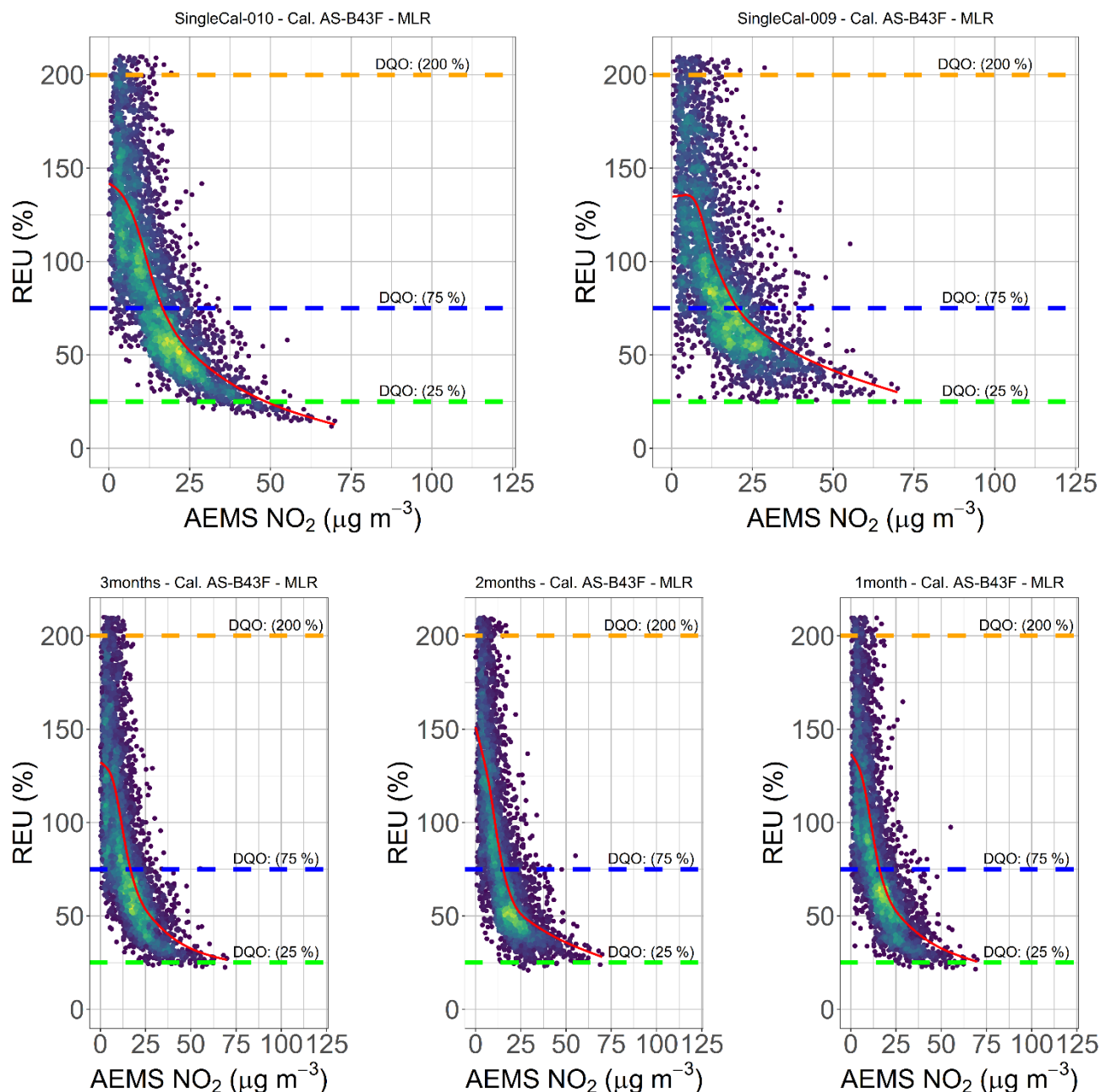


Figure S11. Calculated REU values for MLR calibrated NO₂ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (NO₂ Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

Performance Metrics CO

Table S17. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.73		0.72/0.76		0.98/0.98		0.99/0.99	0.89/0.91
R ²	0.48/0.58		0.61/0.70		0.95/0.97		0.98/0.99	0.96/0.97
RMSE [ppb]	16.09/13.85		26.76/24.42		37.40/30.76		43.64/42.49	32.70/29.75
MAE [ppb]	12.45/10.88		21.54/20.06		30.14/25.51		34.23/34.71	24.59/22.79
Slope	0.65/0.65		0.59/0.66		0.89/0.92		0.85/0.86	0.84/0.86
Delta Slope	0.35/0.35		0.41/0.34		0.11/0.08		0.15/0.14	0.16/0.14
Intercept	33.14/33.42		32.79/25.05		-6.88/-9.36		2.08/-0.68	4.34/3.46
Intercept	33.14/33.42		32.79/25.05		6.88/9.36		2.08/0.68	4.34/3.46
AELCM009								
Rs		0.66/0.72		0.92/0.96		1.00/1.00		0.93/0.95
R ²		0.47/0.61		0.95/0.97		0.99/0.99		0.97/0.98
RMSE [ppb]		22.47/20.61		18.55/18.50		23.97/30.40		21.78/23.74
MAE [ppb]		16.80/15.77		13.56/13.53		20.69/25.73		17.02/18.34
Slope		0.49/0.61		0.90/0.86		0.97/0.89		0.93/0.88
Delta Slope		0.51/0.39		0.10/0.14		0.03/0.11		0.07/0.12
Intercept		52.66/37.26		4.06/9.50		-11.28/5.23		-1.19/5.53
Intercept		52.66/37.26		4.06/9.50		11.28/5.23		1.19/5.53

Table S18. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.68/0.74		0.72/0.78		0.98/0.98		0.99/0.99	0.89/0.91
R ²	0.52/0.60		0.62/0.73		0.97/0.98		0.99/0.99	0.97/0.98
RMSE [ppb]	19.77/17.06		18.02/15.11		18.30/15.01		16.97/15.77	18.29/15.76
MAE [ppb]	14.84/13.47		13.65/11.56		13.29/10.88		10.43/10.55	13.05/11.61
Slope	0.82/0.76		0.69/0.76		0.97/1.01		0.97/0.99	0.95/0.97
Delta Slope	0.18/0.24		0.31/0.24		0.03/0.01		0.03/0.01	0.05/0.03
Intercept	32.48/37.08		38.24/28.18		3.31/-1.60		6.05/-1.31	9.98/5.70
Intercept	32.48/37.08		38.24/28.18		3.31/1.60		6.05/1.31	9.98/5.70
AELCM009								
Rs		0.65/0.73		0.93/0.96		0.98/1.00		0.93/0.95
R ²		0.48/0.61		0.93/0.95		0.97/0.99		0.96/0.98
RMSE [ppb]		21.44/17.82		17.84/15.57		28.66/11.74		23.09/15.25
MAE [ppb]		16.60/13.79		10.90/7.79		18.79/8.31		15.43/9.96
Slope		0.64/0.69		0.96/0.91		1.07/0.96		1.05/0.95
Delta Slope		0.36/0.31		0.04/0.09		0.07/0.04		0.05/0.05
Intercept		47.65/38.28		7.83/13.43		-6.99/6.26		-2.91/7.19
Intercept		47.65/38.28		7.83/13.43		6.99/6.26		2.91/7.19

Table S19. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.67		0.78/0.78		0.99/0.99		0.99/0.99	0.90/0.90
R ²	0.50/0.50		0.60/0.61		0.99/0.99		0.99/0.99	0.91/0.91
RMSE [ppb]	40.22/39.59		34.90/33.44		12.83/15.43		31.67/35.43	31.64/32.32
MAE [ppb]	32.27/32.46		25.45/24.85		9.09/11.51		17.00/18.81	20.95/21.91
Slope	1.84/1.77		1.41/1.35		0.92/0.89		0.83/0.80	0.89/0.85
Delta Slope	0.84/0.77		0.41/0.35		0.08/0.11		0.17/0.20	0.11/0.15
Intercept	-84.96/-73.30		-52.20/-41.62		18.05/26.71		26.38/34.49	18.51/26.86
Intercept	84.96/73.30		52.20/41.62		18.05/26.71		26.38/34.49	18.51/26.86
AELCM009								
Rs		0.67/0.67		0.98/0.98		1.00/1.00		0.93/0.93
R ²		0.45/0.46		0.96/0.96		0.99/0.99		0.91/0.91
RMSE [ppb]		46.09/44.23		12.64/13.37		24.89/27.58		31.11/31.07
MAE [ppb]		36.06/35.02		6.85/7.83		16.50/18.27		19.80/20.38
Slope		1.44/1.40		0.95/0.92		0.85/0.82		0.90/0.87
Delta Slope		0.44/0.40		0.05/0.08		0.15/0.18		0.10/0.13
Intercept		-58.74/-49.92		9.49/15.90		26.51/31.88		12.23/18.93
Intercept		58.74/49.92		9.49/15.90		26.51/31.88		12.23/18.93

Table S20. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.65/0.66		0.77/0.78		0.99/0.99		0.99/0.99	0.90/0.91
R ²	0.54/0.56		0.68/0.70		0.98/0.99		0.98/0.99	0.97/0.97
RMSE [ppb]	20.04/20.53		16.64/16.56		23.18/15.92		19.57/19.95	19.99/18.35
MAE [ppb]	16.22/16.75		12.86/12.83		15.16/11.40		12.49/11.81	14.18/13.20
Slope	0.90/0.98		0.79/0.85		0.82/0.89		0.99/1.05	0.92/0.98
Delta Slope	0.10/0.02		0.21/0.15		0.18/0.11		0.01/0.05	0.08/0.02
Intercept	22.63/13.76		27.72/20.55		27.03/18.01		-1.97/-12.39	13.46/6.09
Intercept	22.63/13.76		27.72/20.55		27.03/18.01		1.97/12.39	13.46/6.09
AELCM009								
Rs		0.63/0.66		0.98/0.99		1.00/1.00		0.94/0.94
R ²		0.50/0.52		0.91/0.93		0.99/0.99		0.97/0.97
RMSE [ppb]		21.45/22.53		21.78/18.05		17.68/13.40		20.39/18.37
MAE [ppb]		17.16/18.17		7.38/6.08		12.37/9.89		12.30/11.38
Slope		0.70/0.82		0.80/0.84		0.94/0.96		0.91/0.93
Delta Slope		0.30/0.18		0.20/0.16		0.06/0.04		0.09/0.07
Intercept		34.74/22.65		26.25/23.75		5.48/0.88		10.14/9.08
Intercept		34.74/22.65		26.25/23.75		5.48/0.88		10.14/9.08

Table S21. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.74	0.57/0.66			0.98/0.99	0.99/0.99		0.90/0.92
R ²	0.48/0.62	0.36/0.47			0.95/0.98	0.98/0.99		0.95/0.97
RMSE [ppb]	16.09/13.25	25.92/23.00			37.40/31.82	47.78/45.91		33.96/30.92
MAE [ppb]	12.45/10.49	19.16/17.03			30.14/26.30	41.55/40.76		25.83/23.65
Slope	0.65/0.77	0.49/0.62			0.89/0.87	0.85/0.85		0.83/0.82
Delta Slope	0.35/0.23	0.51/0.38			0.11/0.13	0.15/0.15		0.17/0.18
Intercept	33.14/21.59	50.13/38.49			-6.88/-0.61	-1.36/-0.77		8.53/11.70
Intercept	33.14/21.59	50.13/38.49			6.88/0.61	1.36/0.77		8.53/11.70
AELCM009								
Rs			0.79/0.85	0.92/0.96			0.99/0.99	0.93/0.96
R ²			0.72/0.82	0.95/0.96			0.99/0.99	0.98/0.98
RMSE [ppb]			22.01/20.41	18.55/20.21			24.22/31.43	21.72/24.58
MAE [ppb]			17.72/17.02	13.56/14.22			19.33/24.27	16.87/18.51
Slope			0.63/0.71	0.90/0.87			0.96/0.90	0.95/0.90
Delta Slope			0.37/0.29	0.10/0.13			0.04/0.10	0.05/0.10
Intercept			31.73/20.74	4.06/6.32			-8.20/0.12	-5.45/0.21
Intercept			31.73/20.74	4.06/6.32			8.20/0.12	5.45/0.21

Table S22. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.68/0.73	0.57/0.66			0.98/0.99	0.99/0.99		0.90/0.92
R ²	0.52/0.57	0.39/0.44			0.97/0.98	0.98/0.99		0.96/0.96
RMSE [ppb]	19.77/21.14	26.39/28.06			18.30/13.25	18.96/16.12		21.11/20.43
MAE [ppb]	14.84/15.61	20.04/19.46			13.29/9.47	12.67/11.11		15.21/13.91
Slope	0.82/0.95	0.64/0.79			0.97/0.98	0.93/0.95		0.91/0.92
Delta Slope	0.18/0.05	0.36/0.21			0.03/0.02	0.07/0.05		0.09/0.08
Intercept	32.48/19.82	52.92/36.99			3.31/3.39	12.41/6.53		18.56/18.05
Intercept	32.48/19.82	52.92/36.99			3.31/3.39	12.41/6.53		18.56/18.05
AELCM009								
Rs			0.78/0.83	0.93/0.97			0.99/0.99	0.93/0.96
R ²			0.73/0.81	0.93/0.94			0.97/0.99	0.96/0.98
RMSE [ppb]			15.80/13.57	17.84/16.74			43.65/15.47	28.71/15.32
MAE [ppb]			12.26/10.25	10.90/7.43			28.53/10.67	17.23/9.45
Slope			0.75/0.82	0.96/0.92			1.13/1.00	1.13/0.99
Delta Slope			0.25/0.18	0.04/0.08			0.13/0.00	0.13/0.01
Intercept			26.29/17.81	7.83/9.14			-8.66/-2.65	-15.12/-1.76
Intercept			26.29/17.81	7.83/9.14			8.66/2.65	15.12/1.76

