

Supplement of Development of Low-Cost Air Quality Stations for Next Generation Monitoring Networks: Calibration and Validation of NO₂ and O₃ Sensors

Table S1. Summary of pre-deployment calibration and field validation procedures performed in the study.

City	Lat. (deg N)	Lon. (deg E)	Time period	Time step	Process	No. records by pollutant (AQ1–AQ2)
Florence	43°47'52"	11°11'31"	2017/07/19–2017/09/27	3 min	Pre-deployment calibration	NO ₂ : 19223–17275 O ₃ : 19223–17275
Montale	43°54'57"	11°00'26"	2018/06/19–2019/08/22	1 H	Field validation	NO ₂ : 7383–9340 O ₃ : 7344–9303

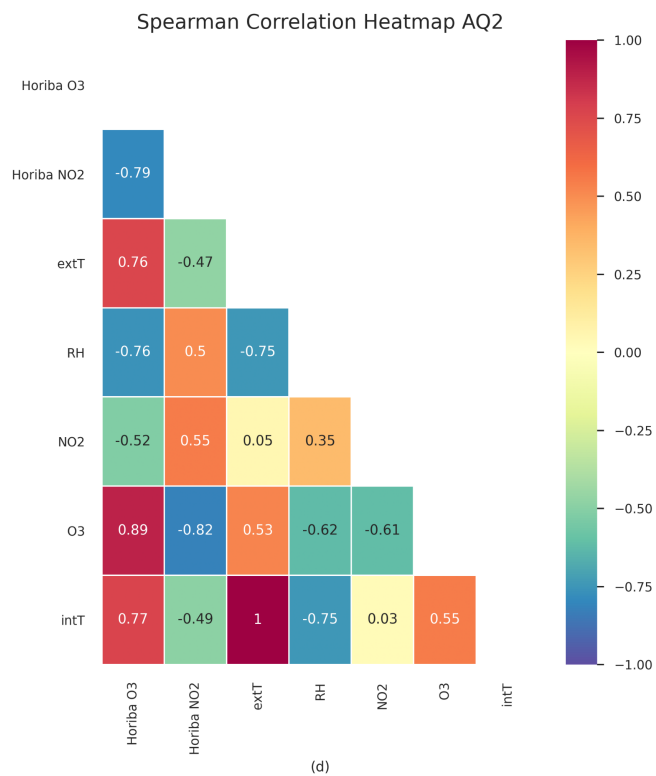
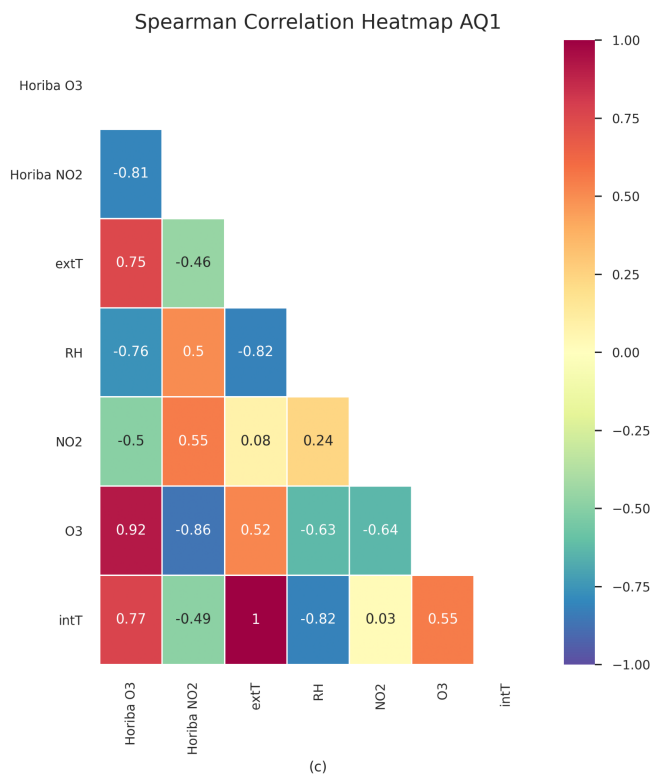
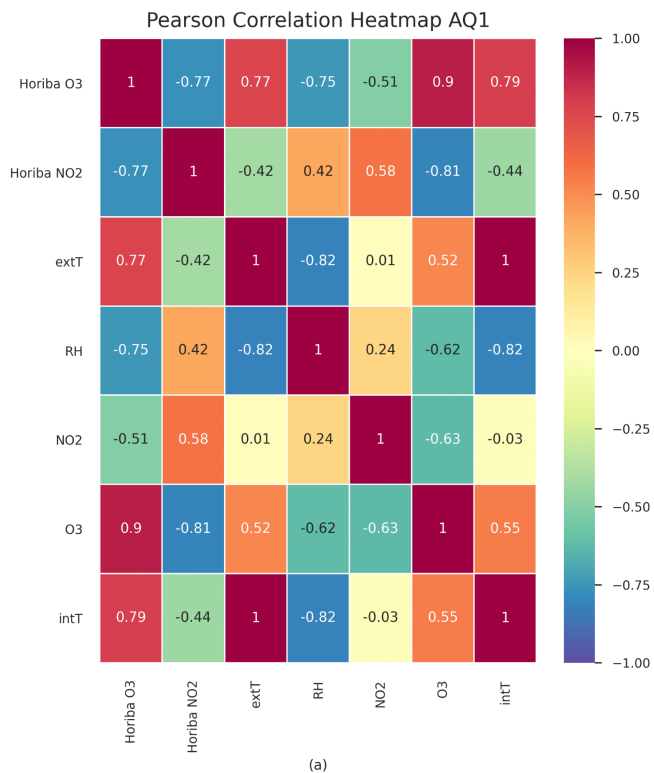


