Supplementary Materials

Improving Air Pollutant Metal Oxide Sensor Quantification Practices through: an Exploration of Sensor Signal Normalization, Multi-sensor and Universal Calibration Model Generation, and Physical Factors Such as Co-location Duration and Sensor Age

Kristen Okorn [1],* and Michael Hannigan [2]

[1] Environmental Engineering, University of Colorado Boulder, Boulder, CO 80309, USA
[2] Mechanical Engineering, University of Colorado Boulder, Boulder, CO 80309, USA;
Michael.Hannigan@Colorado.edu
*Correspondence: E: Kristen.Okorn@colorado.edu, P: (303) 735-8054

Table S1. Colocation Reference Instruments.

| Location		Gas	Reference Instrument	Responsible Agency
Boulder, CO – South Boulder Creek		O_3	Teledyne Model 400E Photometric Ozone Analyzer	Colorado Department of Public Health & Environment (CDPHE)
Boulder, CO – Boulder Campus		O_3	Continuous UV absorption Thermo-Scientific Ozone Monitor (49c, 3711)	National Oceanic and Atmospheric Administration (NOAA)
Shafter, CA		O_3	Teledyne API T400 Ozone Analyzer	California Air Resources Board
Los Angeles, CA		CH_4	Picarro CRDS*	South Coast Air Quality Management District (SCAQMD)
Los Angeles, CA		CH_4	Thermo Scientific 55i	South Coast Air Quality Management District (SCAQMD)
Wiggins, CO		O_3	N/A	N/A
Greeley, CO		CH_4	Los Gatos	South Coast Air Quality Management District (SCAQMD)

* - Primary reference instrument
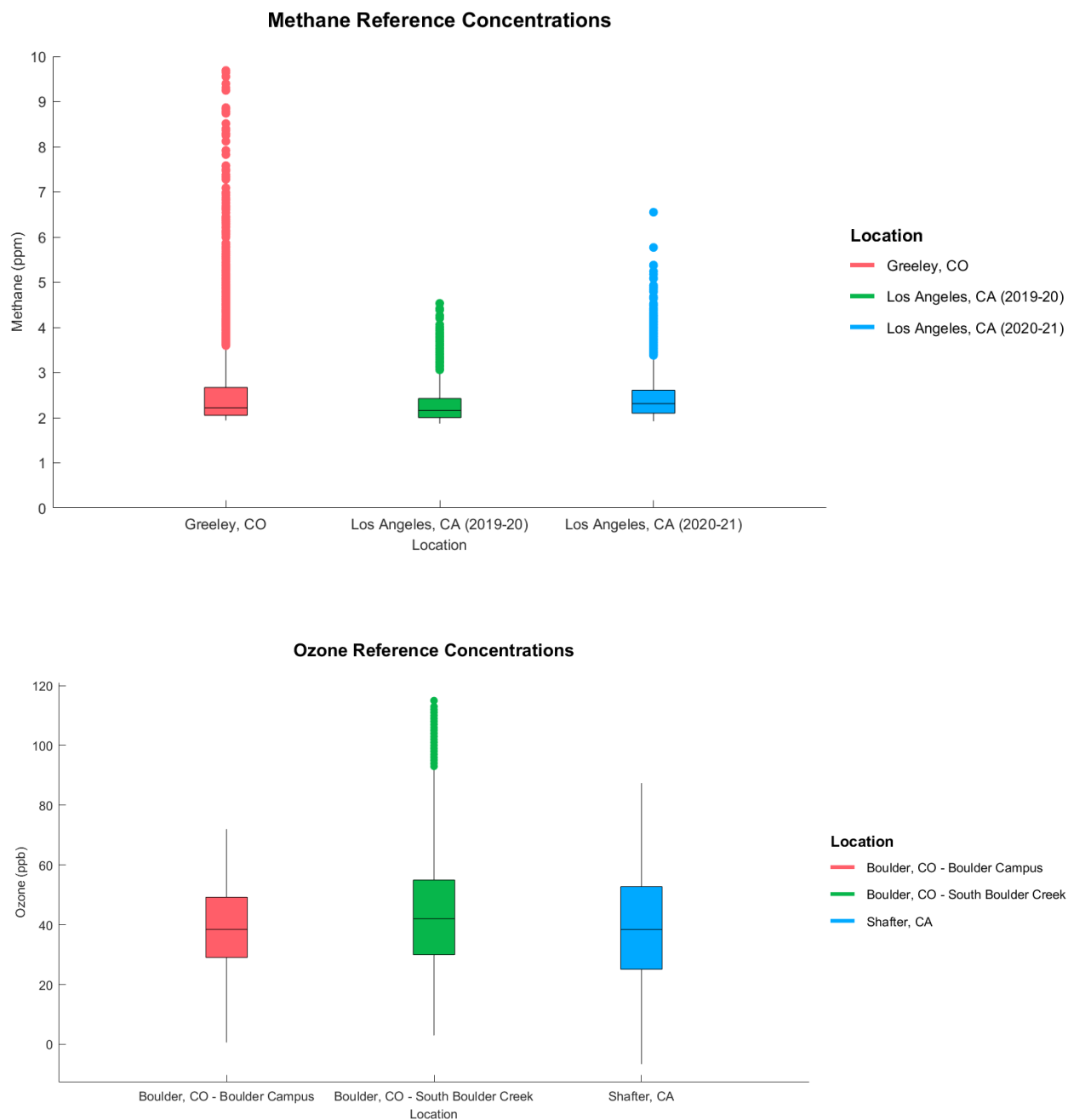
Figure S1. Reference Instrument Concentrations for methane (top) and ozone (bottom).