Table S23. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.67	0.63/0.63			0.99/0.99	1.00/1.00		0.89/0.89
R ²	0.50/0.51	0.37/0.38			0.99/0.99	0.99/0.99		0.86/0.85
RMSE [ppb]	40.22/40.77	59.93/60.17			12.83/13.43	29.40/28.21		39.49/39.56
MAE [ppb]	32.27/32.92	47.63/48.17			9.09/10.10	21.05/20.07		27.51/27.81
Slope	1.84/1.85	1.59/1.59			0.92/0.93	0.83/0.83		0.88/0.88
Delta Slope	0.84/0.85	0.59/0.59			0.08/0.07	0.17/0.17		0.12/0.12
Intercept	-84.96/-83.17	-66.93/-64.70			18.05/19.68	27.04/27.12		19.94/22.62
Intercept	84.96/83.17	66.93/64.70			18.05/19.68	27.04/27.12		19.94/22.62
AELCM009								
Rs			0.82/0.82	0.98/0.99			1.00/1.00	0.95/0.95
R ²			0.70/0.70	0.96/0.96			0.99/0.99	0.96/0.96
RMSE [ppb]			27.92/25.02	12.64/13.97			29.38/35.14	24.51/26.18
MAE [ppb]			20.09/18.17	6.85/8.46			15.74/18.30	14.23/14.97
Slope			1.33/1.26	0.95/0.90			0.85/0.80	0.89/0.84
Delta Slope			0.33/0.26	0.05/0.10			0.15/0.20	0.11/0.16
Intercept			-49.10/-34.90	9.49/20.00			22.82/32.21	13.29/23.98
Intercept			49.10/34.90	9.49/20.00			22.82/32.21	13.29/23.98

Table S24. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.65/0.66	0.60/0.62			0.99/0.99	0.99/0.99		0.90/0.90
R ²	0.54/0.56	0.45/0.46			0.98/0.99	0.98/0.99		0.96/0.96
RMSE [ppb]	20.04/23.03	24.57/29.21			23.18/14.61	24.67/20.48		23.19/22.45
MAE [ppb]	16.22/18.85	19.86/23.97			15.16/10.63	16.95/15.58		17.05/17.26
Slope	0.90/1.11	0.71/0.91			0.82/0.89	0.90/0.94		0.85/0.89
Delta Slope	0.10/0.11	0.29/0.09			0.18/0.11	0.10/0.06		0.15/0.11
Intercept	22.63/0.18	42.83/19.77			27.03/18.08	11.38/2.28		25.31/20.64
Intercept	22.63/0.18	42.83/19.77			27.03/18.08	11.38/2.28		25.31/20.64
AELCM009								
Rs			0.81/0.82	0.98/0.99			0.99/0.99	0.95/0.95
R ²			0.76/0.78	0.91/0.93			0.99/0.99	0.97/0.98
RMSE [ppb]			15.86/14.44	21.78/18.82			16.15/17.90	18.14/17.16
MAE [ppb]			12.39/11.14	7.38/6.04			12.04/11.54	10.60/9.58
Slope			0.80/0.84	0.80/0.84			1.02/1.07	0.98/1.03
Delta Slope			0.20/0.16	0.20/0.16			0.02/0.07	0.02/0.03
Intercept			18.84/15.79	26.25/22.84			-10.14/-18.82	-2.66/-7.06
Intercept			18.84/15.79	26.25/22.84			10.14/18.82	2.66/7.06

Table S25. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.66	0.57/0.60	0.72/0.74				0.99/0.99	0.78/0.78
R ²	0.48/0.51	0.36/0.42	0.61/0.69				0.98/0.99	0.95/0.96
RMSE [ppb]	16.09/15.92	25.92/24.55	26.76/23.80				43.64/43.30	29.80/28.71
MAE [ppb]	12.45/12.57	19.16/18.27	21.54/19.54				34.23/35.27	21.84/21.41
Slope	0.65/0.75	0.49/0.64	0.59/0.75				0.85/0.85	0.82/0.83
Delta Slope	0.35/0.25	0.51/0.36	0.41/0.25				0.15/0.15	0.18/0.17
Intercept	33.14/22.59	50.13/35.96	32.79/14.32				2.08/0.41	8.68/9.98
Intercept	33.14/22.59	50.13/35.96	32.79/14.32				2.08/0.41	8.68/9.98
AELCM009								
Rs				0.92/0.94	0.98/0.99	1.00/1.00		0.98/0.99
R ²				0.95/0.96	0.96/0.98	0.99/0.99		0.97/0.99
RMSE [ppb]				18.55/16.94	23.84/20.64	23.97/27.49		22.26/22.13
MAE [ppb]				13.56/12.33	16.68/14.31	20.69/22.65		16.98/16.43
Slope				0.90/0.88	1.01/0.90	0.97/0.89		0.96/0.89
Delta Slope				0.10/0.12	0.01/0.10	0.03/0.11		0.04/0.11
Intercept				4.06/7.72	-12.05/7.37	-11.28/7.92		-5.70/7.28
Intercept				4.06/7.72	12.05/7.37	11.28/7.92		5.70/7.28

Table S26. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.68/0.68	0.57/0.61	0.72/0.73				0.99/0.99	0.78/0.78
R ²	0.52/0.54	0.39/0.41	0.62/0.69				0.99/0.99	0.95/0.95
RMSE [ppb]	19.77/22.12	26.39/30.77	18.02/17.18				16.97/15.61	20.62/22.22
MAE [ppb]	14.84/16.23	20.04/22.16	13.65/13.29				10.43/10.24	14.74/15.48
Slope	0.82/0.99	0.64/0.81	0.69/0.87				0.97/0.99	0.94/0.95
Delta Slope	0.18/0.01	0.36/0.19	0.31/0.13				0.03/0.01	0.06/0.05
Intercept	32.48/14.27	52.92/36.32	38.24/17.00				6.05/-0.21	14.05/13.62
Intercept	32.48/14.27	52.92/36.32	38.24/17.00				6.05/0.21	14.05/13.62
AELCM009								
Rs				0.93/0.95	0.99/0.99	0.98/1.00		0.98/0.99
R ²				0.93/0.93	0.97/0.98	0.97/0.99		0.97/0.98
RMSE [ppb]				17.84/17.06	21.11/15.73	28.66/12.48		22.99/15.21
MAE [ppb]				10.90/8.83	13.59/11.36	18.79/7.40		14.43/9.19
Slope				0.96/0.92	1.08/0.94	1.07/0.96		1.07/0.95
Delta Slope				0.04/0.08	0.08/0.06	0.07/0.04		0.07/0.05
Intercept				7.83/13.74	-8.51/16.46	-6.99/10.77		-6.32/11.94
Intercept				7.83/13.74	8.51/16.46	6.99/10.77		6.32/11.94

Table S27. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.67/0.67	0.63/0.63	0.78/0.78				0.99/0.99	0.79/0.79
R ²	0.50/0.50	0.37/0.37	0.60/0.60				0.99/0.99	0.80/0.80
RMSE [ppb]	40.22/41.46	59.93/61.67	34.90/36.26				31.67/28.55	43.10/43.74
MAE [ppb]	32.27/33.34	47.63/48.98	25.45/26.41				17.00/15.04	30.59/30.94
Slope	1.84/1.88	1.59/1.63	1.41/1.44				0.83/0.85	0.88/0.90
Delta Slope	0.84/0.88	0.59/0.63	0.41/0.44				0.17/0.15	0.12/0.10
Intercept	-84.96/-90.91	-66.93/-73.03	-52.20/-57.34				26.38/25.41	17.78/14.60
Intercept	84.96/90.91	66.93/73.03	52.20/57.34				26.38/25.41	17.78/14.60
AELCM009								
Rs				0.98/0.99	0.99/0.99	1.00/1.00		0.99/0.99
R ²				0.96/0.97	0.99/0.99	0.99/0.99		0.98/0.98
RMSE [ppb]				12.64/14.33	14.98/18.35	24.89/30.89		18.29/22.33
MAE [ppb]				6.85/9.04	11.80/14.98	16.50/20.80		11.72/14.94
Slope				0.95/0.89	0.93/0.88	0.85/0.80		0.88/0.83
Delta Slope				0.05/0.11	0.07/0.12	0.15/0.20		0.12/0.17
Intercept				9.49/21.56	21.05/32.75	26.51/35.86		22.24/33.61
Intercept				9.49/21.56	21.05/32.75	26.51/35.86		22.24/33.61

Table S28. Performance metrics of the single CO LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.65/0.67	0.60/0.63	0.77/0.78				0.99/0.99	0.79/0.79
R ²	0.54/0.55	0.45/0.44	0.68/0.68				0.98/0.99	0.95/0.93
RMSE [ppb]	20.04/26.68	24.57/36.24	16.64/21.98				19.57/15.82	20.40/26.26
MAE [ppb]	16.22/21.83	19.86/29.97	12.86/16.93				12.49/9.88	15.36/19.65
Slope	0.90/1.35	0.71/1.12	0.79/1.09				0.99/1.03	0.95/1.01
Delta Slope	0.10/0.35	0.29/0.12	0.21/0.09				0.01/0.03	0.05/0.01
Intercept	22.63/-28.13	42.83/-7.59	27.72/-10.99				-1.97/-9.76	11.46/3.33
Intercept	22.63/28.13	42.83/7.59	27.72/10.99				1.97/9.76	11.46/3.33
AELCM009								
Rs				0.98/0.99	0.99/0.99	1.00/1.00		0.99/0.99
R ²				0.91/0.91	0.99/0.99	0.99/0.99		0.98/0.98
RMSE [ppb]				21.78/21.45	18.10/17.52	17.68/16.44		19.27/18.60
MAE [ppb]				7.38/7.21	11.68/11.95	12.37/11.23		10.48/10.13
Slope				0.80/0.79	0.86/0.85	0.94/0.94		0.90/0.89
Delta Slope				0.20/0.21	0.14/0.15	0.06/0.06		0.10/0.11
Intercept				26.25/30.52	23.14/27.00	5.48/6.34		14.06/17.51
Intercept				26.25/30.52	23.14/27.00	5.48/6.34		14.06/17.51

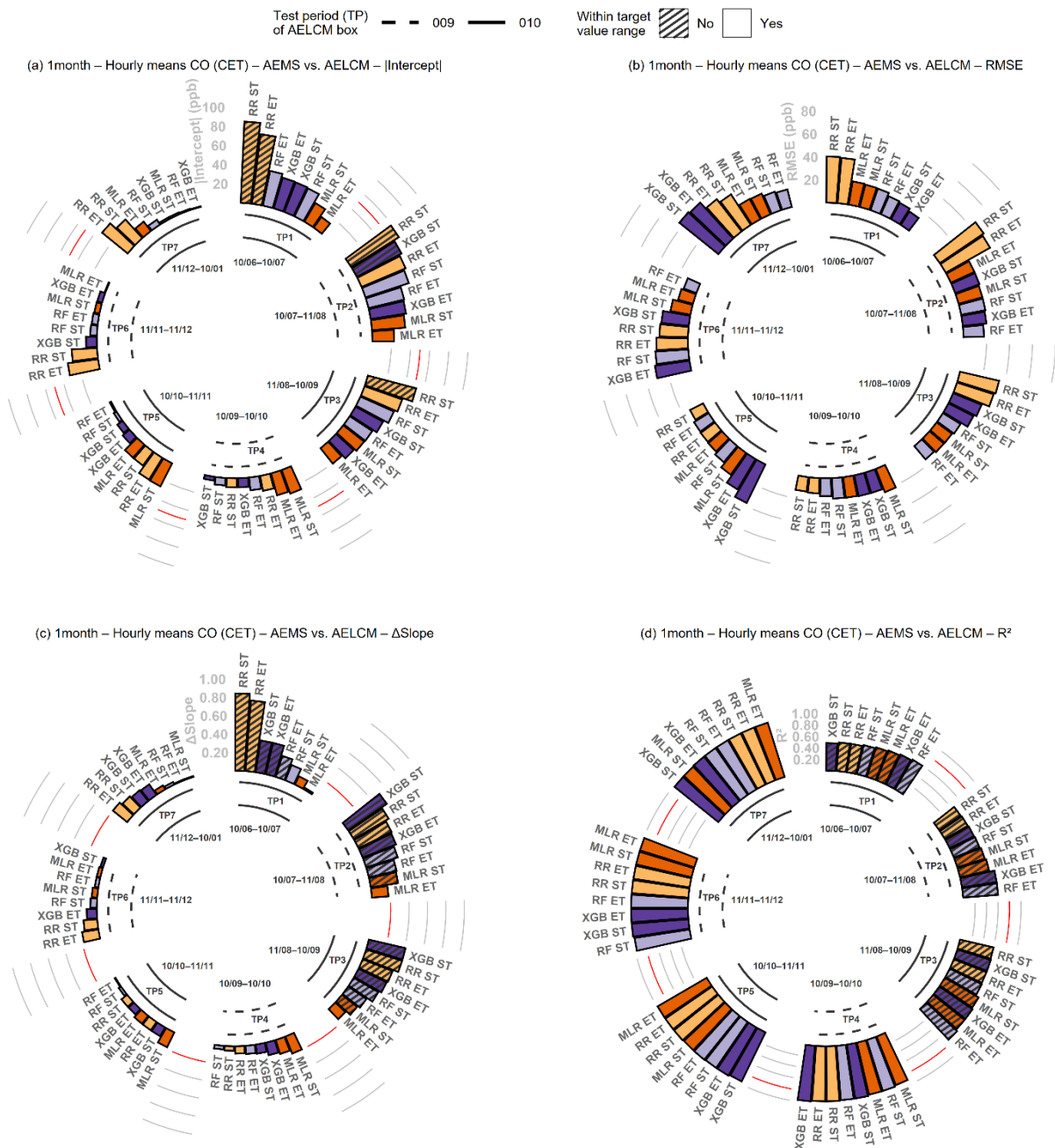


Figure S12. Performance metrics of the single CO LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the one-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric (|Intercept| (a), RMSE (b), Δ Slope (c), R^2 (d)).

