Continuous OTM 33A Analysis of Controlled Releases of Methane with Various Time Periods, Data Rates and Wind Filters

Supplementary Materials: Figures, Tables and Equations

Descriptions:

Figure S1. Data acquisition setup is composed of the devices in Table S3. The tower was deployed at multiple sites at different wind angles with respect to controlled methane releases throughout the data acquisition campaign. These details are presented in Tables S2 and S3.

Table S1. Controlled release test matrix presents the various controlled release rates of methane high pressure bottles and the distances that those releases were from the DAQ tower.

Table S2.-Various distances and differences in height between the controlled release and the tower.

Table S3. Relevant specifications of the data acquisition equipment that was used during the data collection campaign. These instruments were placed on the tower presented in Figure S1.

Table S4. Results of OTM 33A emissions quantification from data released by the EPA. These data were used for verification of the method to ensure it was carried out properly within this works data processing code.

Equation S1. Calculation of root mean squared error (RMSE) in grams per second (g/s) where y_i is the estimated rate in g/s from the OTM 33A calculations and $\hat{y}_i$ is the actual release rate during that period.-N is the number of periods evaluated in the calculation.

Equation S2. Calculation of normalized root mean square deviation (NRMSD) as a percentage (%). This shows the percentage error of the RMSE assessment of the periods in question. $\bar{y}$ is the average actual release rate of the scenario evaluated. When the calculation of RMSE involved multiple release rates, the average ($\bar{y}$) was a weighted sum of the different release rates for that scenario.

Figure S2. Effect of the wind filter used in data analysis. The wind filter was designed to eliminate periods of data that occurred when the mean wind direction of that period was not within (± the bearing direction from the release to the tower) in degrees (°) East of North. The black line represents the bearing from the release to the tower for various scenarios. The points are the mean wind direction (°EoN) of the period. The red points are those that are eliminated by the filter and the green points are those accepted by the filter.

Equation S3. Mathematical representation of the wind filter described in Figure S2.-WF is the wind filter in (±°).

Tables S5-7. Breakdown of the various evaluations performed for wind filter, period length and data frequency, sorted by actual release rate. Presented is the number of periods evaluated for the scenario, the RMSE in g/s and the NRMSD in %.

Table S8. Breakdown of the various evaluations performed for wind filter, period length, data frequency and data quality indicator (DQI) sorted by distance from the release to the tower. Presented is the number of periods evaluated and the RMSE in g/s.

Figure S1. Data acquisition setup.

Table S1. Controlled release test matrix.

Release Rate (g/s)	Distances (m)		
0.04	42	72	119
0.12	57	72	119
0.24	42	72	119

Table S2. Details of data acquisition locations.

Distance (m)	Release		Tower	
	Altitude (m)	Height (m)	Altitude (m)	Height (m)
42	522	2.3	522	4.5
72	522	2.3	524	4.5
57	524	2.3	524	4.5
119	524	2.3	529	4.5

Table S3. Data acquisition equipment specifications.

Device	Manufacturer	Detection Method	Max Rate/ Used Rate	Parameters Measured	Range	Resolution (res) /Accuracy (acc)	Operating Limits
Gill WindMaster	Gill Instruments, Ltd.	Ultrasonic Pulse	20 Hz/10 Hz	3-D Wind Speed	0–50 m/s	<1.5% RMS	T: −40–70 °C RH: <5–100%
LI-7700	LI-COR Biosciences	Wavelength Modulation Spectroscopy	20 Hz/10 Hz	CH_4 conc. Temperature Pressure	CH_4:0–40 ppm at 25 °C	5 ppb res. <1% linearity	T: −25–50 °C P: 50–110 kPa RH: 0–100%
LI-7500	LI-COR Biosciences	Non-dispersive spectroscopy	20 Hz/10 Hz	CO_2 conc. H_2O conc. Temperature Pressure	CO_2:0–3000 µmol/mol H_2O: 0–60 µmol/mol T: −20–7 °C P: 50–110 kPa	CO_2: <1% of reading H_2O: <1% of reading T: ±0.3 °C P: 0.4 kPa	RH: 0–95% T: −25–50 °C P: 50–110 kPa
LI-200R	LI-COR Biosciences	Photovoltaic	1e5 Hz/10 Hz	Solar Loading	0–3000 W/m²	±3% over reading	T: −40–65 °C RH: 0–100%
Omega iBTHx	Omega™ Engineering	Various	0.25 Hz/0.25 Hz	Temperature Pressure Relative Humidity	T: 0–70 °C P: 0–110 kPa RH: 0–100%	T: ±2 °C acc. 0.01 °C res. P: ±0.2 kPa acc. 0.01 kPa res. RH: 2% for 10–90 acc. 0.03% res.	T: 0–70 °C P: 0–110 kPa RH: 0–100%

