Title: Measurements of volatile organic compounds at two locations in the Northern Colorado Front Range during Spring 2022

Abstract: This dataset was collected by Colorado State University (CSU) graduate students during the spring 2022 semester as part of a course in the Department of Atmospheric Science (ATS-716: Air Quality Characterization). Measurements of volatile organic compounds (VOCs) were collected at two locations in Northern Colorado using low-cost sensors called SENSIT SPODs. The SENSIT SPOD sensor package combines wind field and air pollutant concentration measurements to detect emission plumes and locate the source of those emissions. The sensor measures non-speciated, uncalibrated concentrations of a subset of VOCs. The sensor also measures temperature, relative humidity, pressure, and wind direction and speed. The SPODs were used to trigger the collection of whole air samples during periods with higher concentrations of VOCs. Air samples from the triggered canisters were analyzed at CSU using Gas Chromatography (GC) to provide a measure of approximately 50 VOCs. An integrated canister was used to measure the average concentration of approximately 50 VOCs over a one-week period. After collection, sample air in the canisters was analyzed at CSU using Gas Chromatography (GC).

Funding: This work was supported by the Monfort Family Foundation.

Keywords: volatile organic compounds (VOCs), triggered events, integrated samples, whole air samples, Northern Colorado, air quality, air monitoring, air pollution, community-based research

Spatial Coverage: Two locations in Northern Colorado. See Data Description.

Temporal Coverage: Spring 2022. See Data Description.

Publications: None as of June 2022

Data contact:

Emily V. Fischer, Associate Professor, Department of Atmospheric Science.
evf@atmos.colostate.edu; 970-491-8587

Please contact Emily V. Fischer (evf@rams.colostate.edu) before using these datasets.

Definitions of acronyms

- ppmv: Parts per million volume
- ppbv: Parts per billion volume
- PID: Photoionization detector (SPOD sensor that measures hydrocarbons)
- SPOD: Sensor Pod (SENSIT Technologies Corp. low cost fenceline sensor)
- VOC: Volatile organic compound

Data Description

This dataset contains information on VOC concentration and meteorological conditions collected at the Hearthfire neighborhood (40.638, -105.054) in Fort Collins, CO from February 11, 2022 to April 25, 2022 and the Bella Romero neighborhood (40.405, -104.659) in Greeley, CO from February 23, 2022 to May 5, 2022. At the Hearthfire neighborhood site, triggered canisters were not installed until February 17, 2022. The dataset includes 3 different files: 1) SPOD_PID_Data.zip; 2) Triggered_Canisters.csv; and 3) Integrated_Canisters.csv. The following provides a description of each of these files:

- SPOD_PID_Data.zip
    - Zipped folder containing two zipped location-specific subfolders with daily comma-delimited CSV files. Each file contains 21 columns.
    - Subfolders naming convention: SPOD_DATA_IDNUMBER_LOCATION.zip
    - File naming convention: SPOD_DATA_EXPORT_IDNUMBER_MMDDYY.csv
    - IDNUMBER:
        - Hearthfire neighborhood: 1263 and 1038
            - 1263 - Primary SPOD used for deployment. Sensor out of service due to mechanical issues from February 23, 2022 to March 9, 2022.
            - 1038 - Replacement SPOD deployed from February 25, 2022 to March 9, 2022.
        - Bella Romero neighborhood: 1264
- Triggered_Canisters.csv
    - VOC concentration and meteorological data associated with SPOD triggered events. PID trigger thresholds were as follows:
        - Hearthfire neighborhood:
            - Initial (February 17-March 16): 120 ppb (static), 60 ppb (differential)
            - Updated (March 16-April 25): 80 ppb (static), 65 ppb (differential)
            - Duration of sample: 2 min (February 17-March 31) and 2.5 min (March 31-April 25)
        - Bella Romero neighborhood:
            - Initial (February 23-March 29): 120 ppb (static), 60 ppb (differential)
            - Updated (March 29-May 5): 125 ppb (static), 65 ppb (differential)
            - Duration of sample: 2 min (February 23- May 5)
    - Data are contained in a comma-delimited CSV file with 59 columns.
- Integrated_Canisters.csv
    - The average concentration of VOCs in whole air samples collected over approximately one-week time periods at each site.
    - Data are contained in a comma-delimited CSV file with 54 columns..