Table S2: Calibration and Validation Data Split and Rationale

Application	Section	Pollutant	Calibration		Validation		Rationale
			Dates	Location	Dates	Location	
Applying Calibration Models	3.1.1, 3.3.1, 3.6	CH_4	9/24/19 - 10/18/19	Los Angeles	11/12/19 - 12/25/19	Los Angeles	Different months of data selected – slight differences in temperature & humidity spaces over time
	3.1.1, 3.3.1, 3.6	CH_4	8/31/20 - 9/24/20	Greeley	4/20/20 - 4/28/20	Wiggins	Reference data needed for calibration (only available at Greeley); Wiggins validation by default
	3.1.2	O_3	2/13/19 - 2/19/19, 9/13/19 - 9/23/19	Shafter	6/12/19 - 6/19/19	Shafter	2 weeks of calibration data "bookend" 1 week of validation data
	3.1.2	O_3	6/15/15 - 6/25/15	South Boulder Creek	6/11/15 - 6/18/15	Boulder Campus	2 different sets of pods and reference instruments; randomly selected one set as calibration and the other as validation
Length of Colocation / Multiple Reference Instruments	3.2	CH_4	11/25/19 - 1/18/20	Los Angeles	11/25/19 - 1/18/20	Los Angeles	Calibration & validation randomly selected during period of greatest instrument overlap; previous calibration becomes validation 2
Co-locating & deploying sensors in different	3.4	CH_4	9/24/19 - 10/18/19	Los Angeles	8/31/20 - 9/24/20	Greeley	Same CA calibration data used, Greeley data used as validation due to lack of a reference instrument at original validation site (Wiggins)

environments							
Age of sensors	3.5	CH_4	11/13/20 - 1/7/21	Los Angeles	9/24/19 - 10/18/19	Los Angeles	New LA calibration data used (post sensor replacement), original 2019 CA data now as validation