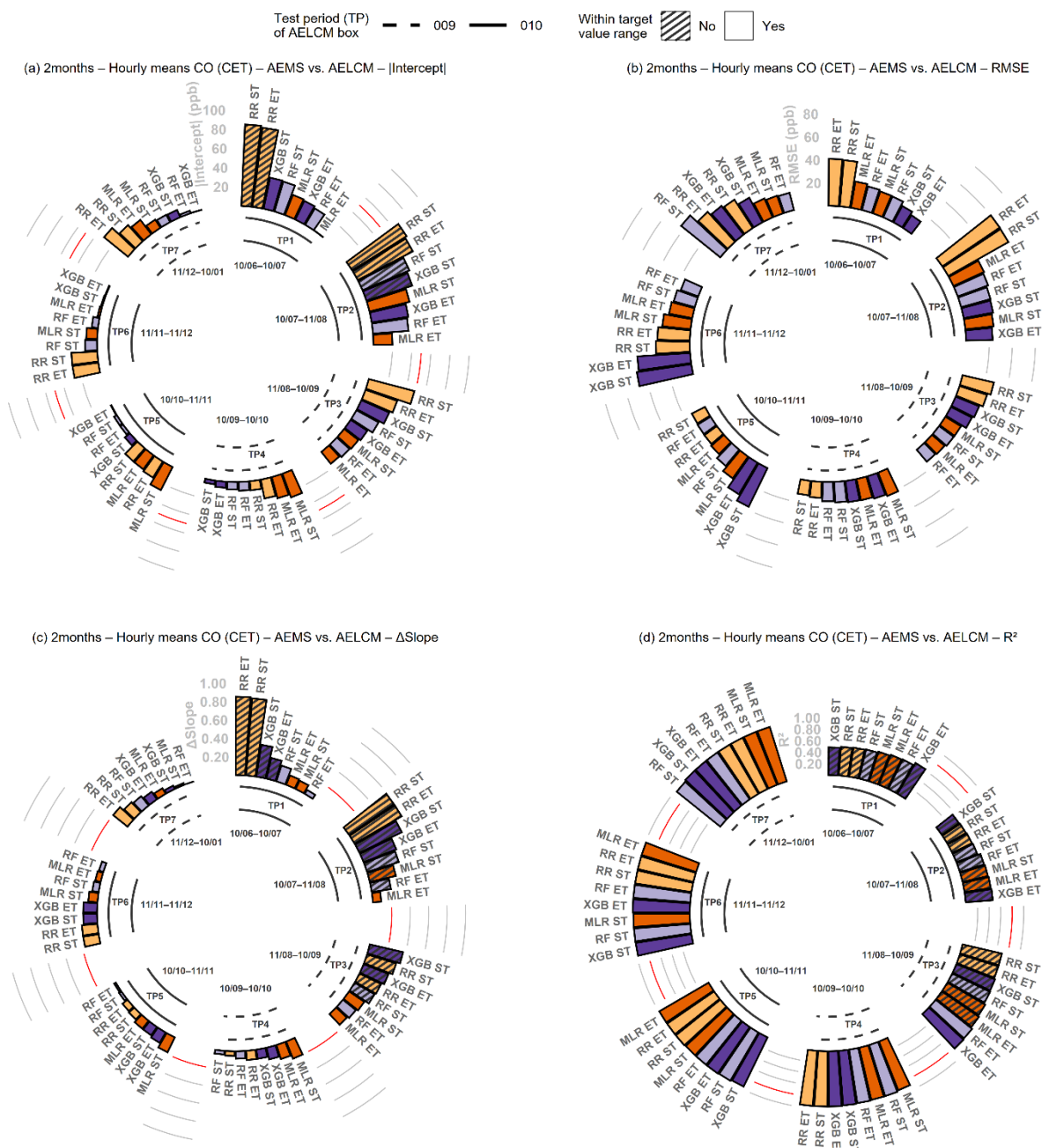


Figure S13. Performance metrics of the single CO LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the two-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric (|Intercept| (a), RMSE (b), Δ Slope (c), R^2 (d)).

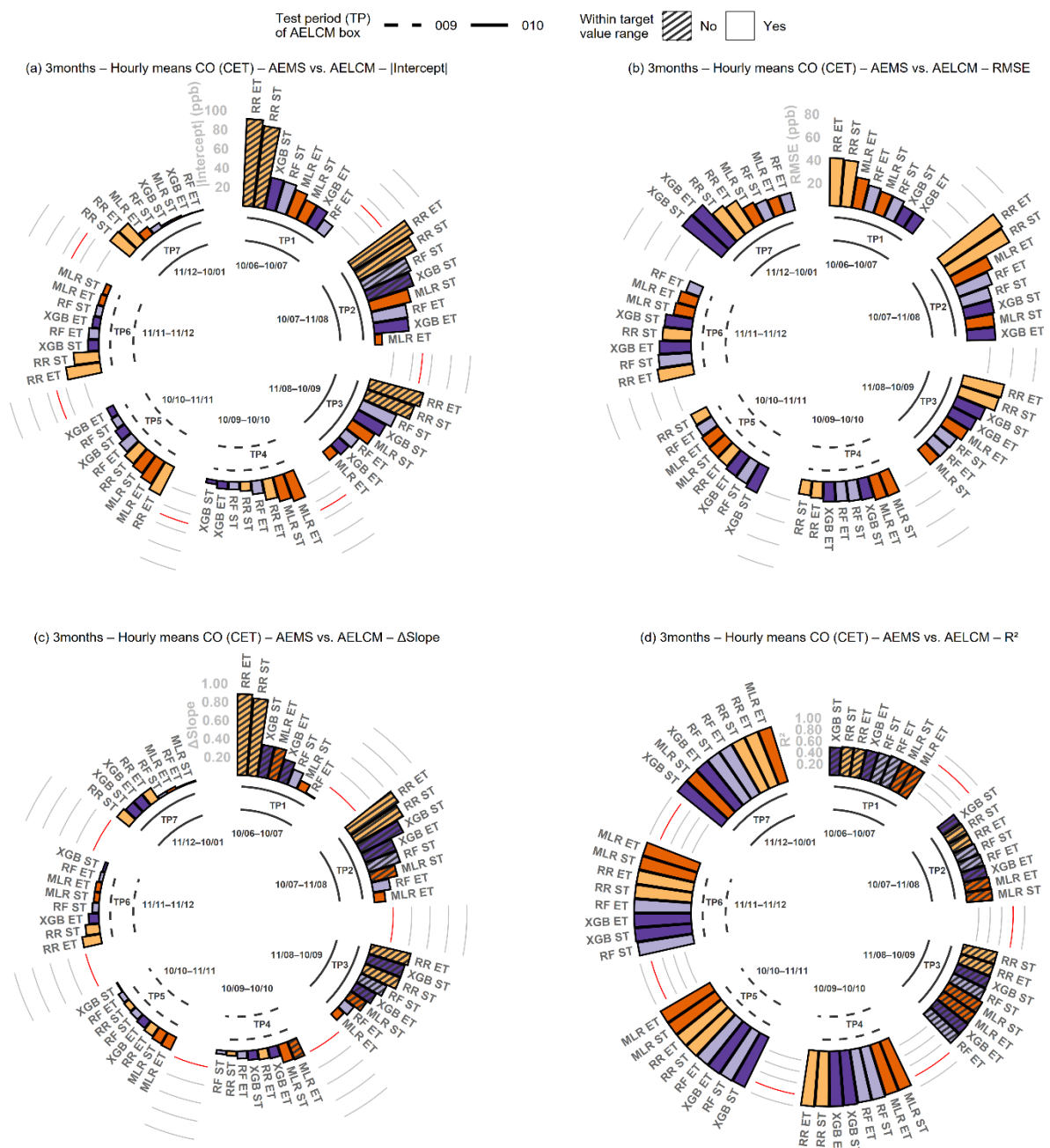


Figure S14. Performance metrics of the single CO LCS in each AELCM box, calculated from hourly mean values after calibration. Metrics are presented for each calibration model, TP, and calibration variant (ST and ET). Models are ordered by performance from highest to lowest in each period. The ET is characterized by the three-month variant for each AELCM box. Values highlighted in red describe the least accepted target value given by EPA for each performance metric ($|Intercept|$ (a), RMSE (b), Δ Slope (c), R^2 (d)).

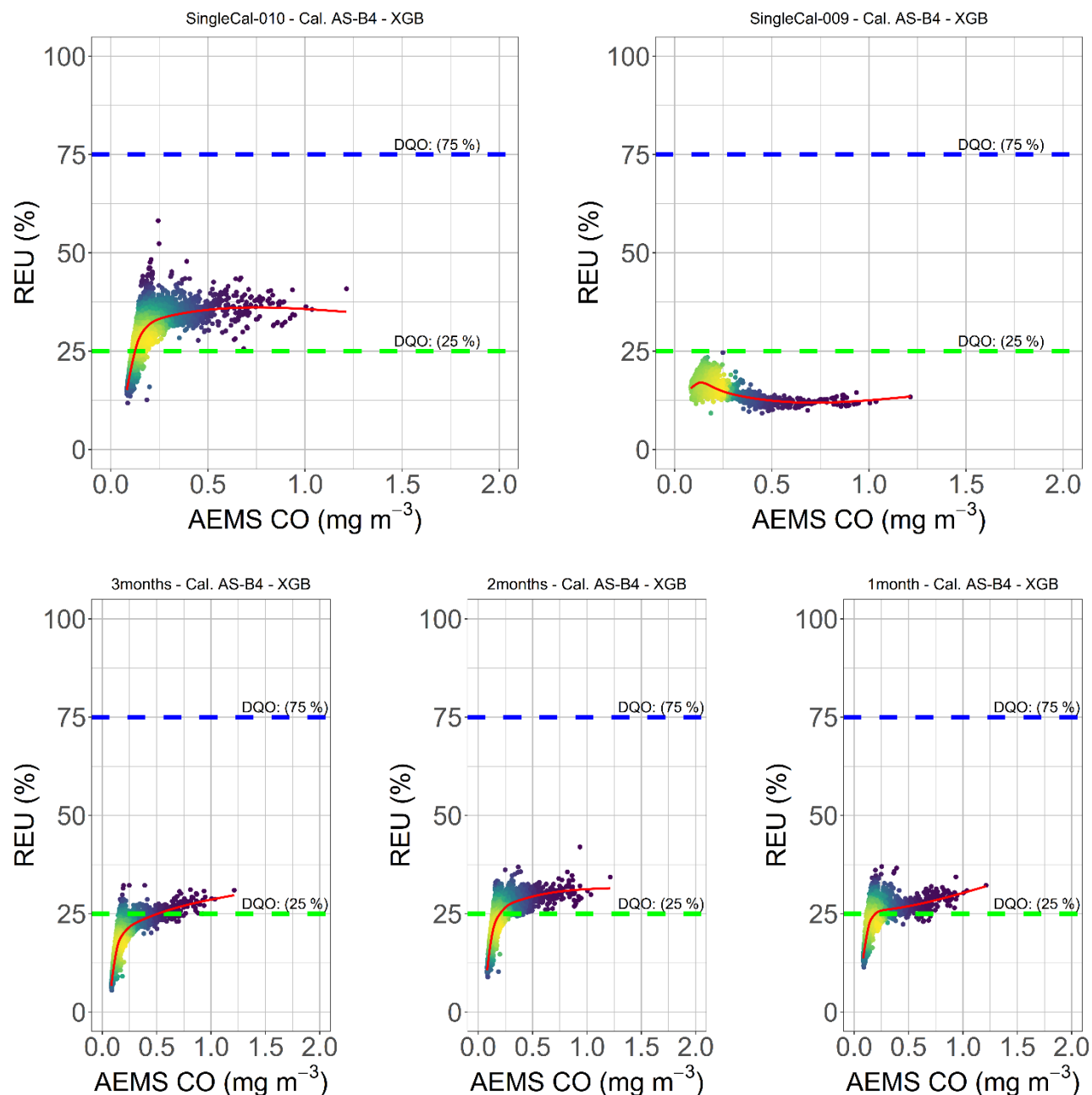


Figure S15. Calculated REU values for XGB calibrated CO LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (CO Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