Variable information:

File Name: SPOD_PID_Data.zip

Variable Name	Units	Description
UTC Date Time	MM/DD/YYYY HH:MM	UTC date time (24-hour)
Local Date Time	MM/DD/YYYY HH:MM	Mountain time zone date time (24-hour)
pid1_PPB_Calc	ppb	Field 1, Sensor 1 VOC
pid1_mvRaw	mV	Field 2, Sensor 1 Raw
temp	Degree Celsius	Temperature
rh_Humd	%	Relative humidity
pressure_mbar	Millibar	Pressure
ws_speed	Miles per hour	Wind speed
ws_direction	Degrees	Wind direction
tc_temp	Arb Units	Sensor Temp
tc_heatOutput	Output 0 = Off, 255 = Fully On	Heater status
tc_setPoint	Arb Units	Sensor Setpoint
batt_voltage	Volt	Battery Voltage
chrg_current	mA	Charging Current
run_current	mA	Operating Current
trig.canister_status	N/A	Port Status
trig.trig_value	N/A	Trigger Flag (1 indicates a trigger event)
trig.trig_activeFlag	N/A	Active Port (1, 2, 4 and 8 correspond with port 1, 2, 3 and 4 respectively)
trig.trig_eventFlag	N/A	Sample Flag
lat	Degrees	GPS Latitude
long	Degrees	GPS Longitude

File Name: Triggered_Canisters.csv

Variable Name	Units	Description
Site		Name of site
trigger_time	MM/DD/YYYY HH:MM	Time of SPOD triggered canister event; Mountain time zone (24-hour)
wind_speed	Miles per hour	Wind speed
wind_dir	Degrees	Wind direction
temperature	Degree Celsius	Temperature
RH	%	Relative humidity
pressure	Millibar	Pressure
ethane	ppb	Concentration of 51 VOCs in 51 columns respectively
…		
acetonitrile		
methane_ppmv	ppm	Methane concentration

File Name: Integrated_Canisters.csv

Variable Name	Units	Description
Site		Name of site
Week	MM/DD to MM/DD	Time period of measuring
ethane	ppb	Concentration of 51 VOCs in 51 columns respectively
…		
acetonitrile		
methane_ppmv	ppm	Methane concentration

Environmental or experimental conditions:

The instrumentation in the Hearthfire neighborhood was in a grassy field directly west of an active oil and gas well pad and north of residential houses. The instrumentation in the Bella Romero neighborhood was located over largely bare ground near livestock. Instruments were placed inside of a cage to prevent interference from livestock. The broader region around Bella Romero has more extensive oil and gas development, agricultural facilities, and industrial facilities than the area around the Hearthfire neighborhood. The Bella Romero site was also located near a road frequently used to access a local school during morning dropoff and afternoon pickup times.

Uncertainty, precision, and accuracy of measurements:

The GC analysis precision, accuracy and combined uncertainty of individual VOCs are listed in the following table. The measurement uncertainty for the methane is 2%. The uncertainty associated with the flow controller used to fill the integrated canisters is +/- 13%.

VOC	Precision (%)	Accuracy (%)	Combined uncertainty (%)	LOD	LOD _unit	Data _unit
ethane	1.8	5.2	5.5	0.0102	ppbv	ppbv
ethene	1.4	5.4	5.6	0.0060	ppbv	ppbv
propane	1.5	5.2	5.4	0.0110	ppbv	ppbv
propene	1.4	5.3	5.5	0.0044	ppbv	ppbv
i-butane	1.3	5.3	5.4	0.0038	ppbv	ppbv
n-butane	1.4	5.2	5.4	0.0057	ppbv	ppbv
ethyne	1.4	5.3	5.5	0.0051	ppbv	ppbv
t-2-butene	1.4	5.2	5.4	0.0015	ppbv	ppbv
1-butene	1.1	5.2	5.3	0.0042	ppbv	ppbv
c-2-butene	1.1	5.2	5.3	0.0030	ppbv	ppbv
cyclopentane	1.3	5.2	5.4	0.0026	ppbv	ppbv
i-pentane	1.2	5.2	5.3	0.0044	ppbv	ppbv

