

**Title:** ReadMe for CAVE 2019 URG Dataset

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**1.0 Data Set Description**

Final data for the University Research Glassware (URG) denuder/filter pack sampling trains run from 7/26/2019 to 9/3/2019 during the CarCavAQS field campaign in Carlsbad Caverns National Park, NM. Data are 24-hour integrated concentrations of gas and particle (PM<sub>2.5</sub>) concentrations. The data are reported at ambient conditions (i.e., not corrected for temperature and pressure). Measured species include:

- Ammonia
- Nitric Acid
- Sulfur Dioxide
- Levoglucosan
- Mannosan
- Galactosan
- Galactose
- Glucose
- Mannose
- Mannitol
- Arabinose
- Xylose
- Chloride
- Nitrite
- Nitrate
- Sulfate
- Sodium-Ethanolamine
- Methylamine
- Diethanolamine
- Potassium
- Dimethylamine
- Allylamine

- Propylamine
- tert-Butylamine
- Trimethylamine
- Diethylamine
- sec-Butylamine
- iso-Butylamine
- Butylamine
- Triethylamine
- Dipropylamine
- Amylamine
- Magnesium
- Calcium
- Ammonium

Measurements were made at the Biology Office and Building 58 (32.18° N, 104.44° W) located within Carlsbad Caverns National Park. The field study took place from Jul. 25-Sept. 5, 2019.

Those interested in using these data are encouraged to contact the authors listed above for more information. In case of planned publication, we request that data users contact Jeff Collett ([collett@colostate.edu](mailto:collett@colostate.edu)) to discuss appropriate recognition of those that collected the data and the agencies that sponsored data collection.

## 2.0 Instrument Description

URG annular denuder and filter pack samplers were used to measure inorganic gas and particle species of aerodynamic size less than 2.5 microns [Allegri *et al.*, 1987, 1994; Fitz, 2021]. The air flow passed through a Teflon coated PM<sub>2.5</sub> cyclone then through a sodium bicarbonate coated annular denuder to collect HNO<sub>3</sub> (g) and SO<sub>2</sub> (g), a phosphorous acid coated denuder to collect NH<sub>3</sub> (g), a 37 mm nylon filter (MTL Nylasorb, 1 µm pore size) to capture PM<sub>2.5</sub> particles, and an additional phosphorous acid coated denuder to capture any volatilized NH<sub>3</sub> from ammonium nitrate initially captured on the filter. The filter effectively retains HNO<sub>3</sub> from this reaction due to the nylon filter's affinity for it [Benedict *et al.*, 2013; Lee *et al.*, 2008; Yu *et al.*, 2005, 2006]. The flow was controlled at 10 L min<sup>-1</sup> and the pressure drop across the sampling train was recorded. A dry gas meter downstream of the sample train measured total flow integrated across the sampling period, which was then corrected for the pressure drop to obtain the ambient sample volume. A schematic of the sampling train set-up at the field site is shown in Figure 1.

After sample collection, annular denuders were extracted in 10 mL 18.2 MΩ deionized water in the field. Filter samples were unloaded into polystyrene test tubes and refrigerated until analysis commenced back in the lab. Each filter was extracted in 6 mL deionized water and sonicated for 40 min without heat. Both sets of extracts were then analyzed in the lab for anion and cation species using ion chromatography. Both systems utilized a Dionex DX-500 ion chromatograph (IC), which includes an isocratic pump, self-regenerating suppressor, and conductivity detector. The injection volume of both methods was 50 µL and analysis time was 17 minutes. The anion IC was used to quantify gas species (HNO<sub>3</sub>, SO<sub>2</sub>), and PM<sub>2.5</sub> species (Cl<sup>-</sup>, NO<sub>2</sub><sup>-</sup>, NO<sub>3</sub><sup>-</sup>, and SO<sub>4</sub><sup>2-</sup>). An IonPac AS14A (4×150 mm) analytical column was used with 1 mM sodium bicarbonate and 8 mM sodium bicarbonate eluent at a flow rate of 1 mL min<sup>-1</sup>. The cation IC was used to

quantify gaseous ammonia ( $\text{NH}_3$ ), and  $\text{PM}_{2.5}$  species:  $\text{Na}^+$ ,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ . A Dionex IonPac CS12A (3x120 mm) analytical column was used with 20 mM methanesulfonic acid eluent at a flow rate of  $0.5 \text{ mL min}^{-1}$ . Each component was quantified using an 8 point calibration curve.