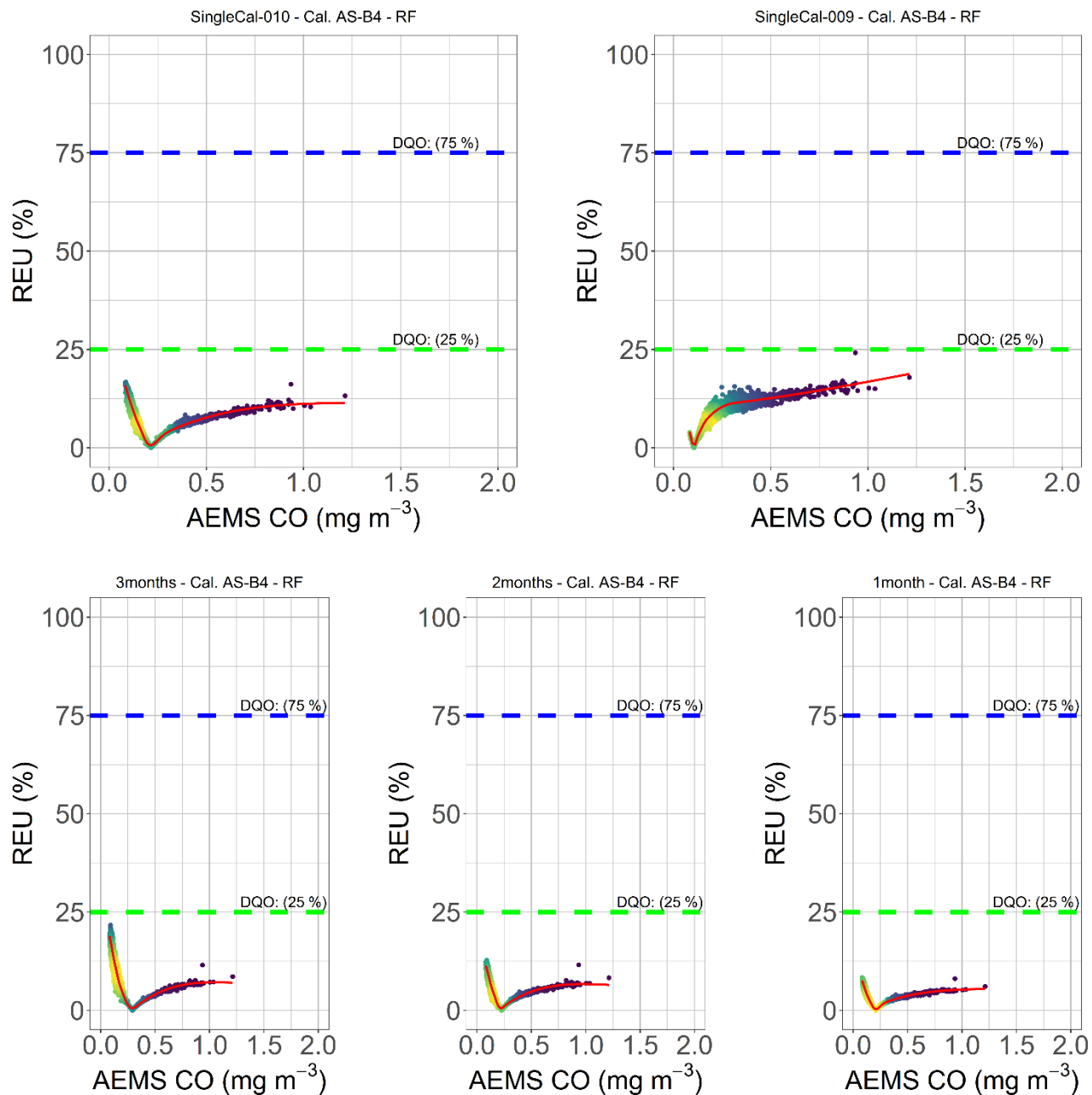


Figure S16. Calculated REU values for RF calibrated CO LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (CO Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

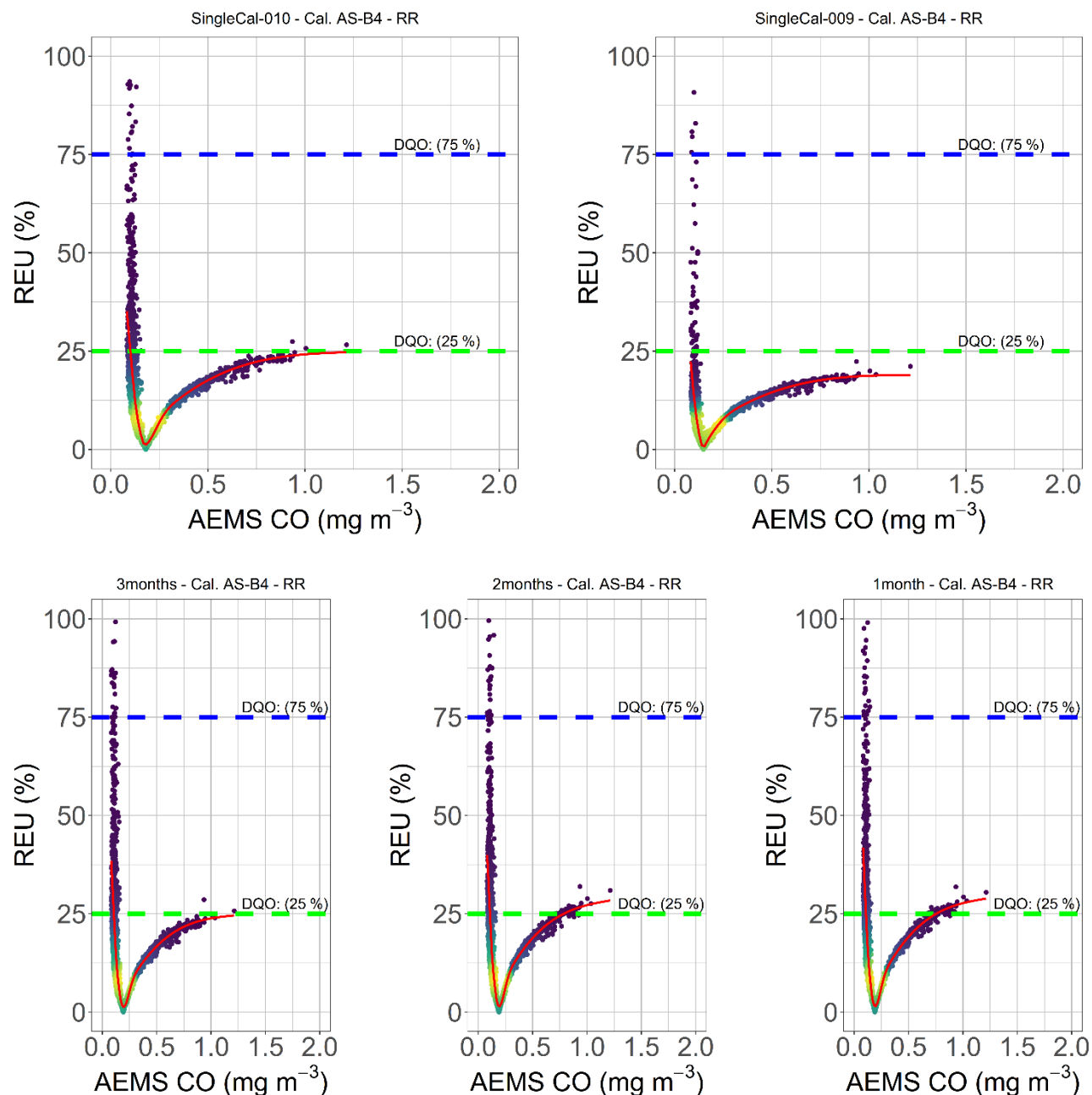


Figure S17. Calculated REU values for RR calibrated CO LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (CO Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

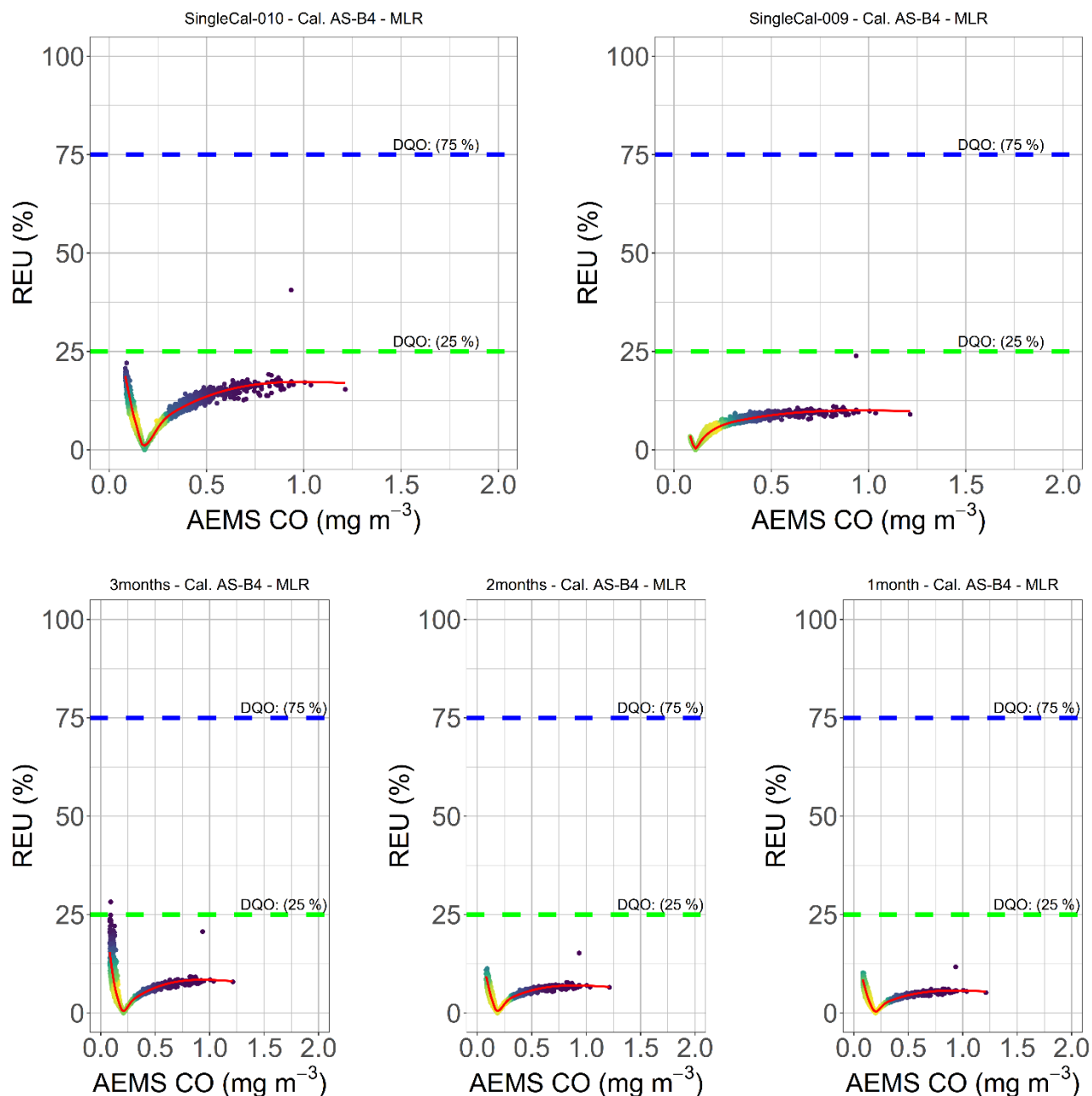


Figure S18. Calculated REU values for MLR calibrated CO LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–10 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (CO Class 1 DQO = 25 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

Performance Metrics O₃

Table S29. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.97		0.97/0.98		0.88/0.92		0.96/0.97	0.96/0.97
R ²	0.89/0.93		0.93/0.95		0.83/0.90		0.90/0.95	0.92/0.95
RMSE [ppb]	6.10/4.42		7.39/5.69		4.33/3.33		4.93/3.53	5.81/4.35
MAE [ppb]	4.60/3.42		5.64/4.50		3.06/2.22		4.02/2.80	4.33/3.24
Slope	0.73/0.87		0.77/0.85		0.90/0.95		0.84/0.90	0.84/0.91
Delta Slope	0.27/0.13		0.23/0.15		0.10/0.05		0.16/0.10	0.16/0.09
Intercept	9.09/5.18		2.93/1.83		1.68/1.31		-0.90/-0.73	1.64/1.00
Intercept	9.09/5.18		2.93/1.83		1.68/1.31		0.90/0.73	1.64/1.00
AELCM009								
Rs		0.98/0.99		0.98/0.98		0.94/0.95		0.99/0.99
R ²		0.95/0.97		0.98/0.97		0.97/0.98		0.98/0.98
RMSE [ppb]		4.43/3.42		2.44/2.09		3.70/1.46		3.62/2.46
MAE [ppb]		3.17/2.51		2.05/1.64		3.37/1.14		2.86/1.76
Slope		0.87/0.95		0.96/1.00		1.02/1.06		0.90/1.00
Delta Slope		0.13/0.05		0.04/0.00		0.02/0.06		0.10/0.00
Intercept		5.55/2.86		2.40/-0.53		3.19/-0.43		3.84/0.05
Intercept		5.55/2.86		2.40/0.53		3.19/0.43		3.84/0.05

Table S30. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.96/0.97		0.98/0.98		0.84/0.91		0.96/0.97	0.96/0.97
R ²	0.91/0.93		0.94/0.96		0.79/0.88		0.92/0.95	0.93/0.95
RMSE [ppb]	5.60/4.80		5.80/4.54		5.56/3.95		3.55/3.03	5.21/4.14
MAE [ppb]	4.52/3.84		4.48/3.57		4.26/2.71		2.82/2.39	4.02/3.13
Slope	0.76/0.88		0.76/0.85		0.87/0.96		0.92/0.92	0.86/0.93
Delta Slope	0.24/0.12		0.24/0.15		0.13/0.04		0.08/0.08	0.14/0.07
Intercept	10.71/6.67		6.47/3.70		4.31/2.04		-0.24/-0.35	3.71/1.80
Intercept	10.71/6.67		6.47/3.70		4.31/2.04		0.24/0.35	3.71/1.80
AELCM009								
Rs		0.96/0.97		0.98/0.98		0.91/0.94		0.98/0.99
R ²		0.91/0.95		0.96/0.97		0.95/0.98		0.96/0.98
RMSE [ppb]		6.31/4.54		2.89/2.02		3.57/1.51		4.51/3.00
MAE [ppb]		4.76/3.32		2.33/1.60		3.05/1.14		3.38/2.02
Slope		0.75/0.89		0.91/0.99		0.91/1.05		0.86/0.98
Delta Slope		0.25/0.11		0.09/0.01		0.09/0.05		0.14/0.02
Intercept		9.93/5.46		3.39/-0.11		3.90/-0.57		4.80/0.53
Intercept		9.93/5.46		3.39/0.11		3.90/0.57		4.80/0.53