Figure S2. Correlation matrices for AQ1 and AQ2 calibration: Pearson correlation for AQ1 (a) and AQ2 (b); Spearman correlation for AQ1 (c) and AQ2 (d).

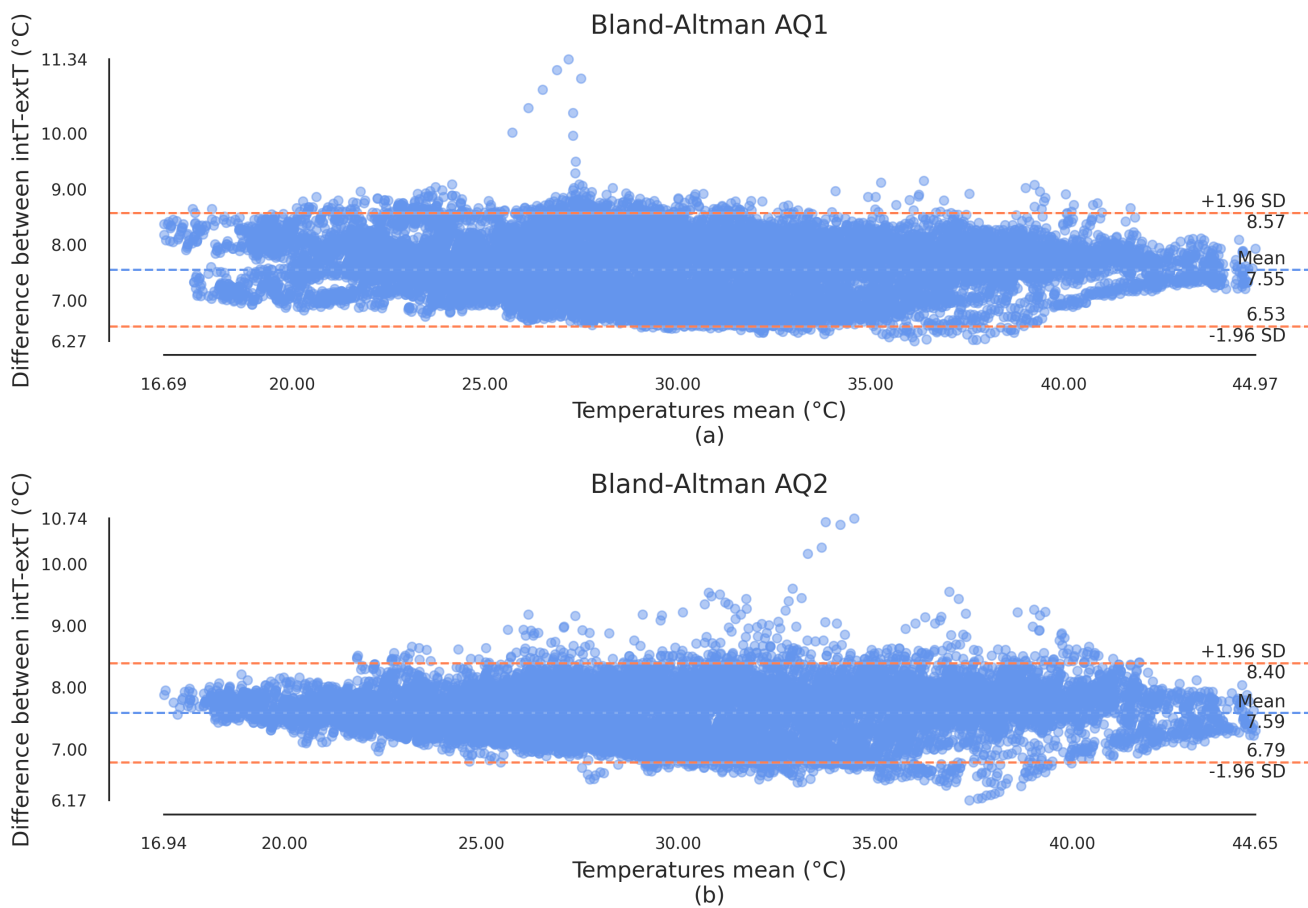


Figure S3. Bland–Altman plots of extT and intT for AQ1 (a) and AQ2 (b). The red lines indicate the limit of agreement (± 1.96 SD) of temperature differences, whilst the blue lines show the average difference between the temperatures.

Table S4. Variance inflation factors (VIF) for the main covariates set.

Pollutant	AQ id	Variables	Intercept	O3	NO2	intT	extT	RH
O3	AQ1	O3,intT	47.38	1.44	-	1.44	-	-
		O3,intT,RH	299.06	1.63	-	3.08	-	3.45
		O3,intT,extT,RH	441.18	1.95	-	151.19	147.78	3.55
		O3,NO2,intT,RH	304.88	3.13	2.25	4.00	-	3.61
		O3,NO2,intT,extT,RH	465.46	3.24	2.35	153.54	154.09	3.77
	AQ2	O3,intT	54.05	1.44	-	1.44	-	-
		O3,intT,RH	210.67	1.63	-	2.30	-	2.52
		O3,intT,extT,RH	472.01	1.92	-	237.86	232.71	2.57
		O3,NO2,intT,RH	221.90	2.97	2.24	3.03	-	2.72
		O3,NO2,intT,extT,RH	484.17	3.25	2.24	238.39	232.72	2.77
NO2	AQ1	NO2,intT	36.86	-	1.00	1.00	-	-
		NO2,intT,RH	241.53	-	1.17	3.37	-	3.58
		NO2,intT,extT,RH	434.86	-	1.42	144.55	149.03	3.70
		NO2,O3,intT,RH	304.88	3.13	2.25	4.00	-	3.61
		NO2,O3,intT,extT,RH	465.46	3.24	2.35	153.54	154.09	3.77
	AQ2	NO2,intT	37.46	-	1.01	1.01	-	-
		NO2,intT,RH	149.67	-	1.23	2.40	-	2.71
		NO2,intT,extT,RH	472.57	-	1.32	211.00	212.93	2.74
		NO2,O3,intT,RH	221.90	2.97	2.24	3.03	-	2.72
		NO2,O3,intT,extT,RH	484.17	3.25	2.24	238.39	232.72	2.77

Table S5. Summary of MLR O3 models for AQ1 and AQ2.