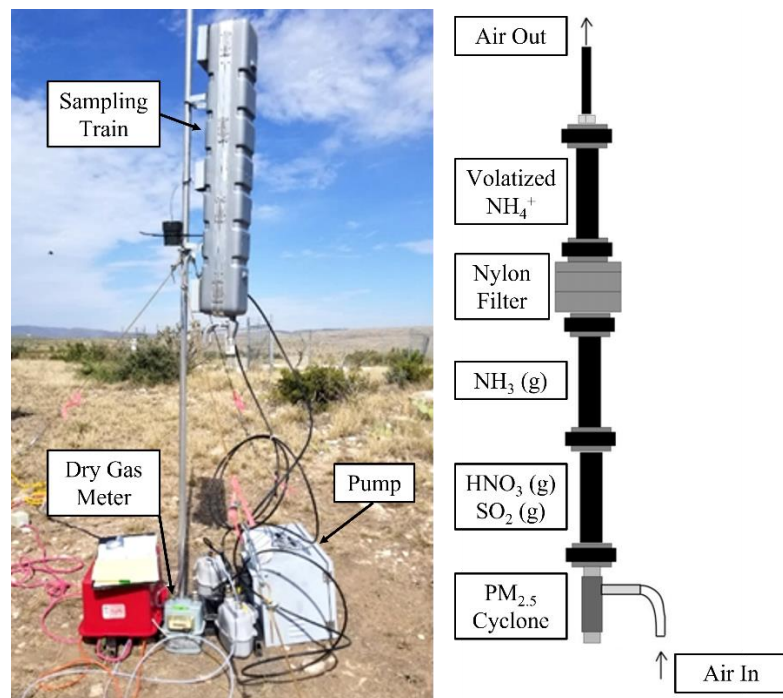


Figure 1. The experimental set-up for URG annular denuder/filter pack sampling is shown. Locations of the URG pump box, dry gas meter, and case which the sampling train is kept in are labeled. A sample train diagram, modified from the diagram in [Yu et al., 2005] is shown on the right-hand side.

### 3.0 Data Collection and Processing

URG samples were collected every 24 hours, from midnight to midnight. Blank samples were collected weekly by loading a denuder/filter pack sampling train into the sampler without the pump running for 24 h. During the IC analysis, A standard replicate and deionized water sample were analyzed after every 10 samples. Based on previous work the relative standard deviations (RSDs) of major aerosol ion concentration measurements ( $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ , and  $\text{NH}_4^+$ ) are estimated to be between 3-5% and the RSDs for replicate denuder gas concentration measurements are estimated to be approximately 10% [Lee et al., 2004]. Denuder and filter data are blank corrected by subtracting the average blank value across the study period.

### 4.0 Data Format

Data can be found in the csv file named CAVE2019\_URG\_final.csv. The file contains the start time, end time, and concentration of all gas and particle species. Concentrations are provided as ambient concentrations (i.e., is not corrected for temperature and pressure). The start and end times are provided in Mountain Daylight Time. Units are  $\mu\text{g m}^{-3}$ . The LOD is  $0.01 \mu\text{g m}^{-3}$  for all denuder data and  $0.01 \text{ ng m}^{-3}$  for all filter data. LODs can also be found in the table in section 6.0 Variable information.

A -8888 indicates data below the detection limit. A -9999 indicates missing data.

## 5.0 Data Remarks

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## 6.0 Description of Variables

Variable Name	Units	Description	Time Resolution	Limit of Detection
Start_time (MDT)	MM/DD/YYYY HH:MM	mountain time zone, beginning of sampling period		
End_time (MDT)	MM/DD/YYYY HH:MM	mountain time zone, end of sampling period		
NH3 (ug/m3)	μg m <sup>-3</sup>	Ammonia gas concentration	24-hour	0.01 μg m <sup>-3</sup>
HNO3 (ug/m3)		Nitric acid gas concentration		
SO2 (ug/m3)		Sulfur dioxide gas concentration		
Levoglucosan (ug/m3)		Concentrations of 33 PM <sub>2.5</sub> species from filter measurements		0.01 ng m <sup>-3</sup>
...				
Calcium (ug/m3)		Total ammonium PM <sub>2.5</sub> concentration (sum of filter and back-up denuder)		0.01 μg m <sup>-3</sup>
Ammonium (ug/m3)				

## 7.0 References

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