Table S31. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.97		0.98/0.98		0.92/0.91		0.97/0.97	0.97/0.97
R ²	0.94/0.94		0.95/0.95		0.88/0.89		0.89/0.90	0.93/0.94
RMSE [ppb]	5.74/5.12		4.85/4.83		4.68/4.37		5.00/4.64	5.08/4.75
MAE [ppb]	4.76/4.16		3.95/3.90		3.79/3.54		3.57/3.60	4.02/3.80
Slope	0.87/0.87		0.83/0.82		0.98/0.92		1.06/0.98	0.97/0.95
Delta Slope	0.13/0.13		0.17/0.18		0.02/0.08		0.06/0.02	0.03/0.05
Intercept	9.08/8.21		6.75/6.08		3.00/3.54		-3.60/-2.45	1.95/2.09
Intercept	9.08/8.21		6.75/6.08		3.00/3.54		3.60/2.45	1.95/2.09
AELCM009								
Rs		0.98/0.98		0.98/0.98		0.95/0.95		0.99/0.99
R ²		0.95/0.95		0.97/0.97		0.93/0.93		0.97/0.97
RMSE [ppb]		5.94/4.81		2.45/2.28		2.95/2.49		4.08/3.39
MAE [ppb]		4.44/3.55		1.97/1.78		2.47/1.97		2.96/2.43
Slope		1.04/1.01		0.92/0.89		0.99/0.95		1.04/1.01
Delta Slope		0.04/0.01		0.08/0.11		0.01/0.05		0.04/0.01
Intercept		2.13/1.73		2.80/2.22		1.83/1.56		1.41/0.93
Intercept		2.13/1.73		2.80/2.22		1.83/1.56		1.41/0.93

Table S32. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

one-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.98		0.98/0.98		0.91/0.91		0.97/0.97	0.97/0.97
R ²	0.92/0.95		0.94/0.95		0.89/0.90		0.94/0.94	0.93/0.94
RMSE [ppb]	5.32/5.09		5.32/4.45		3.80/3.50		6.07/4.87	5.19/4.52
MAE [ppb]	4.37/4.22		4.16/3.60		2.82/2.65		5.33/4.21	4.17/3.67
Slope	0.87/0.91		0.81/0.86		1.03/0.95		1.10/0.99	0.99/0.98
Delta Slope	0.13/0.09		0.19/0.14		0.03/0.05		0.10/0.01	0.01/0.02
Intercept	7.93/6.91		4.80/3.99		0.28/1.79		-6.74/-3.83	-0.47/0.35
Intercept	7.93/6.91		4.80/3.99		0.28/1.79		6.74/3.83	0.47/0.35
AELCM009								
Rs		0.99/0.99		0.99/0.99		0.96/0.97		0.99/0.99
R ²		0.95/0.96		0.98/0.98		0.98/0.98		0.97/0.98
RMSE [ppb]		6.41/5.27		1.60/1.79		2.74/1.56		4.13/3.34
MAE [ppb]		3.92/2.89		1.31/1.38		2.45/1.28		2.56/1.85
Slope		1.12/1.10		0.99/1.01		0.98/1.03		1.06/1.06
Delta Slope		0.12/0.10		0.01/0.01		0.02/0.03		0.06/0.06
Intercept		-1.57/-2.17		0.66/-0.95		2.54/0.72		0.70/-0.61
Intercept		1.57/2.17		0.66/0.95		2.54/0.72		0.70/0.61

Table S33. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.96	0.93/0.94			0.88/0.93	0.93/0.93		0.97/0.98
R ²	0.89/0.92	0.86/0.88			0.83/0.89	0.92/0.96		0.93/0.95
RMSE [ppb]	6.10/4.96	8.58/7.02			4.33/3.64	2.95/1.85		5.88/4.76
MAE [ppb]	4.60/3.89	6.08/5.16			3.06/2.35	2.28/1.41		4.01/3.21
Slope	0.73/0.82	0.68/0.74			0.90/0.99	0.82/0.99		0.84/0.92
Delta Slope	0.27/0.18	0.32/0.26			0.10/0.01	0.18/0.01		0.16/0.08
Intercept	9.09/8.07	9.90/10.22			1.68/1.07	0.21/-0.50		2.47/2.26
Intercept	9.09/8.07	9.90/10.22			1.68/1.07	0.21/0.50		2.47/2.26
AELCM009								
Rs			0.99/0.99	0.98/0.98			0.98/0.98	0.99/0.99
R ²			0.97/0.98	0.98/0.97			0.98/0.98	0.97/0.98
RMSE [ppb]			3.89/3.19	2.44/2.39			2.95/2.03	3.15/2.58
MAE [ppb]			2.94/2.39	2.05/1.88			2.42/1.61	2.47/1.96
Slope			0.86/0.95	0.96/1.00			1.11/1.06	0.91/0.97
Delta Slope			0.14/0.05	0.04/0.00			0.11/0.06	0.09/0.03
Intercept			3.95/0.30	2.40/-0.85			-0.01/-1.26	2.80/-0.27
Intercept			3.95/0.30	2.40/0.85			0.01/1.26	2.80/0.27

Table S34. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.96/0.96	0.94/0.96			0.84/0.91	0.88/0.93		0.96/0.98
R ²	0.91/0.92	0.89/0.92			0.79/0.88	0.92/0.96		0.94/0.95
RMSE [ppb]	5.60/5.39	7.37/6.06			5.56/4.19	2.46/1.83		5.54/4.66
MAE [ppb]	4.52/4.42	5.76/4.79			4.26/2.77	2.06/1.44		4.15/3.35
Slope	0.76/0.85	0.69/0.80			0.87/1.00	0.87/1.00		0.87/0.96
Delta Slope	0.24/0.15	0.31/0.20			0.13/0.00	0.13/0.00		0.13/0.04
Intercept	10.71/8.66	12.41/10.02			4.31/1.73	1.13/-0.27		4.22/2.42
Intercept	10.71/8.66	12.41/10.02			4.31/1.73	1.13/0.27		4.22/2.42
AELCM009								
Rs			0.98/0.99	0.98/0.98			0.98/0.98	0.98/0.99
R ²			0.96/0.98	0.96/0.97			0.97/0.97	0.96/0.98
RMSE [ppb]			5.04/3.30	2.89/2.19			2.45/1.95	3.64/2.55
MAE [ppb]			3.85/2.40	2.33/1.72			1.79/1.45	2.66/1.86
Slope			0.79/0.92	0.91/0.98			1.03/1.02	0.87/0.95
Delta Slope			0.21/0.08	0.09/0.02			0.03/0.02	0.13/0.05
Intercept			6.55/1.64	3.39/-0.17			0.74/-0.57	3.76/0.48
Intercept			6.55/1.64	3.39/0.17			0.74/0.57	3.76/0.48

Table S35. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.97	0.97/0.97			0.92/0.91	0.94/0.94		0.98/0.98
R ²	0.94/0.94	0.93/0.94			0.88/0.89	0.87/0.89		0.95/0.96
RMSE [ppb]	5.74/5.53	5.92/5.74			4.68/4.69	3.37/2.81		5.03/4.84
MAE [ppb]	4.76/4.57	4.85/4.70			3.79/3.84	2.22/2.16		3.90/3.82
Slope	0.87/0.87	0.82/0.81			0.98/0.92	1.00/0.91		0.98/0.96
Delta Slope	0.13/0.13	0.18/0.19			0.02/0.08	0.00/0.09		0.02/0.04
Intercept	9.08/8.86	10.11/10.15			3.00/4.12	-0.33/1.17		2.79/3.53
Intercept	9.08/8.86	10.11/10.15			3.00/4.12	0.33/1.17		2.79/3.53
AELCM009								
Rs			0.99/0.98	0.98/0.98			0.98/0.98	0.99/0.98
R ²			0.97/0.96	0.97/0.96			0.94/0.93	0.97/0.96
RMSE [ppb]			3.59/4.11	2.45/2.59			3.03/3.27	3.06/3.38
MAE [ppb]			2.89/3.27	1.97/2.02			2.15/2.42	2.34/2.57
Slope			0.94/0.89	0.92/0.87			1.06/1.00	0.98/0.92
Delta Slope			0.06/0.11	0.08/0.13			0.06/0.00	0.02/0.08
Intercept			3.37/2.85	2.80/2.41			-0.82/-1.09	1.43/0.98
Intercept			3.37/2.85	2.80/2.41			0.82/1.09	1.43/0.98

Table S36. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.98	0.95/0.97			0.91/0.91	0.95/0.95		0.97/0.98
R ²	0.92/0.95	0.88/0.94			0.89/0.90	0.95/0.95		0.94/0.96
RMSE [ppb]	5.32/5.54	6.81/5.67			3.80/3.95	4.23/2.40		5.17/4.59
MAE [ppb]	4.37/4.69	5.12/4.56			2.82/3.03	3.73/1.77		4.01/3.51
Slope	0.87/0.88	0.76/0.80			1.03/0.97	1.07/0.98		0.99/0.98
Delta Slope	0.13/0.12	0.24/0.20			0.03/0.03	0.07/0.02		0.01/0.02
Intercept	7.93/8.54	10.05/10.24			0.28/2.46	-4.25/-1.12		0.27/2.08
Intercept	7.93/8.54	10.05/10.24			0.28/2.46	4.25/1.12		0.27/2.08
AELCM009								
Rs			0.99/0.99	0.99/0.99			0.99/0.99	0.99/0.99
R ²			0.98/0.98	0.98/0.98			0.98/0.98	0.98/0.98
RMSE [ppb]			2.80/3.12	1.60/2.04			2.09/1.78	2.22/2.39
MAE [ppb]			2.02/2.39	1.31/1.60			1.59/1.30	1.64/1.76
Slope			0.99/0.96	0.99/0.99			1.05/1.06	1.00/0.98
Delta Slope			0.01/0.04	0.01/0.01			0.05/0.06	0.00/0.02
Intercept			0.79/0.00	0.66/-0.83			0.29/-1.22	0.72/-0.40
Intercept			0.79/0.00	0.66/0.83			0.29/1.22	0.72/0.40

Table S37. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

three-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95	0.93/0.93	0.97/0.97				0.96/0.97	0.96/0.97
R ²	0.89/0.90	0.86/0.86	0.93/0.93				0.90/0.95	0.91/0.92
RMSE [ppb]	6.10/6.01	8.58/8.82	7.39/7.24				4.93/3.55	6.89/6.69
MAE [ppb]	4.60/4.60	6.08/6.30	5.64/5.44				4.02/2.83	5.09/4.79
Slope	0.73/0.73	0.68/0.67	0.77/0.75				0.84/0.89	0.82/0.80
Delta Slope	0.27/0.27	0.32/0.33	0.23/0.25				0.16/0.11	0.18/0.20
Intercept	9.09/9.27	9.90/10.20	2.93/4.22				-0.90/-0.64	2.68/3.59
Intercept	9.09/9.27	9.90/10.20	2.93/4.22				0.90/0.64	2.68/3.59
AELCM009								
Rs				0.98/0.99	0.92/0.94	0.94/0.96		0.95/0.96
R ²				0.98/0.98	0.95/0.95	0.97/0.98		0.96/0.97
RMSE [ppb]				2.44/1.78	4.93/3.10	3.70/1.79		3.83/2.31
MAE [ppb]				2.05/1.41	4.36/2.40	3.37/1.41		3.26/1.74
Slope				0.96/0.98	0.91/0.95	1.02/1.02		0.93/0.96
Delta Slope				0.04/0.02	0.09/0.05	0.02/0.02		0.07/0.04
Intercept				2.40/0.25	5.29/2.79	3.19/0.98		4.04/1.69
Intercept				2.40/0.25	5.29/2.79	3.19/0.98		4.04/1.69

Table S38. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

three-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.96/0.96	0.94/0.94	0.98/0.98				0.96/0.97	0.97/0.97
R ²	0.91/0.92	0.89/0.88	0.94/0.94				0.92/0.95	0.92/0.92
RMSE [ppb]	5.60/5.41	7.37/7.34	5.80/5.80				3.55/2.96	5.74/5.60
MAE [ppb]	4.52/4.38	5.76/5.63	4.48/4.37				2.82/2.34	4.39/4.18
Slope	0.76/0.76	0.69/0.71	0.76/0.77				0.92/0.93	0.84/0.84
Delta Slope	0.24/0.24	0.31/0.29	0.24/0.23				0.08/0.07	0.16/0.16
Intercept	10.71/10.24	12.41/11.51	6.47/5.92				-0.24/-0.38	4.59/4.26
Intercept	10.71/10.24	12.41/11.51	6.47/5.92				0.24/0.38	4.59/4.26
AELCM009								
Rs			0.98/0.98	0.91/0.94	0.91/0.95			0.94/0.96
R ²			0.96/0.98	0.91/0.94	0.95/0.98			0.94/0.96
RMSE [ppb]			2.89/1.92	5.54/3.65	3.57/1.72			4.15/2.58
MAE [ppb]			2.33/1.55	4.67/2.82	3.05/1.37			3.35/1.92
Slope			0.91/0.96	0.85/0.93	0.91/0.99			0.87/0.94
Delta Slope			0.09/0.04	0.15/0.07	0.09/0.01			0.13/0.06
Intercept			3.39/1.10	6.21/3.37	3.90/1.32			4.75/2.18
Intercept			3.39/1.10	6.21/3.37	3.90/1.32			4.75/2.18

Table S39. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

three-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.97	0.97/0.97	0.98/0.98				0.97/0.97	0.97/0.97
R ²	0.94/0.94	0.93/0.94	0.95/0.95				0.89/0.91	0.93/0.93
RMSE [ppb]	5.74/5.18	5.92/5.38	4.85/4.63				5.00/4.73	5.40/4.99
MAE [ppb]	4.76/4.22	4.85/4.36	3.95/3.75				3.57/3.70	4.28/4.01
Slope	0.87/0.89	0.82/0.84	0.83/0.85				1.06/0.99	0.97/0.97
Delta Slope	0.13/0.11	0.18/0.16	0.17/0.15				0.06/0.01	0.03/0.03
Intercept	9.08/7.49	10.11/8.78	6.75/5.12				-3.60/-2.96	2.39/1.56
Intercept	9.08/7.49	10.11/8.78	6.75/5.12				3.60/2.96	2.39/1.56
AELCM009								
Rs			0.98/0.98	0.93/0.93	0.93/0.95			0.96/0.96
R ²			0.97/0.97	0.93/0.93	0.93/0.93			0.95/0.95
RMSE [ppb]			2.45/2.69	4.40/4.39	2.95/3.01			3.37/3.44
MAE [ppb]			1.97/2.11	3.78/3.69	2.47/2.53			2.74/2.78
Slope			0.92/0.85	0.92/0.84	0.99/0.92			0.93/0.86
Delta Slope			0.08/0.15	0.08/0.16	0.01/0.08			0.07/0.14
Intercept			2.80/3.74	4.45/5.07	1.83/2.66			3.15/3.89
Intercept			2.80/3.74	4.45/5.07	1.83/2.66			3.15/3.89

