**Title:**

Model data associated with manuscript, "Source regions contributing to excess reactive nitrogen deposition in the Greater Yellowstone Area (GYA) of the United States"

**Abstract:**

Research has shown that excess reactive nitrogen (Nr) deposition in the Greater Yellowstone Area (GYA) of the United States has passed critical load (CL) thresholds and is adversely affecting sensitive ecosystems in this area. To better understand the sources causing excess Nr deposition, the Comprehensive Air Quality Model with extensions (CAMx), using Western Air Quality Study (WAQS) emission and meteorology inputs, was used to simulate Nr deposition in the GYA. CAMx's Particulate Source Apportionment Technology (PSAT) was employed to estimate contributions from agriculture (AG), oil and gas (OG), fire (Fire), and other (Other) source sectors from 27 regions, including the model boundary conditions (BC) to the simulated Nr for 2011. The BC were outside the conterminous United States and thought to represent international anthropogenic and natural contributions. Emissions from the AG and Other source sectors are predominantly from reduced N and oxidized N compounds, respectively. The model evaluation revealed a systematic underestimation in ammonia (NH3) concentrations by 65% and overestimation in nitric acid concentrations by 108%. The measured inorganic N wet deposition at National Trend Network sites in the GYA was overestimated by 31–49%, due at least partially to an overestimation of precipitation. These uncertainties appear to result in an overestimation of distant source regions including California and BC and an underestimation of closer agricultural source regions including the Snake River valley. Due to these large uncertainties the relative contributions from the modelled sources and their general patterns are the most reliable results. Source apportionment results showed that the AG sector was the single largest contributor to the GYA total Nr deposition, contributing 34% on an annual basis. Seventy-four percent of the AG contributions originated from the Idaho Snake River valley, with Wyoming, California, and northern Utah contributing another 7%, 5%, and 4%, respectively. Contributions from the OG sector were small at about 1% over the GYA, except in the southern Wind River Mountain Range during winter where they accounted for more than 10%, with 46% of these contributions coming from OG activities in Wyoming. Wild and prescribed fires contributed 18% of the total Nr deposition, with fires within the GYA having the highest impact. The Other source category was the largest winter contributor (44%) with high contributions from California, Wyoming and northern Utah.

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**Format of data files:**

Comma Separated Values (.csv files, in total 4 files)

Network Common Data Form (.NetCDF files, in total 10 files)

Please refer to link: https://www.unidata.ucar.edu/software/netcdf for the structure of NetCDF files.

**Data source:**

The data achieved here are from CAMx model (www.camx.com) simulation results. Please refer to the manuscript on the journal *Atmospheric Chemistry and Physic* for the detail model configuration,

**Time period of the data:**

2011, full year simulation; report the results in aggregated seasonal values. The definition of season is Spring (March, April, May), Summer (June, July, August), Fall (September, October, November), and Winter (December, January, February).

**Methods:**

Modeling simulations for 2011 were conducted using the CAMx version 6.10 with two nested grids. The outer domain (36 km) covered the contiguous United States (CONUS), as well as portions of Canada and Mexico, while the inner domain (12 km) encompassed the western United States and focused on states within the Western Regional Air Partnership (WRAP) (see Figure "GYA_source_region_map.tiff").

The hourly meteorological inputs for 2011 were generated by the Weather Research and Forecasting (WRF) model (WRF-ARW, version 3.5.1) and were obtained from the

Intermountain West Data Warehouse (IWDW) (http://views.cira.colostate.edu/tsdw/). This meteorological simulation performed comparably to other recent prognostic model applications used in air quality planning.

The emission inventory used by CAMx was primarily derived from the 2011 NEI version 2 (NEI2011v2) with the Sparse Matrix Operator Kernel Emissions (SMOKE) processing system version 3.0 for anthropogenic emissions, the Model of Emissions of Gases and Aerosols from Nature (MEGAN) version 2.10 for biogenic emissions, and the WRAP Windblown Dust Model (WRAP-WBD) to estimate wind-driven dust. Emissions from the oil and gas sector were further updated by the IWDW to represent the best-available inventory for oil and gas activity in the western United States at the time of modeling. The emissions for fire activities include agricultural fires, prescribed fires, and wildfires and were generated by the Particulate Matter Deterministic and Empirical Tagging and Assessment of Impacts on Levels (PMDETAIL) study. PMDETAIL developed 2011 fire emissions using satellite data, ground detects, and burn scar and estimated the plume rise, depending on fire size and type. The hourly, non-surface fire emissions were allocated to the proper CAMx vertical layers based on the model-predicted planetary boundary layer (PBL) height and the spanning of the plume top and bottom above the ground.