Table S4. EPA MATLAB® and Python code analysis differences.

EPA Release Excel Filename	Distance (m)	EPA MATLAB® Results (g/s)	Python Results (g/s)	% Difference
STR_4042011_01.xls	40	0.43	0.43	0.0%
STR_4042011_03.xls	60	0.54	0.77	42.7%
STR_4042011_05.xls	35	0.75	0.75	0.0%
STR_4042011_06.xls	97	0.38	0.38	0.0%
STR_4042011_07.xls	57	0.53	0.53	0.0%
STR_5050611_01.xls	88	0.64	0.65	0.0%
STR_5050611_02.xls	88	0.61	0.61	0.0%
STR_5050611_03.xls	98	0.38	0.37	3.2%
STR_5050611_04.xls	98	0.74	0.74	0.0%
STR_5050611_05.xls	103	0.64	0.64	0.0%
STR_5050611_06.xls	103	0.31	0.31	0.0%
STR_5050611_07.xls	103	0.35	0.35	0.0%
STR_5050611_08.xls	82	0.61	0.61	0.0%
STR_5050611_09.xls	57	0.80	0.75	5.7%
STR_5050611_10.xls	57	0.63	0.63	0.0%
STR_6061411_01.xls	81	0.59	0.59	0.0%
STR_6061411_03.xls	98	0.32	0.32	0.0%
STR_6061411_04.xls	65	0.51	0.76	47.8%
STR_6061411_05.xls	41	0.49	0.49	0.0%
STR_6061411_06.xls	93	0.60	0.60	0.0%

Equation (S1). Root mean squared error.

$$\mathrm{RMSE}(y, \hat{y}) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2} \tag{S1}$$

Equation (S2). Normalized root mean square deviation.