Table S40. Performance metrics of the single O₃ LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from hourly mean values.

three-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.97/0.97	0.95/0.96	0.98/0.98				0.97/0.97	0.96/0.97
R ²	0.92/0.94	0.88/0.92	0.94/0.95				0.94/0.94	0.91/0.93
RMSE [ppb]	5.32/4.96	6.81/5.94	5.32/4.98				6.07/4.89	5.91/5.21
MAE [ppb]	4.37/4.09	5.12/4.60	4.16/4.01				5.33/4.20	4.74/4.22
Slope	0.87/0.87	0.76/0.78	0.81/0.82				1.10/1.03	0.95/0.94
Delta Slope	0.13/0.13	0.24/0.22	0.19/0.18				0.10/0.03	0.05/0.06
Intercept	7.93/8.00	10.05/9.69	4.80/4.97				-6.74/-4.36	0.52/1.41
Intercept	7.93/8.00	10.05/9.69	4.80/4.97				6.74/4.36	0.52/1.41
AELCM009								
Rs			0.99/0.99	0.93/0.94	0.96/0.97			0.96/0.96
R ²			0.98/0.98	0.96/0.97	0.98/0.98			0.97/0.97
RMSE [ppb]			1.60/1.63	4.05/3.23	2.74/1.95			2.97/2.37
MAE [ppb]			1.31/1.28	3.53/2.70	2.45/1.71			2.43/1.90
Slope			0.99/0.97	0.92/0.90	0.98/1.00			0.93/0.93
Delta Slope			0.01/0.03	0.08/0.10	0.02/0.00			0.07/0.07
Intercept			0.66/0.40	4.38/3.66	2.54/1.56			3.00/2.30
Intercept			0.66/0.40	4.38/3.66	2.54/1.56			3.00/2.30

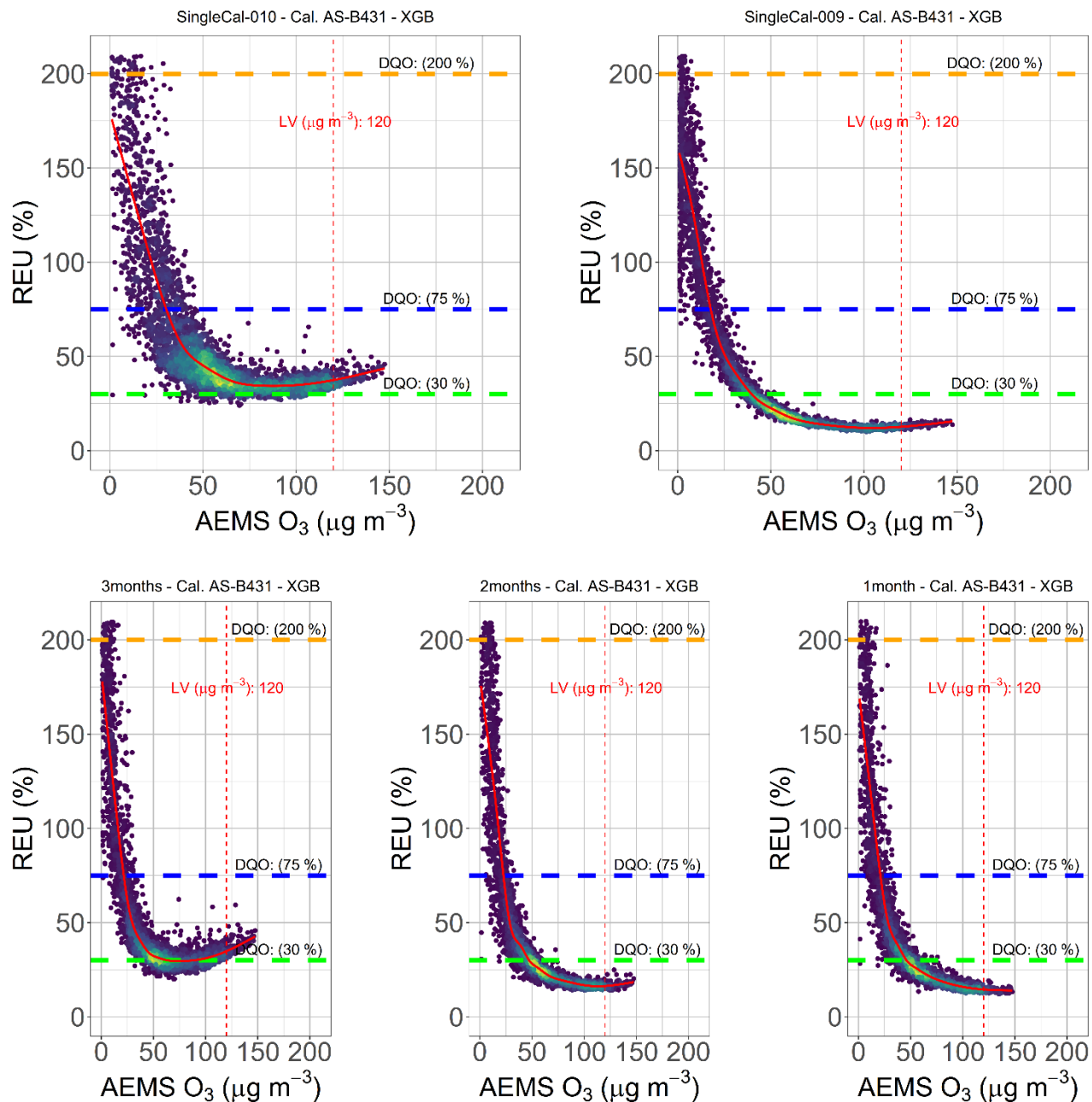


Figure S19. Calculated REU values for XGB calibrated O₃ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–11 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (O₃ Class 1 DQO = 30 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The vertical dashed line describes the limit value for O₃ (LV = 120 μg m⁻³). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

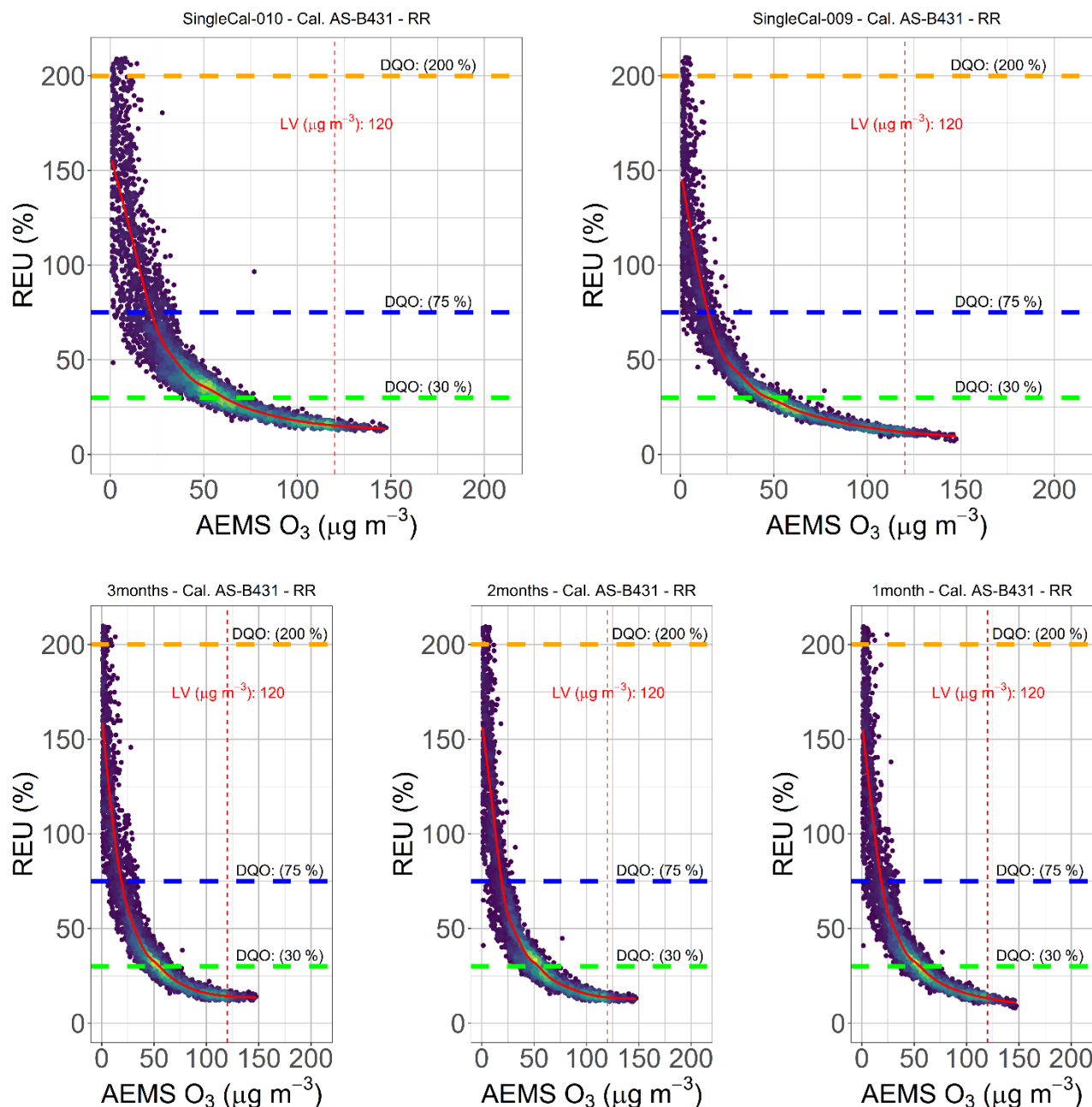


Figure S20. Calculated REU values for RR calibrated O₃ LCS hourly data belonging to the TPs (TP1–TP7, 10 June 2022–11 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs (O₃ Class 1 DQO = 30 %, Class 2 DQO = 75 % and Class 3 DQO = 200 %). The vertical dashed line describes the limit value for O₃ (LV = 120 μg m⁻³). The fitted smooth curve (red) is based on a generalized additive model (GAM). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

Performance Metrics PM_{2.5}

Table S41. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

one-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.94/0.95		0.92/0.92		0.90/0.90		0.97/0.97	0.96/0.96
R ²	0.86/0.86		0.86/0.87		0.89/0.89		0.95/0.95	0.93/0.93
RMSE (µg m ⁻³)	2.12/1.93		1.30/1.12		2.53/2.42		3.28/3.23	2.42/2.30
MAE (µg m ⁻³)	1.28/1.12		0.92/0.77		2.07/1.97		1.88/1.79	1.53/1.41
Slope	0.52/0.55		0.80/0.83		0.76/0.78		0.81/0.81	0.79/0.80
Delta Slope	0.48/0.45		0.20/0.17		0.24/0.22		0.19/0.19	0.21/0.20
Intercept	2.01/2.02		0.76/0.78		0.07/0.05		0.69/0.79	0.42/0.56
Intercept	2.01/2.02		0.76/0.78		0.07/0.05		0.69/0.79	0.42/0.56
AELCM009								
Rs		0.94/0.93		0.96/0.97		0.95/0.95		0.96/0.95
R ²		0.92/0.92		0.95/0.96		0.93/0.94		0.93/0.92
RMSE (µg m ⁻³)		1.53/1.34		0.79/0.86		1.34/1.37		1.26/1.21
MAE (µg m ⁻³)		1.25/1.10		0.68/0.75		1.06/1.07		0.99/0.98
Slope		0.71/0.71		0.87/0.90		0.89/0.93		0.87/0.91
Delta Slope		0.29/0.29		0.13/0.10		0.11/0.07		0.13/0.09
Intercept		1.13/1.41		0.72/1.04		0.98/1.27		0.57/0.81
Intercept		1.13/1.41		0.72/1.04		0.98/1.27		0.57/0.81

Table S42. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

one-month variant Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.96		0.93/0.93		0.89/0.89		0.97/0.97	0.95/0.95
R ²	0.88/0.88		0.87/0.88		0.89/0.89		0.98/0.98	0.95/0.95
RMSE (µg m ⁻³)	1.64/1.54		0.98/0.96		2.14/2.07		1.72/1.70	1.67/1.61
MAE (µg m ⁻³)	0.95/0.87		0.68/0.70		1.72/1.63		0.88/0.88	1.06/1.02
Slope	0.62/0.64		0.90/0.94		0.81/0.83		0.95/0.95	0.91/0.92
Delta Slope	0.38/0.36		0.10/0.06		0.19/0.17		0.05/0.05	0.09/0.08
Intercept	1.93/1.93		0.60/0.50		0.08/0.03		0.12/0.19	0.05/0.15
Intercept	1.93/1.93		0.60/0.50		0.08/0.03		0.12/0.19	0.05/0.15
AELCM009								
Rs		0.97/0.96		0.98/0.98		0.95/0.96		0.97/0.97
R ²		0.96/0.96		0.96/0.96		0.95/0.95		0.96/0.96
RMSE (µg m ⁻³)		0.97/0.64		0.85/0.81		1.63/1.31		1.20/0.96
MAE (µg m ⁻³)		0.81/0.53		0.63/0.58		1.27/0.99		0.90/0.70
Slope		0.83/1.01		0.87/1.02		0.88/1.04		0.86/1.02
Delta Slope		0.17/0.01		0.13/0.02		0.12/0.04		0.14/0.02
Intercept		0.65/0.05		0.34/0.21		0.15/-0.14		0.36/0.06
Intercept		0.65/0.05		0.34/0.21		0.15/0.14		0.36/0.06