n-pentane	1.4	5.2	5.4	0.0014	ppbv	ppbv
t-2-pentene	2.3	5.5	6.0	0.0021	ppbv	ppbv
1-pentene	4.0	5.3	6.6	0.0022	ppbv	ppbv
cis-2-pentene	2.3	6.2	6.6	0.0036	ppbv	ppbv
n-hexane	2.1	5.2	5.6	0.0058	ppbv	ppbv
isoprene	1.3	5.3	5.5	0.0008	ppbv	ppbv
2,4-dimethylpentane	1.3	5.3	5.5	0.0022	ppbv	ppbv
n-heptane	1.6	5.2	5.5	0.0063	ppbv	ppbv
benzene	2.3	5.6	6.0	0.0045	ppbv	ppbv
cyclohexane	2.3	6.0	6.4	0.0042	ppbv	ppbv
2,3-dimethylpentane	1.7	5.3	5.5	0.0100	ppbv	ppbv
2-methylhexane	1.6	5.2	5.5	0.0084	ppbv	ppbv
3-methylhexane	2.0	5.3	5.7	0.0026	ppbv	ppbv
2,2,4-trimethylpentane	2.6	5.4	6.0	0.0050	ppbv	ppbv
methylcyclohexane	1.6	5.2	5.5	0.0062	ppbv	ppbv
2,3,4-trimethylpentane	2.1	5.3	5.7	0.0091	ppbv	ppbv
toluene	2.1	5.2	5.6	0.0055	ppbv	ppbv
2-methylheptane	2.4	5.3	5.8	0.0046	ppbv	ppbv
3-methylheptane	2.2	5.2	5.7	0.0074	ppbv	ppbv
n-octane	2.3	5.3	5.8	0.0024	ppbv	ppbv

ethylbenzene	2.2	5.2	5.7	0.0032	ppbv	ppbv
m+p-xylene	2.5	5.3	5.8	0.0022	ppbv	ppbv
styrene	2.4	5.4	5.9	0.0054	ppbv	ppbv
o-xylene	11.0	5.4	12.3	0.0002	ppbv	ppbv
n-nonane	2.5	5.2	5.8	0.0060	ppbv	ppbv
isopropylbenzene	2.8	5.3	6.0	0.0058	ppbv	ppbv
n-propylbenzene	11.1	5.4	12.3	0.0001	ppbv	ppbv
3-ethyltoluene	12.2	5.2	13.2	0.0003	ppbv	ppbv
4-ethyltoluene	10.2	5.2	11.4	0.0003	ppbv	ppbv
1,3,5-trimethylbenzene	9.7	5.4	11.1	0.0003	ppbv	ppbv
2-ethyltoluene	9.8	5.3	11.1	0.0004	ppbv	ppbv
1,2,4-trimethylbenzene	10.8	5.2	12.0	0.0005	ppbv	ppbv
n-decane	10.4	5.5	11.8	0.0006	ppbv	ppbv
1,2,3-trimethylbenzene	2.9	5.2	6.0	0.0069	ppbv	ppbv
1,3-diethylbenzene	10.8	5.2	12.0	0.0004	ppbv	ppbv
1,4-diethylbenzene	10.2	5.3	11.5	0.0004	ppbv	ppbv
trichloroethene_C2HCl3	10.9	5.5	12.2	0.0010	ppbv	ppbv
tetrachloroethylene_C2Cl4	7.0	10.0	12.2	0.25	pptv	pptv
acetonitrile	9.3	5.0	10.6	0.02	pptv	pptv

Standards, calibrations, and quality controls:

All whole air samples have been analyzed as described in Benedict et al. (2019) and Hecobian et al., (2019).

Benedict, K. B., Zhou, Y., Sive, B. C., Prenni, A. J., Gebhart, K. A., Fischer, E. V., Evanoski-Cole, A., Sullivan, A. P., Callahan, S., Schichtel, B. A., Mao, H., Zhou, Y., and Collett Jr., J. L.: Volatile organic compounds and ozone in Rocky Mountain National Park during FRAPPÉ, Atmos. Chem. Phys., 2019, 19, 499–521, https://doi.org/10.5194/acp-19-499-2019.

Hecobian, A.; Clements, A. L.; Shonkwiler, K. B.; Zhou, Y.; MacDonald, L. P.; Hilliard, N.; Wells, B. L.; Bibeau, B.; Ham, J. M.; Pierce, J. R.; Collett, J. L. Air Toxics and Other Volatile Organic Compound Emissions from Unconventional Oil and Gas Development. *Environ. Sci. Technol. Lett.* 2019, *6*, 720– 726, DOI: 10.1021/acs.estlett.9b00591

Additional Information:

Plume extrapolation of the triggered events:

In each triggered event, an approximately two-minute whole air sample was collected and analyzed. A preliminary extrapolation of the two-minute VOC sample into a one-hour concentration was performed but is not reported here. The performance of plume extrapolation varied due to the number of samples collected during each plume and the different assumptions made during calculations (i.e., the extrapolation methodology used). Contact the PI for more information about plume extrapolation.