

# Metadata

## Dataset Title:

Cary\_AQ\_Chemistry\_Data.csv

Cary Environmental Monitoring Program Air Quality Chemistry Data

## Abstract

This dataset is a contribution to the Cary Institute of Ecosystem Studies Environmental Monitoring Program. This program is a long-term data collection program designed to understand how the environment changes over time. The program includes monitoring of climate including temperature and precipitation, as well as variables related to air pollution, such as acid deposition and ozone, and water pollution and other streamwater chemistry. Our program also includes solar radiation monitoring, which includes diffuse and global photosynthetically active radiation (PAR), diffuse and global shortwave radiation, net radiation and UV. Long-term monitoring of solar radiation provides us with an understanding of atmospheric energy dynamics, which can affect natural and human systems.

Data provided in this dataset include air chemistry data.

The Cary Institute of Ecosystem Studies, Environmental Monitoring Program furnishes data under the following conditions: The data have received quality assurance scrutiny by our program, and, although we are confident of the accuracy of these data, Cary Institute will not be held liable for errors in these data. Data are subject to change resulting from updates in data screening or models used. Data citation: Data citation: Please click on the Cite button on the Figshare repository.

Those wishing to publish data from Cary Institute of Ecosystem Studies, Environmental Monitoring Program are encouraged to contact data manager Vicky Kelly, [kellyv@caryinstitute.org](mailto:kellyv@caryinstitute.org).

## Investigators

First Name	Middle Initial	Last Name	Organization	e-mail address	ORCID ID
Victoria	R	Kelly	Cary Institute of Ecosystem Studies	<a href="mailto:kellyv@caryinstitute.org">kellyv@caryinstitute.org</a>	0000-0003-3418-9211

## Keywords

Cary Institute, Cary Institute of Ecosystem Studies, data, climate, chemistry, dry deposition, air quality, sulfur dioxide, nitric acid vapor, aerosol, particulate matter, calcium, magnesium, potassium, sodium, chloride, sulfate, nitrate, ammonium, phosphate

## Timeframe

The data in this file start January 1988 and end December 2022. Data collection is ongoing.

## Geographic location

The air quality sampler is located in a flat, open field at an elevation of 128 m. GPS coordinates for the site are: N41.785823 W073.741447.

## Methods

Aerosol concentrations,  $\text{HNO}_3$  and  $\text{SO}_2$  are sampled using Teflon filter packs. Three 47-mm diameter filters are placed in each filter pack: a Teflon filter (1988-February 2004 Zefluor, 2 micron, Gelman Sciences, Inc.; February 2004-present Whatman, 1 micron) for collection of aerosols, a Nylasorb 1 micron nylon filter (Gelman Sciences, Inc.) for collection of  $\text{HNO}_3$  vapor and a potassium carbonate-coated cellulose filter for collection of  $\text{SO}_2$ . The cellulose filters are Whatman 41, >20-25  $\mu\text{m}$  particle retention, coarse porosity, ASTM, 12 sec, (Whatman number 1441-047). The cellulose filters are cleaned before coating by rinsing and soaking overnight in double-deionized water. The three filters are placed in line so that the Teflon filter is exposed to incoming ambient air first, the nylon filter second and the carbonate filter last. The filter packs are placed in an inverted stainless steel pot (from 1988 - July 1993 it was an inverted plastic funnel) on a tower approximately 10 m above a mowed grass surface. A continuous flow of air is drawn through the filter pack at 3.00 lpm using a Gast, Inc. oil-less vacuum pump (model 1031, upgraded to model 1531-107B-6288 in 1998), which is regulated by a mass flow controller (Tylan General Inc., model FC280V, upgraded to model FC2604S in 1998 and to Aalborg model GFC 17 in September 2002). When the mass flow controller is off line for any reason, either a needle valve or another mass flow controller regulates flow. During this time, flow is measured using a rotameter (Gilmont Instruments, Inc., or Scienceware®), and the flow measurements are corrected for instantaneous temperature and atmospheric pressure. Clean filter packs are exchanged for exposed ones every Tuesday.