Table S3: Measures of fit for methane calibration models

Method	Colorado Calibration				California Calibration				California Validation			
	R²	MBE	CRMSD	RMSE	R²	MBE	CRMSD	RMSE	R²	MBE	CRMSD	RMSE
Individual	0.696	0.000	0.279	0.269	0.823	0.000	0.138	0.0471	0.780	0.388	0.148	0.0453
	0.685	0.000	0.294	0.274	0.785	0.000	0.148	0.0319	0.786	0.044	0.152	0.0369
	0.673	0.000	0.279	0.279	0.793	0.000	0.140	0.0485	0.793	-0.980	0.222	0.0465
	0.665	0.000	0.290	0.290	0.808	0.000	0.142	0.0344	0.799	-0.821	0.193	-
	0.690	0.000	-	0.272	0.807	-	-	-	-	-	-	-
	0.694	0.000	-	0.270	0.774	-	-	-	-	-	-	-
	-	-	-	-	0.806	-	-	-	-	-	-	-
	-	-	-	-	0.785	-	-	-	-	-	-	-
	-	-	-	-	0.811	-	-	-	-	-	-	-
Z-individual	0.708	0.000	0.061	0.264	0.798	0.000	0.135	0.135	0.791	0.041	0.149	0.1703
	0.699	0.000	0.069	0.268	0.793	0.000	0.137	0.137	0.794	0.041	0.149	0.1703
	0.709	0.038	0.074	0.263	0.797	0.000	0.135	0.136	0.804	-0.027	0.162	0.187
	0.672	0.000	0.082	0.287	0.805	0.000	0.133	0.133	-	0.013	0.151	0.1712
	0.721	0.000	0.084	0.258	-	-	-	-	-	-	-	-
	0.712	-	-	0.262	-	-	-	-	-	-	-	-
Median	0.705	0.000	0.264	0.261	0.822	0.009	0.140	0.040	0.687	-0.044	0.163	0.0413
	0.696	0.000	0.268	0.271	0.773	-0.005	0.137	0.042	0.677	-0.052	0.164	0.0682
	0.672	0.000	0.263	0.282	0.778	-0.008	0.156	0.048	0.595	-0.056	0.175	0.1481
	0.697	0.000	0.000	0.270	0.801	0.038	0.137	0.111	0.463	0.028	0.191	0.0456
	0.702	0.000	0.258	0.276	0.804	0.016	0.140	0.053	0.648	-0.051	0.165	-
	-	0.000	0.262	-	0.765	-0.009	0.149	0.053	-	-	-	-
	-	-	-	-	0.805	-0.004	0.130	0.046	-	-	-	-
	-	-	-	-	0.782	0.006	0.142	0.034	-	-	-	-
	-	-	-	-	0.804	0.003	0.136	0.031	-	-	-	-
	0.696	-0.022	0.279	0.279	0.781	0.000	0.142	0.508	0.768	0.213	0.154	0.0431
	0.651	-0.018	0.293	0.294	0.791	0.000	0.138	0.037	0.783	0.192	0.169	0.0378

Sensor Signal Normalization	0.687	-0.007	0.279	0.279	0.765	0.004	0.140	0.060	0.791	0.211	0.154	0.0421
	0.694	-0.079	0.279	0.290	0.798	0.000	0.137	0.038	-	-	-	-
One-Cal	0.676	-0.026	0.276	0.272	0.827	0.009	-0.099	0.043	0.757	0.146	0.164	0.2028
	0.637	-0.014	0.297	0.300	0.778	-0.004	-0.100	0.042	0.759	0.140	0.159	0.1935
	0.639	-0.017	0.280	0.300	0.795	-0.008	-0.107	0.050	0.745	0.140	0.156	0.1906
	0.656	-0.026	0.274	0.291	0.778	0.016	-	0.101	0.729	0.139	-	-
	0.668	-	-	0.295	0.798	-0.009	-	0.056	0.761	0.146	-	-
One-Hop	0.678	-0.043	0.336	0.275	0.827	0.006	0.109	0.027	0.757	0.000	0.133	0.1821
	0.716	-0.129	0.333	0.242	0.797	0.003	0.141	0.039	0.700	0.000	0.138	0.1038
	0.514	0.068	0.380	0.381	0.806	0.005	0.110	0.039	0.688	0.000	0.141	0.1161
	0.583	-0.160	0.442	0.316	0.845	-0.004	0.139	0.027	0.635	0.000	0.138	0.1473
	0.380	-	-	0.401	0.782	-	-	-	0.705	0.000	0.136	-
	0.643	-	-	0.421	-	-	-	-	-	-	-	-

Table S4: Measures of fit for ozone calibration methods

Method	Colorado Calibration				Colorado Validation				California Calibration				California Validation			
	R²	MBE	CRMSD	RMSE	R²	MBE	CRMSD	RMSE	R²	MBE	CRMSD	RMSE	R²	MBE	CRMSD	RMSE
Individual	0.934	0.000	4.895	4.988	0.960	0.000	10.816	4.333	0.816	-0.933	8.544	7.959	0.635	19.302	11.615	20.073
	0.885	0.051	6.478	6.572	0.901	0.000	10.859	6.149	0.804	-1.153	8.508	7.994	0.735	18.959	10.754	19.736
	0.797	0.070	8.548	8.723	0.800	0.000	2.508	8.748	0.829	-1.257	8.539	7.676	0.770	21.636	11.803	25.685
	0.652	0.000	9.988	10.666	0.765	0.000	10.516	7.647	0.832	-2.974	8.542	7.600	0.700	20.416	10.853	30.093
	0.470	-	-	9.225	0.148	0.021	10.638	12.874	0.820	-1.579	8.804	7.867	0.674	14.918	10.360	30.697
	0.465	-	-	9.222	0.093	0.019	10.714	13.251	0.802	-2.560	8.666	7.910	0.726	16.113	10.816	9.080
	0.473	-	-	9.132	0.103	-	-	13.092	0.834	-0.547	8.558	7.369	0.765	19.827	11.562	33.456
	0.492	-	-	9.018	0.116	-	-	13.201	0.817	-1.216	8.600	7.738	0.576	19.163	11.427	36.961
	0.469	-	-	9.191	0.120	-	-	13.076	0.863	-2.230	8.550	6.868	0.767	18.767	10.846	47.966
	-	-	-	-	-	-	-	-	0.840	-0.816	8.848	6.886	0.762	11.924	11.083	27.298
	-	-	-	-	-	-	-	-	0.849	-0.816	8.848	7.198	0.786	21.505	11.925	26.491
	-	-	-	-	-	-	-	-	0.849	-	-	5.148	0.760	-	-	24.753
	-	-	-	-	-	-	-	-	0.937	-	-	-	0.918	-	-	32.885