Pollutant	AQ id	Variables	Coefficient					R ²	RMSE	AIC	Stat.		
			β_0	β_1	β_2	β_3	β_4				AdjR ²	MAE	MBE
O3	AQ1	O3	-146.10	0.40	-	-	-	0.81	16.92	1.09E+05	0.81	13.42	-0.28
		intT	-109.92	5.46	-	-	-	0.61	24.33	1.19E+05	0.62	19.56	0.21
		RH	165.02	-1.71	-	-	-	0.57	25.61	1.21E+05	0.57	20.35	-0.17
		NO2	97.15	-0.31	-	-	-	0.27	33.63	1.27E+05	0.27	27.42	-0.46
		O3,intT	-186.58	0.30	2.88	-	-	0.94	9.92	9.52E+04	0.94	7.39	-0.06
		O3,RH	-61.47	0.32	-0.71	-	-	0.88	13.61	1.04E+05	0.88	10.69	-0.26
		NO2,O3	-162.73	0.05	0.43	-	-	0.82	16.74	1.09E+05	0.82	13.24	-0.23
		RH,intT	-12.71	-0.71	3.70	-	-	0.65	23.07	1.17E+05	0.65	18.21	0.09
		NO2,intT	-84.20	-0.29	5.36	-	-	0.86	14.52	1.05E+05	0.86	11.35	-0.11
		NO2,RH	170.74	-0.21	-1.52	-	-	0.69	21.88	1.17E+05	0.69	17.50	-0.39
	AQ2	O3,RH,intT	-193.19	0.30	0.04	2.97	-	0.94	9.93	9.52E+04	0.94	7.39	-0.06
		NO2,O3,intT	-159.76	-0.10	0.23	3.44	-	0.95	8.69	9.18E+04	0.95	6.39	-0.12
		NO2,O3,RH	-64.32	0.01	0.32	-0.71	-	0.88	13.60	1.04E+05	0.88	10.69	-0.26
		NO2,RH,intT	-87.77	-0.29	0.03	5.42	-	0.86	14.52	1.05E+05	0.86	11.36	-0.11
		NO2,O3,RH,intT	-180.76	-0.11	0.23	0.15	3.79	0.95	8.62	9.14E+04	0.95	6.30	-0.10
		O3	-140.53	0.31	-	-	-	0.77	17.58	9.93E+04	0.77	14.11	0.14
		intT	-90.68	5.04	-	-	-	0.64	22.12	1.04E+05	0.64	18.07	-0.24
		RH	148.13	-1.37	-	-	-	0.55	24.62	1.07E+05	0.55	19.48	-0.29
		NO2	101.33	-0.34	-	-	-	0.31	30.43	1.12E+05	0.31	24.74	0.23
		O3,intT	-174.35	0.23	2.86	-	-	0.91	10.86	8.83E+04	0.91	8.18	-0.05
O3,RH	-59.90	0.24	-0.61	-	-	0.84	14.77	9.51E+04	0.84	11.96	-0.03		
NO2,O3	-139.86	-0.00	0.31	-	-	0.77	17.58	9.93E+04	0.77	14.11	0.14		
RH,intT	-9.43	-0.60	3.52	-	-	0.69	20.50	1.03E+05	0.69	16.33	-0.30		
NO2,intT	-62.83	-0.30	4.79	-	-	0.89	12.22	9.07E+04	0.89	9.52	-0.08		
NO2,RH	150.72	-0.21	-1.15	-	-	0.65	21.64	1.04E+05	0.65	17.38	-0.13		
O3,RH,intT	-155.80	0.22	-0.12	2.62	-	0.91	10.76	8.81E+04	0.91	8.18	-0.07		
NO2,O3,intT	-129.74	-0.16	0.14	3.51	-	0.94	8.59	8.30E+04	0.95	6.51	-0.04		
NO2,O3,RH	-53.73	-0.02	0.24	-0.62	-	0.84	14.76	9.51E+04	0.84	11.96	-0.03		
NO2,RH,intT	-60.82	-0.30	-0.02	4.76	-	0.89	12.21	9.07E+04	0.89	9.52	-0.09		
NO2,O3,RH,intT	-133.43	-0.16	0.14	0.03	3.58	0.94	8.58	8.29E+04	0.95	6.50	-0.03		

Table S6. Summary of MLR NO₂ models for AQ1 and AQ2.

