

Title: Data associated with “Volatile organic compounds and ozone at four national parks in the southwestern United States”

Abstract:

This file contains the sample information and concentrations of data collected during a study to characterize volatile organic compounds at four national parks in the southwestern US. These data are associated with the article:

Benedict, K.B., Prenni, A.J. El-Sayed, M.M.H., Hecobian, A., Zhou, Y., Gebhart, K.A., Sive, B.C., Schichtel, B.A., Collett Jr, J.L. (2020). Volatile organic compounds and ozone at four national parks in the southwestern United States. *Atmospheric Environment*, 239.
<https://doi.org/10.1016/j.atmosenv.2020.117783>

The abstract from the published article is as follows:

The National Park Service is tasked with protecting the lands it oversees, including from impacts from air pollutants. While ozone is regularly monitored in many parks across the United States, precursors to ozone formation are not routinely measured. In this work we characterize volatile organic compounds (VOCs) at four national parks in the southwestern United States: Carlsbad Caverns (CAVE), Great Basin (GRBA), Grand Canyon (GRCA), and Joshua Tree (JOTR). Whole air samples were collected for VOC analysis for five months (mid-April through mid-September) in 2017. Samples were collected from 3 p.m. to 5 p.m. local time, corresponding approximately to the time of expected peak ozone concentrations, and were analyzed using gas chromatography for a variety of compounds including alkanes, alkenes, aromatics, biogenics, and alkyl nitrates. Among the four parks, the total measured VOC mixing ratio was greatest at CAVE, mostly due to an abundance of light alkanes (on average 94% of all VOCs measured) from oil and gas sources. VOC concentrations at the other three parks were similar to each other and approximately 7–10 times lower than at CAVE. While VOC sources varied across sites, VOC-OH reactivity was dominated by biogenic compounds at all sites except CAVE, which had similar contributions from biogenics and from light alkanes. JOTR had the highest levels of ozone, and the highest concentrations of biogenic VOCs among the parks studied. Back trajectory analysis suggests that the high levels of ozone occurred when air flow came from the west, in the direction of the greater Los Angeles area. The two parks most removed from oil and gas and urban sources, GRBA and GRCA, had the lowest concentrations of total VOCs, and were likely influenced by long range transport of pollutants. To better characterize source influences at the park with the highest VOC concentrations, intensive measurements were conducted in and around CAVE for one week in September 2017. These measurements showed an oil and gas influence throughout the region and indicated that the whole air samples collected over the five-month study did not capture the full range of VOC mixing ratios present at other times of the day.

Contact: Katherine B. Benedict (katherine.benedict@colostate.edu, 970-491-8966)

Recommended data citation: Benedict, Katherine B; Prenni, Anthony J.; El-Sayed, Marwa M.H.; Hecobian, Arsineh; Zhou, Yong; Gebhart, Kristi A.; Sive, Barkley C.; Schichtel, Bret A.; Collett Jr, Jeffrey L. (2020). Data associated with “Volatile organic compounds and ozone at four national parks in the southwestern United States”. Colorado State University. Libraries.
<http://dx.doi.org/10.25675/10217/206528>

Description: SWNP2017_VOCS_FinalDataSet.csv, final data of all sample locations, times and concentrations

Location of where data were collected:

Carlsbad Caverns National Park, NM (32.1479°, -104.5567°)

Great Basin National Park, NV (38.9833°, -114.3000°)

Grand Canyon National Park, AZ (36.1070°, -112.1130°)

Joshua Tree National Park– Black Rock, CA (34.0694°, -116.3889°)

Joshua Tree National Park– Cottonwood Canyon, CA (33.7411°, -115.8206°)

Guadalupe Mountain National Park, NM (31.89143°, -104.83067°)

Bitter Lake National Wildlife Refuge, NM (33.5988°, -104.4031°)

Various locations around Carlsbad Caverns National Park in New Mexico and Texas

Time Period of Collection: 2017-04-2017-09

Definitions of site names and abbreviations:

Carlsbad Caverns National Park (CAVE)

Great Basin National Park (GRBA)

Grand Canyon National Park (GRCA)

Joshua Tree National Park - Black Rock (JOTR-BR)

Joshua Tree National Park - Cottonwood Canyon (JOTR-CC)

CAVE Intensive - Mobile (collected by A.J. Prenni)

CAVE Intensive - PlumeTracker (collected by A. Hecobian)

CAVE Intensive - CAVE (additional samples collected Carlsbad Caverns National Park)

CAVE Intensive - Bitter Lake (Bitter Lake National Wildlife Refuge)

