Description

These files contain observed and CMAQ estimated gas species data that were used in the analysis documented in the manuscript "Evaluation of 15 years of modeled NOX across the contiguous United States". The files are packages as a set of .csv, .zip and .tar.gz files that correspond to different plots and analyses in the paper.

2014 Emissions Inventory Summary for NOX

File name: NOX_2014NEIv2.zip

Used for Figure 1

The data provided in files 2014NEIv2_National_Tier3_nonroad.csv and 2014NEIv2_nox_totals_bysector.csv was downloaded from the National Emissions Inventory site using the Query tool (https://www.epa.gov/air-emissions-inventories/2014-national-emissions-inventory-nei-data). The files are provided in comma-separated value (csv) format and contain annual NOx emissions information in US tons by sector for the year 2014.

The data provided in 2014fd_onroad_NOX_bySCC.csv was provided by Alison Eyth (US EPA-OAQPS) and contains annual NOx emissions in US tons by Source Classification Code (SCC) for the onroad sector specific to the year 2014.

2002-2016 Onroad and Nonroad NOX Trends

File name: NOX_onroad_nonroad_emissions_trends.zip

Used for Figure 2

The data provided in the file US_NOX_ModelingPlatforms_20022016.csv contains annual NOx inventories by sector from EPA emissions modeling platforms for 2002-2016.

The data provided in MOVES2014b_Onr_Nr_Total_NOx_20022016.csv contains annual estimates of NOX for both onroad and nonroad sectors that were calculated from 2-month national model runs using the official version of MOVES2014b and its default database

https://www.epa.gov/moves/moves-versions-limited-current-use

Modeled oxidized nitrogen species for 2015

File name: Modeled_NOX_NOY_NOZ_2015.zip

Used for Figure 3

The zipped file contains 4 .csv files: annual_panel1_NOX.csv, annual_panel2_NOZ.csv, annual_panel3_NOY.csv, annual_panel4_NOX_to_NOY_ratio.csv

Each file contains the gridded model data shown in the four maps in Figure 3. The model grid is 395 x 246 and uses a Lambert conformal projection. The projection information is provided below.

Lambert conformal projection:
true latitudes of 33.000 and 45.000

with a center at -97.000 40.000
XORG=-2412000.000 m
YORG=-1620000.000 m
DELTAX= 12000.000 m
DELTAY= 12000.000 m
NX=396
NY=246

Matched AQS and CMAQ Hourly NOx

File names: AQS_full_site_list.csv, AQS_CMAQ_matched_YYYY.tar.gz (YYYY is the placeholder for years 2002-2017)

Used for Figures 4 and 5

The data are provided as monthly files for each of the 16 years of model simulation (2002-2016 with two model versions used for 2016). Each file is in comma-separated value (csv) format and contains paired hourly gas species observed and simulated mixing ratios for days on which monitoring data were available during that month. The .csv data file names are in the following format:

AQS_CMAQvXX_Hourly_YYYYMM.csv

- XX is the CMAQ version, e.g. 502, 51
- YYYYMM: year and month of the matched observed and modeled data

The first six lines of each file contain header information. Variable units are provided on line 4 and variable names are on line 6. The species names are part of the variable names, e.g., NOX_ob corresponds to the observed NOX value, NOX_mod corresponds to the CMAQ estimate. The monthly .csv files are tar and zipped into annual .tar.gz files. The file AQS_full_site_list.csv provides additional meta data about each AQS monitoring location site. The column 'co_network' was used to determine whether a site was part of the EPA's near road network (these sites were excluded from the analysis).

Information on the CMAQ simulation used for each of the years is summarized in Table 1 below.

Table 1: Details of CMAQ model simulations used in this study.

Year	Air Quality Model	Chemical Mechanism Aerosol Module	Meteorological Model	NEI version (Emissions Platform)	Onroad Model	Reference/Metadata
2002	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2002 NEI v3 (2002af)	MOVES2010b	https://doi.org/10.15139/S3/IF4U6D
2003	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2002 NEI v3 (2003af)	Interpolated between 2002 and 2005	https://doi.org/10.15139/S3/E08VGK
2004	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2005 NEI v3 (2005ct_04)	Interpolated between 2002 and 2005	https://doi.org/10.15139/S3/Z0XTML
2005	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2005 NEI v3 (2005ct)	MOVES2010b	https://doi.org/10.15139/S3/GLQYWT