Pollutant	AQ id	Variables	Coefficient					R ²	RMSE	AIC	Stat		
			β_0	β_1	β_2	β_3	β_4				AdjR ²	MAE	MBE
NO ₂	AQ1	NO2	13.03	0.15	-	-	-	0.34	14.22	1.05E+05	0.34	10.91	0.09
		intT	70.28	-1.36	-	-	-	0.19	15.72	1.07E+05	0.19	12.14	-0.16
		RH	2.19	0.42	-	-	-	0.18	15.81	1.08E+05	0.18	12.25	-0.07
		O3	111.52	-0.16	-	-	-	0.66	10.22	9.61E+04	0.66	7.74	-0.01
		NO2,intT	57.18	0.15	-1.30	-	-	0.52	12.14	1.01E+05	0.52	9.17	0.01
		NO2,RH	-1.44	0.13	0.30	-	-	0.42	13.28	1.03E+05	0.42	9.99	0.08
		NO2,O3	101.09	0.03	-0.14	-	-	0.67	10.09	9.57E+04	0.67	7.64	0.01
		RH,intT	47.73	0.17	-0.95	-	-	0.20	15.59	1.07E+05	0.20	12.02	-0.13
		O3,intT	111.23	-0.16	0.02	-	-	0.66	10.22	9.61E+04	0.66	7.74	-0.01
		O3,RH	127.09	-0.18	-0.13	-	-	0.67	10.10	9.57E+04	0.67	7.67	-0.01
	NO2,RH,intT	89.29	0.16	-0.24	-1.90	-	0.53	11.96	1.00E+05	0.53	9.09	-0.02	
	NO2,O3,intT	100.92	0.04	-0.13	-0.19	-	0.67	10.06	9.57E+04	0.67	7.61	0.01	
	NO2,O3,RH	116.25	0.02	-0.16	-0.11	-	0.67	10.01	9.55E+04	0.67	7.61	0.01	
	O3,RH,intT	150.78	-0.17	-0.27	-0.54	-	0.68	9.97	9.53E+04	0.67	7.57	-0.05	
	NO2,O3,RH,intT	144.78	0.05	-0.14	-0.32	-0.93	0.69	9.68	9.45E+04	0.69	7.36	-0.03	
	AQ2	NO2	11.81	0.16	-	-	-	0.38	12.86	9.22E+04	0.38	9.83	-0.09
		intT	66.88	-1.31	-	-	-	0.21	14.45	9.49E+04	0.21	10.91	0.07
		RH	4.94	0.35	-	-	-	0.19	14.67	9.54E+04	0.19	11.09	0.08
		O3	113.00	-0.13	-	-	-	0.64	9.79	8.58E+04	0.64	7.35	-0.04
		NO2,intT	52.45	0.16	-1.19	-	-	0.55	10.91	8.85E+04	0.55	8.19	-0.01
NO2,RH		3.19	0.14	0.20	-	-	0.43	12.28	9.12E+04	0.43	9.25	-0.03	
NO2,O3		97.76	0.05	-0.11	-	-	0.66	9.53	8.52E+04	0.66	7.15	-0.06	
RH,intT		47.54	0.14	-0.95	-	-	0.23	14.28	9.47E+04	0.23	10.73	0.08	
O3,intT		114.00	-0.13	-0.08	-	-	0.64	9.78	8.58E+04	0.64	7.34	-0.04	
O3,RH		123.40	-0.14	-0.08	-	-	0.64	9.72	8.56E+04	0.64	7.32	-0.07	
NO2,RH,intT	77.38	0.17	-0.20	-1.67	-	0.57	10.71	8.79E+04	0.57	8.07	-0.04		
NO2,O3,intT	96.78	0.06	-0.10	-0.34	-	0.67	9.41	8.50E+04	0.67	7.04	-0.04		
NO2,O3,RH	107.47	0.04	-0.12	-0.07	-	0.66	9.48	8.51E+04	0.66	7.14	-0.08		
O3,RH,intT	137.80	-0.13	-0.15	-0.39	-	0.65	9.63	8.53E+04	0.65	7.26	-0.06		
NO2,O3,RH,intT	126.78	0.08	-0.10	-0.23	-0.87	0.69	9.07	8.40E+04	0.69	6.83	-0.08		