CAVE Intensive - GUMO (Guadalupe Mountain National Park)

Variable Information:

Data Codes-

-9999; No data collected or data removed due to contamination

-8888; Concentrations below limit of detection

NA; Not applicable

List of Variables-

Site Name

Start Time, m/d/yyyy hh:mm

Stop Time, m/d/yyyy hh:mm

Location Notes, included for grab samples about where operator stopped

Latitude, decimal degrees

Longitude, decimal degree

Sample Notes, notes specific to sample regarding weather conditions or issues with sample

Ethane, pptv

Ethene, pptv

Propane, pptv

Propene, pptv

i-butane, pptv

n-butane, pptv

Ethyne, pptv

t-2-butene, pptv

1-butene, pptv

c-2-butene, pptv

cyclopentane, pptv

i-pentane, pptv

n-pentane, pptv

n-hexane, pptv

isoprene, pptv

n-heptane, pptv

n-octane, pptv

n-nonane, pptv

n-decane, pptv

Benzene, pptv

Toluene, pptv

Ethylbenzene, pptv

m+p-xylene, pptv

Styrene, pptv

o-xylene, pptv

i-propylbenzene, pptv

n-propylbenzene, pptv

3-ethyltoluene, pptv

4-ethyltoluene, pptv

1,3,5-trimethylbenzene, pptv

2-ethyltoluene, pptv

1,2,4-trimethylbenzene, pptv

1,2,3-trimethylbenzene, pptv

1,3-diethylbenzene, pptv

1,4-diethylbenzene, pptv

1,2-diethylbenzene, pptv

a-pinene, pptv

b-pinene, pptv

Methane, ppmv

OCS, pptv

CH₃CN, pptv

MeCHCl₃, pptv

F113, pptv

MeONO₂, pptv

CHCl₃, pptv

EtONO₂, pptv

C₂HCl₃, pptv

i-PrONO₂, pptv

CH₂Br₂, pptv

CHBrCl₂, pptv

n-PrONO₂, pptv

C₂Cl₄, pptv

2-BuONO₂, pptv

3-PenONO₂, pptv

2-PenONO₂, pptv

CHBr₃, pptv

Uncertainty, precision, and accuracy of measurements:

- C₂ to C₆ Non-methane hydrocarbons have limits of detection of 2 pptv
- C₇ and greater Non-methane hydrocarbons have limits of detection of 1 pptv.
- The measurement precision, represented by the relative standard deviation (RSD) of the peak areas for each compound in the whole air standards, was 1 - 8% for the hydrocarbons, 3 - 10% for halocarbons, and 3 - 5% for the alkyl nitrates.

Methods:

Whole air samples were collected three days per week (Monday, Thursday, and Saturday) at all sites except JOTR-CC, which sampled once per week. Stainless steel Silonite®-coated 1.4 L canisters (Entech Instruments, Simi Valley, CA, USA) were cleaned by repeated filling and evacuating of ultra-high purity (UHP) nitrogen gas while heating under vacuum. Canisters were shipped to each site where National Park Service (NPS) site operators installed the canisters for the week each Tuesday. Timers coupled with a flow controller (Restek, Bellefonte, PA, USA) were used to automatically collect air into individual canisters from 3 PM to 5 PM (local time) on each sampling day.

A five-channel, three-GC (gas chromatograph) analytical system, which employed three flame ionization detectors (FIDs), one electron capture detector (ECD) and one mass spectrometer (MS) was used to analyze sampled canisters. This system was used to measure 56 individual VOCs, including light alkanes (C₂-C₅), heavy alkanes (more than C₅), C₁-C₂ halocarbons, C₁-C₅ alkyl nitrates, alkenes, branched alkanes, branched alkenes, cyclic alkanes, biogenic VOCs, and aromatic VOCs.

The analytical system and sample analysis methodology used for this study are similar to those used in previous studies (see references in associated manuscript). Briefly, multiple standards were used during sample analysis (analyzed every 10 samples) to track system drift over time. The measurement precision, represented by the relative standard deviation (RSD) of the peak areas for each compound in the whole air standards, was 1 - 8% for the hydrocarbons, 3 - 10% for halocarbons, and 3 - 5% for the alkyl nitrates. System blanks were measured every day prior to analysis and were analyzed in the same manner as other sampled canisters. Site blank canisters were shipped to and from each site in the same shipment as samples but were not installed in the field. These were filled with UHP nitrogen after arriving in the lab and were analyzed in the same batch as the samples with which they travelled.

Date dataset was last modified: 2020 May 6