The boundary conditions for the 36-km domain were estimated from a 2011 global model run using the Model for Ozone and Related chemical Tracers (MOZART) version 4.6. The simulation year of 2011 was preceded by 15 days of "spin-up" time to minimize the effects of initial conditions. A more-detailed description of the WRF-SMOKE-CAMx modeling platform applied in this study is summarized in Table S1 as well as the 2011 Three-State Air Quality Study (3SAQS).

For the source apportionment estimates, 27 source regions (see the Figure "GYA_source_region_map.tiff"), as well as the lateral boundary conditions (BC), were "tagged" in the CAMx PSAT simulation. In addition, the emissions for each region were further subdivided into four source sectors: 1) agriculture (AG), 2) oil and gas activity (OG), 4) fire activity, including wildfires and prescribed fires (Fire), and 4) the remaining sources labeled as Other. The Other source sector primarily comes from mobile and large point sources, with smaller contributions from natural sources such as lightning.

CAMx-PSAT treats nitrogen-containing compounds as one of seven species: gaseous NH3; particulate ammonium (PNH4); reactive gaseous nitrogen (RGN), which includes primary emissions of NOx, nitrous acid (HONO), nitrate radical (NO3), and dinitrogen pentoxide (N2O5); gaseous nitric acid (HNO3); gaseous peroxy nitrogen (TPN), including peroxyacetyl nitrate (PAN) and peroxynitric acid (PNA); gas-phase organic nitrate (NTR); and particulate nitrate (PNO3). PSAT maintains the source-group identity (i.e., source region and source sector) by apportioning the secondary species to the precursor emissions (ENVIRON, 2014). In the source apportionment comparison results, we report the reduced Nr deposition as the sum of NH3 and PNH4 and the oxidized Nr deposition as the sum of RGN, HNO3, PNO3, TPN, and NTR in units of kg N $ha^{-1}$.

**File information:**

1. "Source_partition_lookup_table.csv": Lookup table for the 27 source region partition in the CAMx modeling. The corresponding Figure is "GYA_source_region_map.tiff".
2. "SA_GYA_totalN_2011_seasonly.csv": CAMx source apportionment results for the average **total** nitrogen deposition (in the unit of g N/ha) at the GYA area in each season contributed by the 4 tagged source sectors (AG, OG, Fire, Other) and 27 tagged source regions as well as lateral boundary conditions (BC).
3. "SA_GYA_wetN_dryN_2011_seasonly.csv": CAMx source apportionment results for the average **dry** and **wet** nitrogen deposition (in the unit of kg N/ha) at the GYA area in each season contributed by 4 tagged source sectors, 27 tagged source regions as well as BC.
4. "SA_GYA_reducedN_oxidizedN _2011_seasonly.csv": CAMx source apportionment results for the average **reduced** and **oxidized** nitrogen deposition (in the unit of kg N/ha) at the GYA area in each season contributed by 4 tagged source sectors, 27 tagged source regions as well as BC.
5. "GYA_PSAT_DNdep_Annual.nc": NetCDF files for the **annual dry** nitrogen deposition over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
6. "GYA_PSAT_DNdep_Spring.nc": NetCDF files for the **dry** nitrogen deposition on **spring** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
7. "GYA_PSAT_DNdep_**Summer**.nc": NetCDF files for the **dry** nitrogen deposition on **summer** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
8. "GYA_PSAT_DNdep_Fall.nc": NetCDF files for the **dry** nitrogen deposition on **fall** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
9. "GYA_PSAT_DNdep_Winter.nc": NetCDF files for the **dry** nitrogen deposition on **winter** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
10. "GYA_PSAT_WNdep_Annual.nc": NetCDF files for the **annual wet** nitrogen deposition over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.

11. “GYA_PSAT_WNdep_Spring.nc”: NetCDF files for the **wet** nitrogen deposition on **spring** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
12. “GYA_PSAT_WNdep_**Summer**.nc”: NetCDF files for the **wet** nitrogen deposition on **summer** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
13. “GYA_PSAT_WNdep_Fall.nc”: NetCDF files for the **wet** nitrogen deposition on **fall** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.
14. “GYA_PSAT_WNdep_Winter.nc”: NetCDF files for the **dry** nitrogen deposition on **winter** over the GYA area from the source apportionment results. See the variable information section below for the list of variables and their definition.

**Variable information**

Due to the data construction of NetCDF, the variables of data recorded in this format with the file names “GYA_PSAT_*Ndep_*.nc” (10 files) are basically self-explanatory.

There are 5 common variables for the 10 files which define the gridded domain structures. They are “lat”, “lon”, “time”, “x” and “y”. The 2D matrix for each variable is in the grid of 41 (columns, y-axis) $\times$35 (rows, x-axis).