$$\mathrm{NRMSD} = \frac{\mathrm{RMSE}}{\bar{y}} \tag{S2}$$

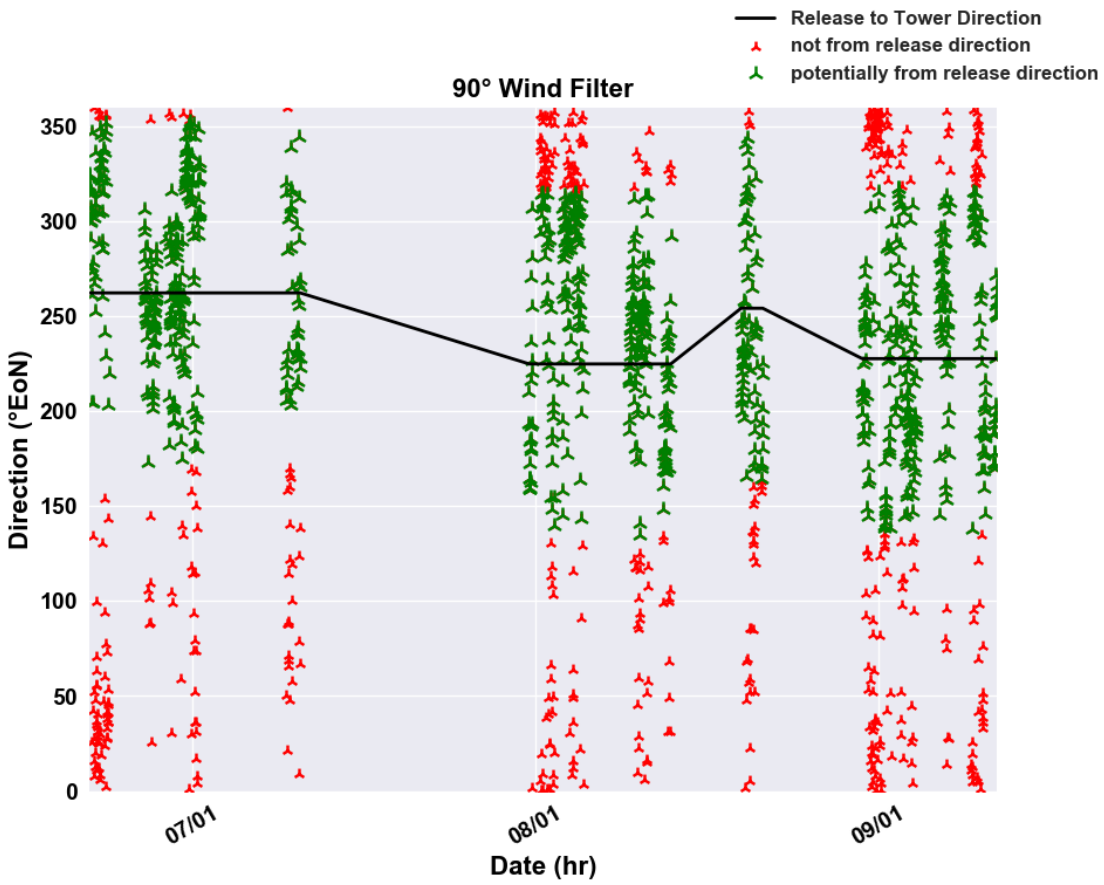

Figure S2. 90° wind filter of 20-minute period, 10-Hz analysis.

Equation (S3). Mathematical representation of the wind filter.

$$|Release\ to\ Tower\ Direction\ (°\text{EoN}) - \text{Mean Wind Direction } (°EoN)| < \text{WF°} \quad \text{(S3)}$$

Table S5. Wind-filtered 20-min, 10-Hz data by release rate.

Wind Filter (±°)	Release Rate (g/s)	Count	RMSE (g/s)	NRMSD (%)
180	All	1451	0.140	177%
	0.04	911	0.106	295%
	0.12	395	0.177	149%
	0.24	145	0.197	82%
120	All	1166	0.139	173%
	0.04	718	0.107	298%
	0.12	328	0.171	144%
	0.24	120	0.196	82%
90	All	969	0.121	148%
	0.04	586	0.058	162%
	0.12	278	0.179	151%
	0.24	105	0.177	74%
60	All	713	0.117	131%
	0.04	400	0.064	177%
	0.12	213	0.152	128%
	0.24	100	0.179	75%
30	All	376	0.122	146%
	0.04	217	0.059	164%
	0.12	120	0.160	135%
	0.24	39	0.210	88%
20	All	250	0.125	158%
	0.04	151	0.056	156%
	0.12	77	0.175	147%
	0.24	22	0.224	94%
10	All	130	0.143	176%
	0.04	78	0.056	155%
	0.12	39	0.206	173%
	0.24	13	0.243	102%

Table S6. Varying period length at 10-Hz by release rate.