2006	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2008 NEI v3 (2007ed_06)	MOVES2010b	https://doi.org/10.15139/S3/56JKOO
2007	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2008 NEI v3 (2007rh)	MOVES2010b	https://doi.org/10.15139/S3/8LVCJM
2008	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2008 NEI v3 (2008ab)	MOVES2010b	https://doi.org/10.15139/S3/JPHKEV
2009	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2008 NEI v3 (2009ef)	MOVES2010b	https://doi.org/10.15139/S3/MEDEWM
2010	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2008 NEI v3 (2007ed_10)	MOVES2010b	https://doi.org/10.15139/S3/YIPTDY
2011	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2011 NEI v1 (2011ed)	MOVES2010b	https://doi.org/10.15139/S3/NS8Y6C
2011	CMAQv5.0.2_met_updates	CB05TUCL AERO6	WRFv3.7	2011 NEI v1 (2011ed)	MOVES201b	Appel et al. 2017
2011	CMAQv5.1	CB05e51 AERO6	WRFv3.7	2011 NEI v1 (2011ed)	MOVES2010b	Appel et al. 2017
2012	CMAQv5.0.2	CB05TUCL AERO6	WRFv3.4	2011 NEI v2 (2011ed_12)	MOVES2014a	https://doi.org/10.15139/S3/YXQNRW
2013	CMAQv5.1	CB05e51 AERO6	WRFv3.7.1	2011 NEI v2 (2013ej)	MOVES2014a	https://doi.org/10.15139/S3/FQO7IS
2014	CMAQv5.2	CB6r3 AERO6NVPOA	WRFv3.8.1	2014 NEI v1 (2014fb)	MOVES2014a	https://doi.org/10.15139/S3/XYW3HL
2015	CMAQv5.2.1	CB6r3 AERO6NVPOA	WRFv3.8	2015 NEI v1 (2015fd)	MOVES2014a	Kelly et al., 2019
2016	CMAQv5.2.1	CB6r3 AERO6	WRFv3.8	2016 NEI alpha (2016fe)	MOVES2014b	Appel et al., 2020
2016	CMAQv5.3	CB6r3 AERO7	WRFv3.8	2016 NEI beta (2016ff)	MOVES2014b	Appel et al., 2020

Diurnal profiles of NOX bias, mobile NOX emissions and modeled boundary layer

File name: Diurnal_profiles.csv

Used for Figure 6

The data is provided in a comma-separated file (.csv) and contains paired hourly NOx observed, simulated NOx mixing ratios, simulated boundary layer heights, gridded NO2 emissions and calculated NOx emissions for days on which monitoring data were available during summer and winter for the 4 locations presented in Figure 6. The column headings and their description are presented below:

site.id	US EPA Air Quality System identifier
LST	Local Std Time
time.on	Time of observation
dow	Day of the Week

start.hour	Integer for hour of observation
tz	Time Zone
nox.obs	NOx observations (ppb)
nox.mod.v502	Modeled NOx (ppb) CMAQv5.0.2
nox.mod.v51	Modeled NOx (ppb) CMAQv5.1
nox.mod.v52	Modeled NOx (ppb) CMAQv5.2
pblh.mod.v51	Modeled Planetary Boundary Layer Height (m) CMAQv5.1
pblh.mod.v502	Modeled Planetary Boundary Layer Height (m) CMAQv5.0.2
pblh.mod.v52	Modeled Planetary Boundary Layer Height (m) CMAQv5.2
nox_mb_v502	Mean Bias (model - obs) NOx (ppb) calculated using CMAQv5.0.2
nox_mb_v51	Mean Bias (model - obs) NOx (ppb) calculated using CMAQv5.1
nox_mb_v52	Mean Bias (model - obs) NOx (ppb) calculated using CMAQv5.2
file	Site identifier
month	month
season	season (Winter = Dec-Jan-Feb; Summer = June-Jul-Aug)
NO2.RPD.onroad	Rate per Hour NO2 onroad emissions (mol s-1) from SMOKE
NO2.RPH.onroad	Rate per Distance NO2 onroad emissions (mol s-1) from SMOKE
NO2.RPV.onroad	Rate per Vehicle NO2 onroad emissions (mol s-1) from SMOKE
NO2.nonroad	Nonroad NO2 emissions (mol s-1) from SMOKE
mylabel	City associated with AQ site
NOX_Running	Calculated NOx emissions from NO2 SMOKE emissions (NO2.RPD.onroad *(1/0.092))
NOX_Idling	Calculated NOx emissions from NO2 SMOKE emissions (NO2.RPH.onroad *(1/0.092))
NOX_Starts	Calculated NOx emissions from NO2 SMOKE emissions (NO2.RPV.onroad *(1/0.092))
NOX_Nonroad	Calculated NOx emissions from NO2 SMOKE emissions (NO2.nonroad *(1/0.092))