There are associated 82 variables for every tagged species in CAMx at each tagged sources regions and source sectors directly from the CAMx-PSAT source apportionment standard outputs. The rule of the variable name definition is follow as:

[Species name][Source sector #][Source region #]_[wet/dry deposition marker]

For example, the variable “NH3001027D” means the contribution of dry deposition of NH3 (ammonia) from Source sector #1 and Source region #27; the variable “NH3000BC_D” means the contribution of dry deposition of NH3 at each grid from boundary conditions; the variable “NH3000IC_D” means the contribution of dry deposition of NH3 at each grid from initial conditions. The gaseous species are in the unit of “moles N/ha” and the particulate species are in the unit of “gram N/ha”.

In total 9 species were tagged in the CAMx-PSAT, they are:

SO2: gaseous sulfur dioxide

PS4:  particulate sulfate

NH3: gaseous ammonia

PN4: particulate ammonium

RGN: reactive gaseous nitrogen

HN3: gaseous nitric acid

TPN: gaseous peroxy nitrogen

NTR: gas-phase organic nitrate

PN3: particulate nitrate

In total 4 source sectors were tagged in the CAMx-PSAT, they are:

000: boundary conditions (BC) or intimal conditions (IC)

001: agriculture source sector

002: oil and gas source sector

003: others source sector

In total 27 source regions were tagged in the CAMx-PSAT, they are:

001: NW Colorado

002: NE Colorado

003: SE Colorado

004: SW Colorado

005: Upper Green River

006: Jackson

007: Eastern Wyoming

008: Western Wyoming

009: Yellowstone

010: Northern Idaho

011: Snake River Valley

012: Northern Utah

013: Southern Utah

014: Nevada

015: Montana

016: Washington

017: Oregon

018: California

019: Mexico

020: New Mexico

021: Arizona

022: Texas &Oklahoma

023: Canada

024: North Dakota

025: Pacific

026: Far East US

027: SD_KS_NE

Beside the standard outputs, there are aggregated variables to show the nitrogen deposition from different species contributed from all source regions or from all source sectors. The definitions of those variables are:

[Species name][Source sector#i, i=1,3]=$\sum_{j=1,27}$[Species name][Source sector #i, i = 1,3][Source region #j, j = 1,27]_[wet/dry deposition marker]

For example,
RGN001=RGN001001+RGN001002+RGN001003+RGN001004+RGN001005+RGN001006+RGN001007+RGN001008+RGN001009+RGN001010+RGN001011+RGN001012+RGN001013+RGN001014+RGN001015+RGN001016+RGN001017+RGN001018+RGN001019+RGN001020+RGN001021+RGN001022+RGN001023+RGN001024+RGN001025+RGN001026+RGN001027

Then the total wet/dry deposition for each nitrogen species in the unit of “kg N/ha” is:

ARGN=RGNBC+RGN001+RGN002+RGN003

ATPN=TPNBC+TPN001+TPN002+TPN003

ANTR=NTRBC+NTR001+NTR002+NTR003

AHN3=HN3BC+HN3001+HN3002+HN3003

APN3=PN3BC+PN3001+PN3002+PN3003

ANH3=NH3BC+NH3001+NH3002+NH3003

APN4=PN4BC+PN4001+PN4002+PN4003

The total wet/dry nitrogen deposition contributed by boundary conditions in the unit of "kg N/ha" is:

ABCON=RGNBC+TPNBC+NTRBC+HN3BC+PN3BC+NH3BC+PN4BC

The total wet/dry nitrogen deposition contributed by AG source sector in the unit of "kg N/ha" is:

A001=RGN001+TPN001+NTR001+HN3001+PN3001+NH3001+PN4001

The total wet/dry nitrogen deposition contributed by OG source sector in the unit of "kg N/ha" is:

A002=RGN002+TPN002+NTR002+HN3002+PN3002+NH3002+PN4002

The total wet/dry nitrogen deposition contributed by Other source sector in the unit of "kg N/ha" is:

A003=RGN003+TPN003+NTR003+HN3003+PN3003+NH3003+PN4003

The total wet/dry oxidized nitrogen deposition contribution in the unit of "kg N/ha" is:

AOXDN=ARGN+ATPN+ANTR+AHN3+APN3

The total wet/dry reduced nitrogen deposition contribution in the unit of "kg N/ha" is:

AREDN=ANH3+APN4

The total wet/dry all nitrogen deposition contribution in the unit of "kg N/ha" is:

ATOTALN=AOXDN+AREDN

**Date dataset was last modified**

5 September, 2018