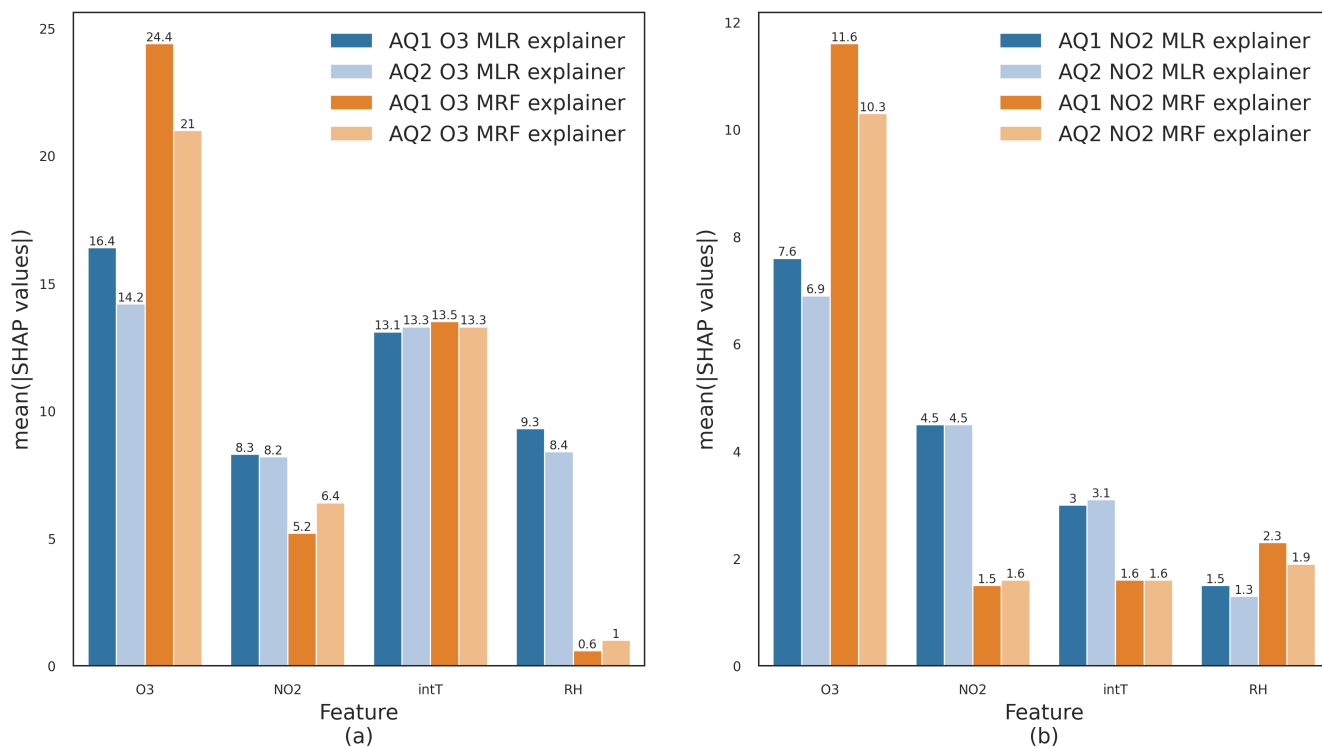


Figure S7. Mean absolute SHAP values of all features for MLR and MRF models for O3 and NO2 concentrations at AQ1 and AQ2 stations. The effect of intT, RH, O3 and NO2 raw data on