Table S43. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

one-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.92/0.92		0.88/0.88		0.89/0.89		0.98/0.98	0.92/0.93
R ²	0.77/0.79		0.81/0.82		0.88/0.88		0.99/0.99	0.94/0.94
RMSE (µg m ⁻³)	2.09/2.06		1.27/1.20		2.24/2.08		1.01/1.02	1.73/1.66
MAE (µg m ⁻³)	1.43/1.44		0.85/0.82		1.77/1.59		0.70/0.76	1.19/1.15
Slope	0.46/0.45		0.72/0.72		0.84/0.82		0.99/0.97	0.94/0.92
Delta Slope	0.54/0.55		0.28/0.28		0.16/0.18		0.01/0.03	0.06/0.08
Intercept	3.12/3.28		1.80/1.91		-0.22/0.11		0.41/0.67	-0.05/0.22
Intercept	3.12/3.28		1.80/1.91		0.22/0.11		0.41/0.67	0.05/0.22
AELCM009								
Rs		0.92/0.96		0.94/0.96		0.95/0.95		0.95/0.97
R ²		0.93/0.96		0.94/0.95		0.95/0.95		0.93/0.94
RMSE (µg m ⁻³)		1.46/1.29		1.31/1.04		1.53/1.19		1.44/1.18
MAE (µg m ⁻³)		1.14/1.06		0.96/0.97		1.19/0.95		1.10/0.99
Slope		0.59/0.61		0.79/0.80		0.93/0.93		0.85/0.85
Delta Slope		0.41/0.39		0.21/0.20		0.07/0.07		0.15/0.15
Intercept		2.57/3.02		0.30/1.69		-0.34/1.06		0.38/1.48
Intercept		2.57/3.02		0.30/1.69		0.34/1.06		0.38/1.48

Table S44. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the one-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

Metric	one-month variant Multiple Linear Regression (AELCM010, AELCM009)							
	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95		0.93/0.93		0.90/0.90		0.98/0.98	0.96/0.96
R ²	0.89/0.90		0.87/0.87		0.88/0.88		0.99/0.99	0.96/0.96
RMSE (µg m ⁻³)	1.67/1.53		1.03/0.98		2.11/2.02		2.02/2.19	1.76/1.75
MAE (µg m ⁻³)	0.96/0.88		0.69/0.65		1.67/1.59		1.28/1.40	1.15/1.13
Slope	0.63/0.65		0.90/0.92		0.83/0.84		0.87/0.85	0.86/0.84
Delta Slope	0.37/0.35		0.10/0.08		0.17/0.16		0.13/0.15	0.14/0.16
Intercept	1.67/1.70		0.46/0.47		-0.02/0.00		0.66/0.76	0.35/0.58
Intercept	1.67/1.70		0.46/0.47		0.02/0.00		0.66/0.76	0.35/0.58
AELCM009								
Rs		0.97/0.96		0.97/0.97		0.95/0.95		0.98/0.97
R ²		0.98/0.96		0.96/0.96		0.95/0.95		0.96/0.96
RMSE (µg m ⁻³)		0.89/0.71		1.01/0.69		1.76/1.16		1.28/0.88
MAE (µg m ⁻³)		0.75/0.58		0.74/0.51		1.36/0.94		0.95/0.68
Slope		0.94/1.08		0.87/1.03		0.85/0.96		0.88/1.00
Delta Slope		0.06/0.08		0.13/0.03		0.15/0.04		0.12/0.00
Intercept		-0.30/-0.56		0.00/-0.08		0.28/0.33		0.06/0.05
Intercept		0.30/0.56		0.00/0.08		0.28/0.33		0.06/0.05

Table S45. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

Metric	two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)							
	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.94/0.94	0.94/0.94			0.90/0.89	0.96/0.97		0.95/0.95
R ²	0.86/0.86	0.95/0.95			0.89/0.89	0.97/0.97		0.90/0.90
RMSE (µg m ⁻³)	2.12/2.01	1.38/1.28			2.53/2.44	1.26/1.14		1.90/1.80
MAE (µg m ⁻³)	1.28/1.18	1.11/1.02			2.07/1.98	1.02/0.94		1.37/1.28
Slope	0.52/0.54	0.78/0.79			0.76/0.78	0.91/0.93		0.80/0.82
Delta Slope	0.48/0.46	0.22/0.21			0.24/0.22	0.09/0.07		0.20/0.18
Intercept	2.01/1.99	0.57/0.60			0.07/0.04	0.16/0.04		0.37/0.33
Intercept	2.01/1.99	0.57/0.60			0.07/0.04	0.16/0.04		0.37/0.33
AELCM009								
Rs			0.92/0.92	0.96/0.97			0.96/0.96	0.97/0.97
R ²			0.80/0.80	0.95/0.96			0.96/0.95	0.95/0.95
RMSE (µg m ⁻³)			1.48/1.27	0.79/0.90			3.04/2.96	2.01/1.93
MAE (µg m ⁻³)			1.10/0.96	0.68/0.80			1.82/1.86	1.20/1.20
Slope			0.77/0.76	0.87/0.86			0.79/0.78	0.81/0.80
Delta Slope			0.23/0.24	0.13/0.14			0.21/0.22	0.19/0.20
Intercept			0.92/1.51	0.72/1.29			1.40/1.89	0.97/1.52
Intercept			0.92/1.51	0.72/1.29			1.40/1.89	0.97/1.52

Table S46. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

Metric	two-month variant Random Forest (AELCM010, AELCM009)							
	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95	0.96/0.95			0.89/0.89	0.97/0.96		0.95/0.95
R ²	0.88/0.88	0.96/0.95			0.89/0.89	0.97/0.97		0.91/0.91
RMSE (µg m ⁻³)	1.64/1.57	0.81/0.73			2.14/2.09	0.96/0.95		1.49/1.44
MAE (µg m ⁻³)	0.95/0.91	0.65/0.58			1.72/1.66	0.77/0.75		1.02/0.97
Slope	0.62/0.63	0.89/0.93			0.81/0.82	0.97/0.99		0.86/0.88
Delta Slope	0.38/0.37	0.11/0.07			0.19/0.18	0.03/0.01		0.14/0.12
Intercept	1.93/1.91	0.42/0.29			0.08/0.02	-0.03/-0.08		0.39/0.35
Intercept	1.93/1.91	0.42/0.29			0.08/0.02	0.03/0.08		0.39/0.35
AELCM009								
Rs			0.93/0.93	0.98/0.97			0.97/0.97	0.98/0.98
R ²			0.85/0.84	0.96/0.96			0.96/0.95	0.96/0.95
RMSE (µg m ⁻³)			1.18/1.19	0.85/0.84			2.98/2.64	1.92/1.74
MAE (µg m ⁻³)			0.86/0.87	0.63/0.61			1.77/1.50	1.09/0.99
Slope			0.84/0.98	0.87/1.01			0.84/0.85	0.84/0.86
Delta Slope			0.16/0.02	0.13/0.01			0.16/0.15	0.16/0.14
Intercept			0.65/0.54	0.34/0.34			0.44/0.87	0.55/1.18
Intercept			0.65/0.54	0.34/0.34			0.44/0.87	0.55/1.18

Table S47. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.92/0.92	0.92/0.94			0.89/0.89	0.96/0.96		0.92/0.93
R ²	0.77/0.79	0.95/0.95			0.88/0.88	0.96/0.96		0.85/0.85
RMSE (µg m ⁻³)	2.09/2.06	1.20/1.19			2.24/2.06	1.12/1.14		1.74/1.67
MAE (µg m ⁻³)	1.43/1.46	0.93/0.95			1.77/1.55	0.83/0.83		1.24/1.20
Slope	0.46/0.45	0.66/0.65			0.84/0.82	1.01/0.99		0.84/0.82
Delta Slope	0.54/0.55	0.34/0.35			0.16/0.18	0.01/0.01		0.16/0.18
Intercept	3.12/3.34	2.36/2.50			-0.22/0.19	0.16/0.51		0.84/1.11
Intercept	3.12/3.34	2.36/2.50			0.22/0.19	0.16/0.51		0.84/1.11
AELCM009								
Rs			0.84/0.90	0.94/0.96			0.98/0.98	0.96/0.97
R ²			0.76/0.81	0.94/0.95			0.98/0.98	0.97/0.97
RMSE (µg m ⁻³)			1.78/1.26	1.31/1.09			1.86/1.65	1.67/1.35
MAE (µg m ⁻³)			1.26/0.93	0.96/1.01			1.25/1.27	1.16/1.07
Slope			0.62/0.66	0.79/0.79			0.92/0.88	0.90/0.87
Delta Slope			0.38/0.34	0.21/0.21			0.08/0.12	0.10/0.13
Intercept			1.80/2.60	0.30/1.82			-0.02/1.51	-0.20/1.28
Intercept			1.80/2.60	0.30/1.82			0.02/1.51	0.20/1.28

Table S48. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the two-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95	0.96/0.96			0.90/0.90	0.96/0.96		0.95/0.95
R ²	0.89/0.90	0.97/0.97			0.88/0.88	0.95/0.95		0.90/0.91
RMSE (µg m ⁻³)	1.67/1.56	0.73/0.63			2.11/2.00	1.10/1.10		1.50/1.42
MAE (µg m ⁻³)	0.96/0.89	0.59/0.50			1.67/1.56	0.90/0.89		1.03/0.96
Slope	0.63/0.65	0.94/0.97			0.83/0.85	0.95/0.97		0.88/0.90
Delta Slope	0.37/0.35	0.06/0.03			0.17/0.15	0.05/0.03		0.12/0.10
Intercept	1.67/1.67	-0.00/-0.08			-0.02/-0.07	0.45/0.43		0.26/0.25
Intercept	1.67/1.67	0.00/0.08			0.02/0.07	0.45/0.43		0.26/0.25
AELCM009								
Rs			0.93/0.93	0.97/0.97			0.98/0.98	0.98/0.98
R ²			0.86/0.84	0.96/0.96			0.98/0.98	0.97/0.96
RMSE (µg m ⁻³)			1.34/1.18	1.01/0.67			3.61/2.76	2.30/1.78
MAE (µg m ⁻³)			1.02/0.84	0.74/0.50			2.53/1.84	1.43/1.06
Slope			0.85/1.02	0.87/1.01			0.77/0.81	0.77/0.82
Delta Slope			0.15/0.02	0.13/0.01			0.23/0.19	0.23/0.18
Intercept			0.28/0.00	0.00/0.01			0.61/0.92	0.64/1.13
Intercept			0.28/0.00	0.00/0.01			0.61/0.92	0.64/1.13

Table S49. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on XGB, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variant Extreme Gradient Boosting (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.94/0.94	0.94/0.93	0.92/0.93				0.97/0.97	0.97/0.96
R ²	0.86/0.84	0.95/0.93	0.86/0.85				0.95/0.95	0.94/0.94
RMSE (µg m ⁻³)	2.12/2.02	1.38/1.27	1.30/1.16				3.28/3.19	2.17/2.07
MAE (µg m ⁻³)	1.28/1.19	1.11/1.03	0.92/0.82				1.88/1.76	1.29/1.20
Slope	0.52/0.52	0.78/0.78	0.80/0.80				0.81/0.81	0.80/0.79
Delta Slope	0.48/0.48	0.22/0.22	0.20/0.20				0.19/0.19	0.20/0.21
Intercept	2.01/2.31	0.57/0.82	0.76/1.08				0.69/0.86	0.56/0.83
Intercept	2.01/2.31	0.57/0.82	0.76/1.08				0.69/0.86	0.56/0.83
AELCM009								
Rs				0.96/0.97	0.87/0.87	0.95/0.95		0.95/0.95
R ²				0.95/0.96	0.85/0.86	0.93/0.94		0.90/0.90
RMSE (µg m ⁻³)				0.79/0.78	2.34/1.99	1.34/1.31		1.62/1.44
MAE (µg m ⁻³)				0.68/0.69	1.82/1.49	1.06/1.03		1.18/1.07
Slope				0.87/0.90	0.75/0.78	0.89/0.93		0.85/0.88
Delta Slope				0.13/0.10	0.25/0.22	0.11/0.07		0.15/0.12
Intercept				0.72/0.90	0.60/0.80	0.98/1.08		0.66/0.81
Intercept				0.72/0.90	0.60/0.80	0.98/1.08		0.66/0.81

Table S50. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RF, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variants Random Forest (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95	0.96/0.93	0.93/0.93				0.97/0.97	0.97/0.97
R ²	0.88/0.85	0.96/0.93	0.87/0.85				0.98/0.97	0.96/0.96
RMSE (µg m ⁻³)	1.64/1.61	0.81/0.83	0.98/1.12				1.72/1.70	1.35/1.36
MAE (µg m ⁻³)	0.95/1.01	0.65/0.67	0.68/0.86				0.88/0.91	0.79/0.86
Slope	0.62/0.61	0.89/0.90	0.90/0.94				0.95/0.94	0.92/0.92
Delta Slope	0.38/0.39	0.11/0.10	0.10/0.06				0.05/0.06	0.08/0.08
Intercept	1.93/2.34	0.42/0.66	0.60/0.80				0.12/0.30	0.24/0.63
Intercept	1.93/2.34	0.42/0.66	0.60/0.80				0.12/0.30	0.24/0.63
AELCM009								
Rs				0.98/0.97	0.90/0.90	0.95/0.95		0.96/0.96
R ²				0.96/0.96	0.88/0.88	0.95/0.95		0.92/0.91
RMSE (µg m ⁻³)				0.85/0.66	2.60/2.23	1.63/1.27		1.84/1.53
MAE (µg m ⁻³)				0.63/0.54	2.08/1.76	1.27/1.01		1.33/1.11
Slope				0.87/0.95	0.73/0.81	0.88/1.04		0.82/0.95
Delta Slope				0.13/0.05	0.27/0.19	0.12/0.04		0.18/0.05
Intercept				0.34/0.10	0.32/0.01	0.15/-0.41		0.29/-0.17
Intercept				0.34/0.10	0.32/0.01	0.15/0.41		0.29/0.17