Diurnal profiles of NOX bias and observations from sensitive and base case

File name: Diurnal_profiles_sensitivities.csv

Used for Figure 7

The data is provided in a comma-separated file (.csv) and contains hourly NOx observed and simulated NOx mixing ratios for the month of July 2011 for monitors representing each of the cities in Figure 6. The column headings and their description are presented below:

site.id	US EPA Air Quality System identifier
County	County
State	State
Month	Month
Ob_hour	Hour of observation

Variable	Mean hourly NOx Bias calculated for each model version/sensitivity case as well as hourly NOx observations
Value	Value in ppb
Site.name	City corresponding to monitoring site

DISCOVER-AQ data files

File names: CMAQ_aircraft_paried_data_CB05e51chemistry.tar.gz, CMAQ_aircraft_paried_data_CB05tuclchemistry.tar.gz, CMAQ_aircraft_paried_data_CB6chemistry.tar.gz

Used for Figures 8 and 9

These files include CMAQ model data and observational data for NOy species measured by aircraft from the DISCOVER-AQ Baltimore campaign (Crawford et al., 2014; Crawford & Pickering, 2014). Please note the PI contact information for the original measurement data listed below:

- NO, NO2, and NOy measurements from National Center for Atmospheric Research four-channel chemiluminescence instrument: Weinheimer, A.J.; Montzka, D.D.; Knapp, D.J., National Center for Atmospheric Research, wein@ucar.edu, 303-497-1444, NCAR, 1850 Table Mesa Dr., Boulder, CO 80305
- NO_2 measured by laser-induced fluorescence (LIF): Cohen, Ronald, University of California, Berkeley, Chemistry Department, University of California, Berkeley, CA 94720; cohen@cchem.berkeley.edu; 510-642-2357
- peroxy nitrates (PNs; $\sum RO_2NO_2$), alkyl nitrates (ANs; $\sum RNO_2$), and nitric acid (HNO_3) measured by Thermal dissociation (TD) coupled with LIF: Cohen, Ronald, University of California, Berkeley, Chemistry Department, University of California, Berkeley, CA 94720; cohen@cchem.berkeley.edu; 510-642-2357

Data file names are in the following format:

CCTM_MMMM_12km.P3B15s_CCC_YYYYMMDD.csv

- MMMM is a placeholder for the chemical mechanism used for the modeling simulation
  - CB6_apr25_tucl: model simulation using the CB05 chemical mechanism
  - CB6_apr25_e51: model simulation using the CB05e51 chemical mechanism
  - CB6cl1: model simulation using CB6 chemical mechanism
- CCC is a placeholder for the NOy species of interest
  - ANs: alkyl nitrates
  - HNO3: nitric acid
  - NO2_LIF: nitrogen dioxide measured by laser-induced fluorescence (UC Berkeley)
  - NO2_NCAR: nitrogen dioxide measured by four-channel chemiluminescence (NCAR)
  - NO: nitric oxide
  - NOy: total NOy measured by four-channel chemiluminescence (NCAR)
  - PNs: peroxy nitrates
- YYYYMMDD: date of the aircraft flight

Data files include the following data fields:

- Site_ID: location name which corresponds to approximate aircraft location
    - Aldino: aircraft vertical spiral near Aldino, MD
    - Beltsville: aircraft vertical spiral near Aldino, MD
    - Edgewood: aircraft vertical spiral near Edgewood, MD
    - Essex: aircraft vertical spiral near Essex, MD
    - Fairhill: aircraft vertical spiral near Fairhill, MD
    - Padonia: aircraft vertical spiral near Padonia, MD
    - Highway: aircraft transect following I-95 interstate between Beltsville and Baltimore
    - ChesapeakBay: aircraft transect over the Chesapeake Bay
    - Onflight: all other aircraft locations
- Datetime(UTC): Date and time of measurement given in UTC. Model data is matched to the nearest hour.
- Lat: Latitude of aircraft at time of measurement. Model data is matched to the nearest 12km resolution grid-cell center.
- Lon: Longitude of aircraft at time of measurement. Model data is matched to the nearest 12km resolution grid-cell center
- Alt(m): Altitude in meters of aircraft at time of measurement. Model data is matched to the nearest model layer
- Mod_layer: Model layer number (layer 1 represents the surface layer)
- MdLyerHgt(m): Mean height above ground level in meters of the model layer matched the aircraft altitude
- P3B_CCC(ppb): aircraft measurement of compound “CCC” given in units of ppb
- CMAQ_CCC(ppb): model prediction of compound “CCC” given in units of ppb
- SpiralNo: this field assigns a categorical number to the Site_ID field

Crawford, J. H., & Pickering, K. E. (2014). DISCOVER-AQ: Advancing strategies for air quality observations in the next decade. Environmental Management, 4– 7.

Crawford, J., Dickerson, R., & Hains, J. (2014). DISCOVER-AQ: Observations and early results. Environmental Management, 8– 15.