the overall output of the training model is also shown.

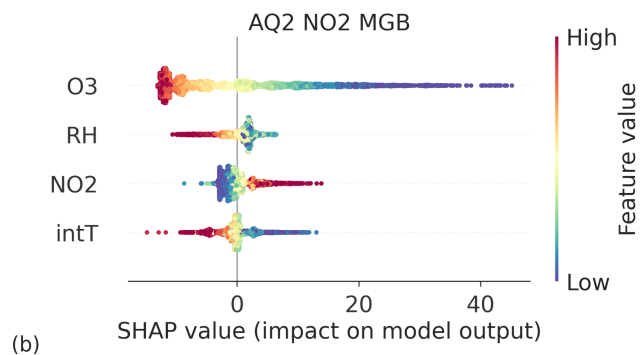
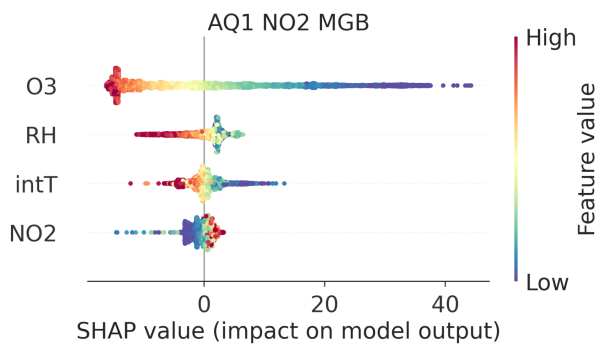
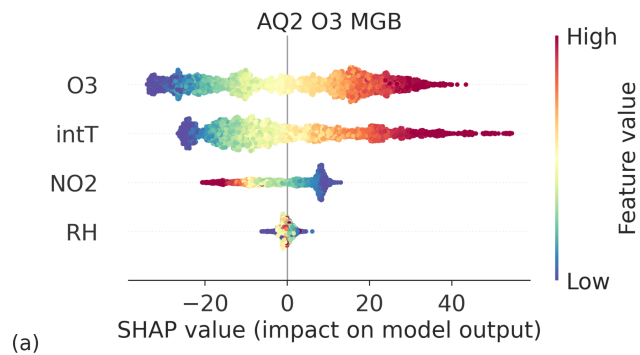
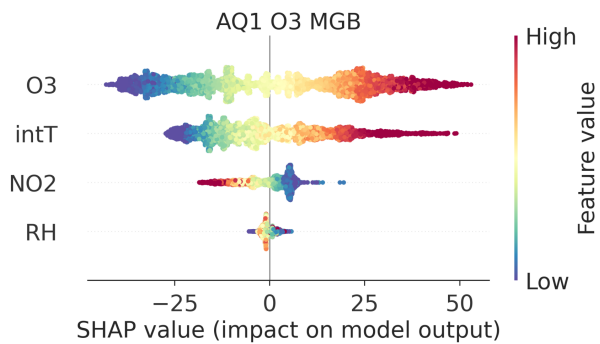