Z-Indiv.	0.938	0.000	4.895	4.895	0.358	0.045	10.048	10.052	0.816	-0.001	7.181	7.959	0.528	-7.223	79.929	80.255
	0.886	0.051	6.478	6.552	0.346	0.000	10.170	10.146	0.806	-0.001	7.181	7.956	0.535	-7.223	79.929	74.248
	0.668	0.000	9.988	9.986	0.928	0.000	2.608	2.609	0.832	0.041	7.713	7.589	0.885	-7.297	45.969	46.545
	-	-	-	-	0.359	0.030	10.053	10.040	0.832	-0.007	8.714	7.600	0.690	7.284	17.782	19.216
	-	-	-	-	0.366	0.043	9.987	9.985	0.820	0.011	7.755	7.866	0.728	-9.295	34.942	36.157
	-	-	-	-	0.354	0.053	10.071	10.079	0.836	0.059	7.595	7.910	0.522	-1.731	122.517	122.529
	-	-	-	-	-	-	-	-	0.817	-0.037	8.110	7.330	0.714	94.202	54.659	108.911
	-	-	-	-	-	-	-	-	0.842	0.011	6.412	7.738	0.140	24.189	15.965	28.983
	-	-	-	-	-	-	-	-	0.849	-0.007	7.529	6.868	0.901	8.418	103.650	103.991
	-	-	-	-	-	-	-	-	-	0.026	6.970	6.852	0.539	-17.142	103.602	105.011
	-	-	-	-	-	-	-	-	-	0.026	6.970	7.198	-	-20.810	67.489	70.624
Median	0.934	-0.996	5.174	5.269	0.633	5.099	21.825	13.202	0.782	-24.375	20.490	28.397	0.344	-18.746	13.949	23.366
	0.884	-1.373	6.732	7.004	0.662	4.684	27.711	4.020	0.826	-3.560	7.295	10.018	0.476	-16.843	18.455	24.986
	0.706	-1.292	10.786	10.617	0.648	-8.461	21.383	11.942	0.825	-3.560	7.295	7.783	0.842	-16.843	18.455	27.316
	0.548	3.783	13.479	13.997	0.636	4.728	26.346	13.498	0.805	1.089	7.563	7.805	0.536	-16.592	18.012	24.489

	-	-	-	-	0.633	4.912	17.967	13.083	0.794	-0.302	8.880	8.468	0.344	-18.704	13.925	23.319
	-	-	-	-	-	4.889	18.990	-	0.822	0.576	7.302	8.086	0.473	-17.140	19.067	25.639
	-	-	-	-	-	-	-	-	0.230	-1.363	7.436	7.644	0.541	-16.561	20.406	26.281
	-	-	-	-	-	-	-	-	0.293	-53.581	8.802	41.011	0.248	-18.674	14.929	23.909
	-	-	-	-	-	-	-	-	0.713	-52.080	9.977	39.333	0.840	-15.506	25.856	30.149
	-	-	-	-	-	-	-	-	0.844	-7.831	6.999	14.407	0.802	-15.280	22.128	26.892
	-	-	-	-	-	-	-	-	0.844	0.895	7.446	7.344	0.603	-15.759	19.327	24.937
	-	-	-	-	-	-	-	-	0.898	0.895	7.446	7.344	0.449	-17.052	14.634	22.471
	-	-	-	-	-	-	-	-	-	-	-	-	0.755	-	-	-
Sensor Signal Norm.	0.882	0.000	4.895	7.217	-	-	-	-	0.775	-0.933	8.544	8.790	0.554	11.615	19.302	22.527
	0.727	2.776	6.711	10.640	-	-	-	-	0.816	-1.153	8.508	8.405	0.615	10.754	18.959	21.797
	0.572	1.279	10.790	11.699	-	-	-	-	0.814	-1.257	8.539	8.453	0.555	11.803	21.636	24.646
	-	-1.140	11.645	-	-	-	-	-	0.813	-2.974	8.542	3.110	0.618	10.853	20.416	23.122
	-	-	-	-	-	-	-	-	0.786	-1.579	8.804	8.641	0.637	10.360	14.918	18.162