The Teflon filters are extracted in 50 ml of double deionized water for 24 hours in the dark at 2 degrees C after sonication for 15 minutes. The solution is then decanted into sample bottles and analyzed at the Cary Institute for pH, nitrate, sulfate, ammonium, phosphate, Chloride, Sodium, Calcium, Magnesium and Potassium for determination of aerosol chemistry (see Table 1 for analytical methods). Nitric acid vapor is determined by extracting each nylon filter in 50 ml of a mixture of  $\text{NaHCO}_3$  (0.28 M) and  $\text{Na}_2\text{CO}_3$  (0.22 M) diluted 1:100 with double deionized water. The filters are sonicated for 15 minutes and then refrigerated for 24 hours before decanting the solutions and analyzing them for nitrate and sulfate. Sulfur dioxide is determined by extracting the carbonate-coated filters in 50 ml of double deionized water with 2 drops of hydrogen peroxide. The filters are sonicated and extracted as described above and the resulting solution is analyzed for sulfate. Concentrations of sulfate from the nylon and carbonate filters are added to determine total sulfur dioxide. From 1993-2015 all sample extractions were preserved with 2 drops of chloroform. No preservative was used from 2016 onward.

Using the total amount of time that each filter was exposed and the average flow rate for the week, weekly concentrations of each component are calculated. For samples that returned less than detection limit concentrations, one half the detection limit is used to calculate air concentrations. Monthly average deposition velocities were estimated for 1988-2013 using a multi-layer dry deposition model (Meyers, T.P., Finkelstein, P., Clarke, J., Ellestad, T.G., Sims, P.F. 1998. A multilayer model for inferring dry deposition using standard meteorological measurements. *Journal of Geophysical Research* 103: 22645-22661). Monthly average deposition velocity values were used to estimate weekly average deposition velocities, which were combined with weekly concentrations to estimate weekly fluxes. Data sets include monthly mean air concentrations, monthly mean deposition velocities and monthly total deposition. For a descriptions of variables, see variable list with units below.

### LOW-VOLUME FILTER PACK AIR CHEMISTRY INSTRUMENT MAKE, MODEL & DATES USED

Pump: Gast, Inc. oil-less vacuum pump model 1031 (1988-1998), model 1531-107B-6288 (1998- present)

Mass Flow Controller: Tylan-Millipore model FC280V (1988-1998) FC2604S (1998-2002) Aalborg GFC17 (2002-present)

### LOW-VOLUME FILTER PACK AIR CHEMISTRY DATA QUALITY ASSURANCE & QUALITY CONTROL PARAMETERS & METHODS

All filter packs and bottles are cleaned by rinsing in deionized water 6 times and finally either dried in a drying oven at no more than 60 degrees C or allowed to sit with caps loosened (bottles) until dry. Every 12 months a filter pack with a set of filters is exposed under a vacuum of 3.00 lpm for 3 minutes. The filter pack and filters are handled and analyzed as regularly exposed filters. This is to ensure that the sample handling procedures introduce no contamination.

When analytical results are received from the Cary Institute analytical lab, data are examined and checked using two methods. First, ion balances and ionic strength are calculated using the following equations:

$$\text{Ion Balance} = ((\text{ANIONS} - \text{CATIONS}) / ((\text{CATIONS} + \text{ANIONS}) / 2)) * 100;$$

$$\text{Ion Strength} = \text{CATIONS} + \text{ANIONS};$$

Where:

$$\text{Cations} = \text{CA}/20 + \text{MG}/12 + \text{NA}/23 + \text{K}/39 + \text{NH}_4/18 + \text{HA};$$

$$\text{Anions} = \text{NO}_3/62 + \text{SO}_4/48 + \text{CL}/35.5;$$

And:

HA is teflon filter H<sup>+</sup> conc (mg/l)  
 CA is teflon filter Ca concentration (mg/L)  
 MG is teflon filter Mg concentration (mg/L)  
 NA is teflon filter Na concentration (mg/L)  
 K is teflon filter K concentration (mg/L)  
 NO<sub>3</sub> is teflon filter NO<sub>3</sub> concentration (mg/L)  
 SO<sub>4</sub> is teflon filter SO<sub>4</sub> concentration (mg/L)  
 CL is teflon filter Cl concentration (mg/L)  
 NH<sub>4</sub> is teflon filter NH<sub>4</sub> concentration (mg/L)

HA is calculated as  $(10^{**\text{PH}}) * 1000$ , where PH = pH of teflon filter extractant.

Ion balances and ionic strength are examined and samples are considered for reanalysis if the following criteria are met:

Ionic Strength (ueq) and Ion Balance (%)  
 Less than 50 greater than 40  
 Between 50 and 100 greater than 20  
 Greater than 100 greater than 10

The second quality control step is to examine time series graphs of sample concentrations for each analyte. If any samples are obvious outliers, they are considered for reanalysis.

Analytical methods, instrument notes including calibration schedule, malfunctions and repairs, new instrumentation, anecdotal information etc. can be made available on request.