Figure S8. Beeswarm MGB

Table S9. Statistics of the MLR and MRF calibrated models assessed during the field validation procedure.

Pollutant	AQ id	Stat.	MLR	MRF
O3	AQ1	r	0.92	0.81
		CRMSD	15.98	24.13
		RMSE	16.52	29.08
		MAE	12.96	22.22
		MBE	4.20	16.23
	AQ2	r	0.93	0.76
		CRMSD	15.35	25.44
		RMSE	17.88	42.98
		MAE	13.99	36.24
		MBE	9.17	34.64
NO2	AQ1	r	0.75	0.65
		CRMSD	11.25	11.83
		RMSE	12.64	13.48
		MAE	9.40	9.97
		MBE	5.75	6.46
	AQ2	r	0.78	0.58
		CRMSD	10.63	11.77
		RMSE	10.65	11.94
		MAE	7.72	9.12
		MBE	-0.69	2.03



Figure S10. Trend analysis of 7-day average O₃ and NO₂ concentrations measured at the validation site by the calibrated AQ1 and AQ2 stations compared to the ARPAT reference station (17 June 2019–22 August 2019).

Table S11. Seasonal analysis of MFR validation. Min–Max ($\mu\text{g m}^{-3}$) represents the minimum and maximum concentrations measured by the reference station, while intT is the average internal temperature measured by the AQ stations.

Year	Season	Pollutant	AQ id	min-max	intT	r	Stat.		
							nRMSE	MAE	MBE
2018	Summer	O ₃	AQ1	6 - 166	34.65	0.90	10.20	12.58	-4.91
			AQ2	6 - 166	34.20	0.84	15.59	20.68	16.52
		NO ₂	AQ1	1 - 47	34.62	0.64	42.26	16.00	15.87
			AQ2	1 - 47	34.16	0.51	18.93	7.27	5.41
	Autumn	O ₃	AQ1	2 - 146	28.06	0.84	21.49	24.43	22.53
			AQ2	2 - 146	25.53	0.76	35.59	46.81	46.57
		NO ₂	AQ1	1 - 62	28.07	0.65	21.83	9.58	6.71
			AQ2	1 - 62	25.54	0.43	18.02	8.85	1.04
	Winter	O ₃	AQ1	2 - 65	16.60	0.88	52.57	22.13	21.12
			AQ2	2 - 72	14.53	0.83	67.43	39.32	39.17
		NO ₂	AQ1	3 - 88	16.59	0.71	17.59	11.65	3.42
			AQ2	2 - 88	14.53	0.57	20.64	13.40	-2.82
2019	Spring	O ₃	AQ1	2 - 132	22.41	0.75	29.11	32.63	31.92
			AQ2	2 - 132	21.14	0.68	35.91	40.38	39.57
		NO ₂	AQ1	2 - 63	22.32	0.67	12.73	5.67	-0.54
			AQ2	2 - 63	21.09	0.34	17.18	8.29	2.31
	Summer	O ₃	AQ1	7 - 185	34.98	0.82	13.42	19.44	12.35
			AQ2	7 - 185	32.29	0.75	20.71	31.31	28.19
		NO ₂	AQ1	0 - 47	34.94	0.50	22.19	8.19	6.81
			AQ2	0 - 47	32.25	0.34	18.00	7.28	5.05