-	-	-	-	-	-	-	-	0.785	-2.560	8.666	8.941	0.613	10.816	16.113	19.406	
-	-	-	-	-	-	-	-	0.802	-0.547	8.558	8.307	0.557	11.562	19.827	22.952	
-	-	-	-	-	-	-	-	0.809	-1.216	8.600	8.627	0.564	11.427	19.163	22.312	
-	-	-	-	-	-	-	-	0.789	-2.230	8.550	8.533	0.611	10.846	18.767	21.676	
-	-	-	-	-	-	-	-	0.806	-0.816	8.848	8.396	0.584	11.083	11.924	16.279	
-	-	-	-	-	-	-	-	-	-0.816	8.848	8.396	-	11.925	21.505	24.590	
One-Cal	0.938	0.000	4.895	4.895	0.075	5.337	21.039	21.705	0.816	8.620	8.621	11.728	0.716	8.202	14.031	16.253
	0.882	-0.377	6.721	6.687	0.087	5.337	24.270	24.850	0.776	8.620	8.621	7.983	0.638	8.202	14.031	16.253
	0.653	-0.279	11.831	11.435	0.045	-12.043	21.078	23.933	0.815	-0.395	8.706	7.983	0.638	8.189	14.232	16.420
	0.531	4.056	13.380	13.978	0.000	5.326	23.333	16.683	0.815	-1.884	8.703	8.337	0.630	8.093	13.142	15.434
	-	-	-	-	0.011	5.424	15.312	18.075	0.801	-0.388	9.041	8.404	0.709	8.117	12.164	14.624
	-	-	-	-	-	5.405	16.991	-	0.781	-2.120	8.827	8.836	0.739	8.038	12.895	15.195
	-	-	-	-	-	-	-	-	0.764	1.982	8.668	8.069	0.692	8.264	14.145	16.382
	-	-	-	-	-	-	-	-	0.802	1.435	8.976	8.241	0.647	8.130	13.036	15.363
	-	-	-	-	-	-	-	-	0.804	1.809	8.930	8.818	0.658	7.987	12.415	14.762

	-	-	-	-	-	-	-	-	0.771	-0.607	8.930	8.197	0.707	7.921	11.879	14.278
	-	-	-	-	-	-	-	-	0.805	-0.607	8.930	8.197	0.708	8.173	14.656	14.279
	-	-	-	-	-	-	-	-	0.805	-	-	-	0.605	-	-	-
	-	-	-	-	-	-	-	-	0.862	-	-	-	0.688	-	-	-
One-Hop	0.938	0.000	6.447	4.895	-	-	-	-	0.816	0.008	8.651	8.462	0.716	-0.352	14.246	14.251
	0.958	-0.003	8.601	3.894	-	-	-	-	0.780	0.008	8.651	7.872	0.642	-0.352	14.246	14.100
	0.912	0.295	10.268	5.656	-	-	-	-	0.820	0.000	8.588	7.881	0.728	6.647	13.502	15.050
	0.731	-	-	8.747	-	-	-	-	0.819	0.008	8.689	7.881	0.652	-1.080	9.384	9.446
	-	-	-	-	-	-	-	-	0.819	0.003	8.853	8.174	0.742	6.504	12.150	13.781
	-	-	-	-	-	-	-	-	0.789	0.011	8.570	7.867	0.720	5.821	13.478	14.682
	-	-	-	-	-	-	-	-	0.811	0.006	8.590	7.960	0.723	8.823	12.084	14.962
	-	-	-	-	-	-	-	-	0.806	0.000	8.610	7.947	0.655	8.161	13.550	15.818
	-	-	-	-	-	-	-	-	0.816	-0.009	8.551	7.661	0.675	4.400	13.070	13.791
	-	-	-	-	-	-	-	-	0.803	0.012	8.881	8.064	0.697	8.074	11.866	14.352
	-	-	-	-	-	-	-	-	0.811	0.012	8.881	8.063	0.726	8.274	14.140	16.383

	-	-	-	-	-	-	-	-	0.811	-	-	-	0.628	-	-	-
	-	-	-	-	-	-	-	-	0.872	-	-	-	0.706	-	-	-