## LOW-VOLUME FILTER PACK AIR CHEMISTRY DATA VARIABLE DESCRIPTIONS WITH UNITS

### Data Table

Column name	Description	Unit or code explanation or date format	Empty value code
STARTDAY	Date & time filter pack placed on tower	Datetime (m/d/yyyy hh:mm format)	NA

ENDDAY	Date & time filter pack taken off tower	Datetime (m/d/yyyy hh:mm format)	NA
SO2	air concentration of gaseous SO2 (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACHNO3	air concentration of gaseous HNO3 (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACNO3	air concentration of particulate NO3 (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACNH4	air concentration of particulate NH4 (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACSO4	air concentration of particulate SO4 (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACCA	air concentration of particulate Ca (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACMG	air concentration of particulate Mg (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACNA	air concentration of particulate Na (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACK	air concentration of particulate K (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
ACCL	air concentration of particulate Cl (ug/m <sup>3</sup> )	ug/m <sup>3</sup>	NA
SO2FLUX	SO2 dry deposition for the week (mol/ha)	mol/ha	NA
HNH3FLUX	HNO3 vapor dry deposition for the week (mol/ha)	mol/ha	NA
NO3FLUX	NO3 particle dry deposition for the week (mol/ha)	mol/ha	NA
SO4FLUX	SO4 particle dry deposition for the week (mol/ha)	mol/ha	NA
NH4FLUX	NH4 particle dry deposition for the week (mol/ha)	mol/ha	NA
TOTAL_S	Total S dry deposition for the week (mol/ha)	mol/ha	NA
TOTAL_N	Total N dry deposition for the week (mol/ha)	mol/ha	NA
CAFLUX	Ca particle dry deposition for the week (mol/ha)	mol/ha	NA
MGFLUX	Mg particle dry deposition for the week (mol/ha)	mol/ha	NA
NAFLUX	Na particle dry deposition for the week (mol/ha)	mol/ha	NA
KFLUX	K particle dry deposition for the week (mol/ha)	mol/ha	NA
CLFLUX	Cl particle dry deposition for the week (mol/ha)	mol/ha	NA
VDSO2	deposition velocity for SO2 (cm/s)	cm/s	NA
VDHNO3	deposition velocity for HNO3 (cm/s)	cm/s	NA
VDTSP	deposition velocity for fine particles (cm/s)	cm/s	NA

## Intellectual Rights

This information is released under the Creative Commons license - Attribution-NonCommercial - CC BY-NC (<https://creativecommons.org/licenses/by/4.0/>).

Methods of Analysis  
Cary Institute of Ecosystem Studies Analytical  
Laboratory

ION	INSTRUMENT	TECHNIQUE
NH <sub>4</sub> <sup>+</sup>	Lachat QuikChem 8000	Phenate method <sup>1</sup> #10-107-06-1-J
SO <sub>4</sub> <sup>=</sup> , NO <sub>3</sub> <sup>-</sup> (PPT, AQ), Cl <sup>-</sup>	Dionex ICS2000 Ion Chromatograph	Ion exchange chromatography, AS18 and AG18 columns, SRS (self-regenerating) suppressor <sup>2</sup> with CRD 200 (carbonate removal device)
K <sup>+</sup> , Na <sup>+</sup>	Perkin Elmer Aanalyst 300 Atomic Absorption Spectrometer	Flame atomization, direct air <sup>3</sup>
Ca <sup>++</sup> , Mg <sup>++</sup>	Leeman Labs Inductively Coupled Plasma/Profile	Emission spectroscopy
NO <sub>3</sub> <sup>-</sup> (WC)	Lachat QuikChem 8000	Cadmium diazotization <sup>1</sup> Method #10-107-04-1-C
PO <sub>4</sub>	Lachat QuikChem 8000	Phosphomolybdate <sup>1</sup> Method #_10-115-01-1-M
pH	Fisher-Accumet AR20 pH meter with Fisher glass electrode, Fisher calomel reference probe	Standardization with Fisher 7.00 and 3.00 buffer solutions; samples and buffers at room temperature
Specific Conductance	Fisher-Accumet AR20 pH/conductivity meter	Conductivity probe w/ 1.0 cm <sup>-1</sup> cell constant
DOC (Dissolved Organic Carbon)	Shimadzu TOC 5050	High temperature combustion of sample; platinum catalyst C to CO <sub>2</sub> , NDIR detect.

<sup>1</sup>Standard Lachat methods, 2000, Lachat Instruments, Milwaukee, WI

<sup>2</sup>Small, H., Stevens, T.S., and Bauman, W.C. *Anal. Chem.* 1975, 47:1801-1809

<sup>3</sup>Slavin, W. *Atomic absorption spectroscopy*. Wiley-Interscience, New York. 1968. PPT=precipitation samples, AQ=air samples, WC=Wappinger Creek samples