Period Length (min)	Release Rate (g/s)	Count	RMSE (g/s)	NRMSD (%)
10	All	1378	0.116	131%
	0.04	778	0.047	132%
	0.12	409	0.158	132%
	0.24	191	0.188	79%
15	All	938	0.148	167%
	0.04	532	0.061	168%
	0.12	278	0.206	173%
	0.24	128	0.228	96%
20	All	713	0.117	131%
	0.04	400	0.064	177%
	0.12	213	0.152	128%
	0.24	100	0.179	75%
25	All	580	0.111	126%
	0.04	327	0.059	163%
	0.12	175	0.151	127%
	0.24	78	0.164	69%
30	All	475	0.130	147%
	0.04	264	0.057	159%
	0.12	149	0.192	161%
	0.24	62	0.164	69%
45	All	333	0.122	141%
	0.04	189	0.066	183%
	0.12	103	0.163	137%
	0.24	41	0.186	78%
60	All	248	0.141	161%
	0.04	140	0.077	213%
	0.12	75	0.211	177%
	0.24	33	0.156	65%

Table S7. Varying data frequency of 20-minute periods by release rate.

Data Frequency (Hz)	Release Rate (g/s)	Count	RMSE (g/s)	NRMSD (%)
10	All	713	0.117	131%
	0.04	400	0.064	177%
	0.12	213	0.152	128%
	0.24	100	0.179	75%
5	All	697	0.115	131%
	0.04	395	0.062	172%
	0.12	208	0.151	127%
	0.24	94	0.178	74%
2	All	695	0.114	130%
	0.04	394	0.063	176%
	0.12	208	0.147	124%
	0.24	93	0.179	75%
1	All	697	0.114	129%
	0.04	395	0.064	178%
	0.12	208	0.146	123%
	0.24	94	0.177	74%
0.5	All	704	0.120	135%
	0.04	396	0.059	165%
	0.12	212	0.163	137%
	0.24	96	0.178	74%
0.2	All	702	0.106	119%
	0.04	393	0.051	143%
	0.12	213	0.132	111%
	0.24	96	0.181	76%
0.1	All	696	0.112	126%
	0.04	388	0.055	153%
	0.12	212	0.149	125%
	0.24	96	0.173	72%

Table S8. RMSE (g/s) and number of periods analyzed by distance.

Distance (m)	**50**		75		120	
Data Frequency (Hz)	#	**RMSE**	#	RMSE	#	RMSE
10	306	0.0947	196	0.0926	211	0.1588
5	296	0.0920	193	0.0940	208	0.1556
2	295	0.0912	192	0.0951	208	0.1532
1	296	0.0886	193	0.0991	208	0.1514
0.5	302	0.0933	195	0.0901	207	0.1682
0.2	301	0.0969	195	0.0930	206	0.1285
0.1	296	0.0896	195	0.0948	205	0.1503
Period Lengths (min)	#	RMSE	#	RMSE	#	RMSE
10	569	0.0834	403	0.0996	406	0.1623
15	399	0.0846	262	0.1364	277	0.2143
20	306	0.0947	196	0.0926	211	0.1588
25	245	0.0718	160	0.1134	175	0.1488
30	203	0.0822	134	0.1596	138	0.1537
45	140	0.0686	94	0.0890	99	0.1899
60	106	0.0744	67	0.0769	75	0.2303
Wind Filters (± °)	#	RMSE	#	RMSE	#	RMSE
180	551	0.0934	436	0.1100	464	0.1983
120	453	0.0915	367	0.0909	346	0.2126
90	397	0.0875	288	0.0810	284	0.1811
60	306	0.0947	196	0.0926	211	0.1588
30	162	0.0775	109	0.1038	105	0.1802
20	110	0.0776	73	0.1061	67	0.1912
15	63	0.0899	41	0.0977	26	0.2608
DQI Filters (< DQI)	#	RMSE	#	RMSE	#	RMSE
5	61	0.0837	30	0.0768	19	0.2397
10	115	0.1118	62	0.0701	83	0.1871
15	184	0.0952	107	0.0850	183	0.1714
20	234	0.0954	201	0.0792	224	0.1574
25	277	0.0894	253	0.0797	259	0.1498
30	360	0.0873	278	0.0798	279	0.1827