Table S51. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on RR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variant Ridge Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.92/0.92	0.92/0.95	0.88/0.89				0.98/0.99	0.95/0.96
R ²	0.77/0.80	0.95/0.96	0.81/0.83				0.99/0.99	0.95/0.95
RMSE (µg m ⁻³)	2.09/2.01	1.20/1.19	1.27/1.16				1.01/1.06	1.45/1.41
MAE (µg m ⁻³)	1.43/1.52	0.93/1.03	0.85/0.88				0.70/0.86	0.98/1.07
Slope	0.46/0.45	0.66/0.66	0.72/0.72				0.99/0.95	0.93/0.90
Delta Slope	0.54/0.55	0.34/0.34	0.28/0.28				0.01/0.05	0.07/0.10
Intercept	3.12/3.64	2.36/2.81	1.80/2.27				0.41/0.93	0.38/1.05
Intercept	3.12/3.64	2.36/2.81	1.80/2.27				0.41/0.93	0.38/1.05
AELCM009								
Rs				0.94/0.96	0.89/0.89	0.95/0.95		0.94/0.95
R ²				0.94/0.95	0.87/0.87	0.95/0.95		0.89/0.90
RMSE (µg m ⁻³)				1.31/0.93	3.18/2.16	1.53/1.16		2.17/1.51
MAE (µg m ⁻³)				0.96/0.85	2.75/1.62	1.19/0.93		1.63/1.13
Slope				0.79/0.80	0.75/0.75	0.93/0.93		0.85/0.85
Delta Slope				0.21/0.20	0.25/0.25	0.07/0.07		0.15/0.15
Intercept				0.30/1.41	-0.51/0.75	-0.34/0.80		-0.30/0.88
Intercept				0.30/1.41	0.51/0.75	0.34/0.80		0.30/0.88

Table S52. Performance metrics of the single PM_{2.5} LCS in each AELCM box (AELCM010 and AELCM009) across different TPs following calibration. The calibration models are based on MLR, using both ST and ET variants. The ET is characterized by the three-month variant for each AELCM box. The ‘All’ column shows performance metrics calculated from data aggregated across all TPs. Performance metrics are calculated from daily mean values.

two-month variant Multiple Linear Regression (AELCM010, AELCM009)								
Metric	TP 1 (ST / ET)	TP 2 (ST / ET)	TP 3 (ST / ET)	TP 4 (ST / ET)	TP 5 (ST / ET)	TP 6 (ST / ET)	TP 7 (ST / ET)	All (ST / ET)
AELCM010								
Rs	0.95/0.95	0.96/0.97	0.93/0.93				0.98/0.98	0.97/0.97
R ²	0.89/0.90	0.97/0.97	0.87/0.87				0.99/0.99	0.97/0.97
RMSE (µg m ⁻³)	1.67/1.33	0.73/0.60	1.03/1.06				2.02/2.25	1.45/1.44
MAE (µg m ⁻³)	0.96/0.82	0.59/0.48	0.69/0.78				1.28/1.47	0.88/0.89
Slope	0.63/0.69	0.94/1.03	0.90/0.99				0.87/0.84	0.87/0.84
Delta Slope	0.37/0.31	0.06/0.03	0.10/0.01				0.13/0.16	0.13/0.16
Intercept	1.67/1.76	-0.00/-0.11	0.46/0.40				0.66/0.92	0.50/1.11
Intercept	1.67/1.76	0.00/0.11	0.46/0.40				0.66/0.92	0.50/1.11
AELCM009								
Rs				0.97/0.97	0.90/0.90	0.95/0.95		0.96/0.96
R ²				0.96/0.96	0.88/0.88	0.95/0.95		0.92/0.92
RMSE (µg m ⁻³)				1.01/0.69	2.79/2.15	1.76/1.24		1.99/1.49
MAE (µg m ⁻³)				0.74/0.57	2.31/1.71	1.36/1.00		1.47/1.09
Slope				0.87/0.98	0.76/0.86	0.85/0.94		0.82/0.91
Delta Slope				0.13/0.02	0.24/0.14	0.15/0.06		0.18/0.09
Intercept				0.00/-0.09	-0.14/-0.30	0.28/0.24		0.04/-0.01
Intercept				0.00/0.09	0.14/0.30	0.28/0.24		0.04/0.01

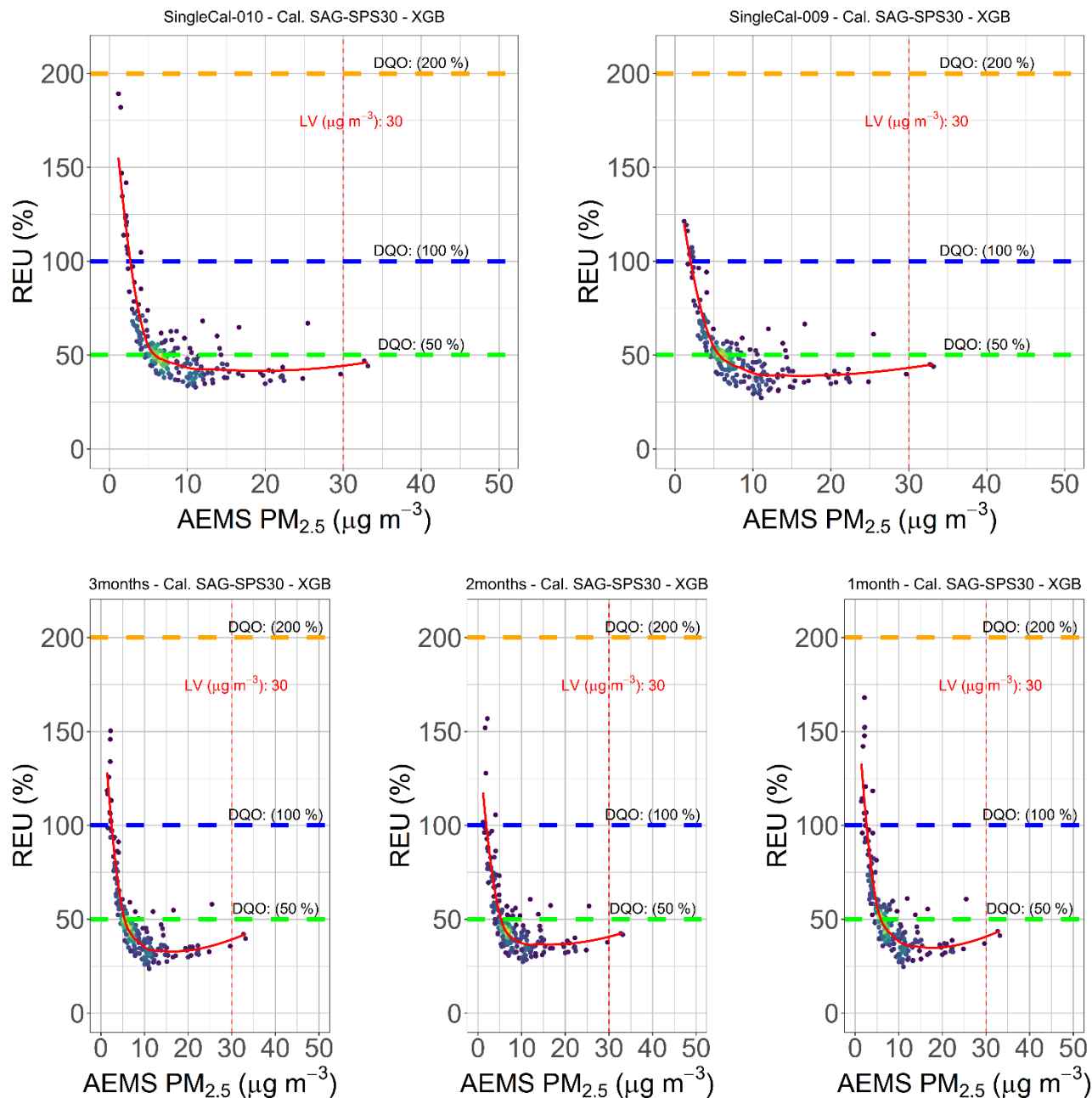


Figure S21. Calculated REU values for XGB calibrated $\text{PM}_{2.5}$ LCS daily data belonging to the TPs (TP1–TP7, 11 June 2022–6 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs ($\text{PM}_{2.5}$ Class 1 DQO = 50 %, Class 2 DQO = 100 % and Class 3 DQO = 200 %). The vertical dashed line describes the limit value for $\text{PM}_{2.5}$ (LV = $30 \mu\text{g m}^{-3}$). The fitted smooth curve (red) is based on locally estimated scatterplot smoothing (LOESS). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

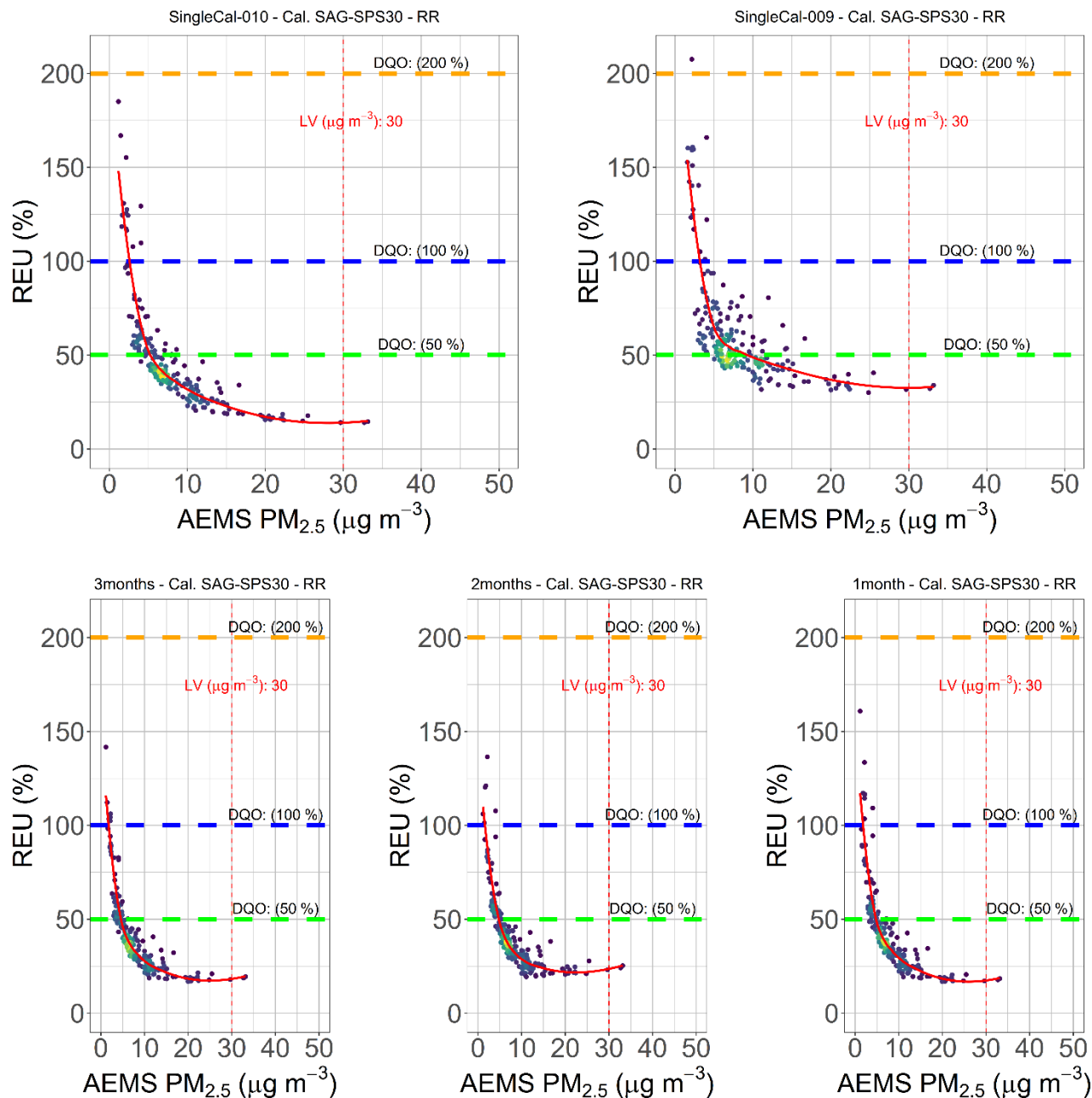


Figure S22. Calculated REU values for RR calibrated $PM_{2.5}$ LCS daily data belonging to the TPs (TP1–TP7, 11 June 2022–6 January 2023) of AELCM009 and AELCM010. The calibration variants are ST (top row) and ET (bottom row). The ET is characterized by ET variants of 1, 2 and 3 months for each AELCM box. Horizontal dashed lines describe the DQOs ($PM_{2.5}$ Class 1 DQO = 50 %, Class 2 DQO = 100 % and Class 3 DQO = 200 %). The vertical dashed line describes the limit value for $PM_{2.5}$ (LV = $30 \mu g m^{-3}$). The fitted smooth curve (red) is based on locally estimated scatterplot smoothing (LOESS). Data density is shown through colour, where darker colours express lower data density and brighter colours express higher data density.

Table S53. Model variables for the development of the calibration functions based on MLR, RR, RF and XGB.

Calibration Model	NO ₂ Model Features	CO Model Features
MLR	V _{NO2} , V _{CO} , RH, T, V _{NO2} * T	V _{CO} , RH, T, V _{CO} * T, $\frac{(V_{CO})^2-1}{2}$
RR	V _{NO2} , V _{CO} , RH, T	V _{CO} , RH, T
RF	V _{NO2} , V _{CO} , RH, T	V _{CO} , RH, T
XGB	V _{NO2} , V _{CO} , RH, T	V _{CO} , RH, T