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EPA's Air Quality Time Series Project (EQUATES) Data Dictionary

Summary

The EPA's Air Quality Time Series (EQUATES) project datasets include 2002–2019 emissions, meteorology, and air quality modeling of the contiguous US (CONUS) over the "12US1" 12-km domain and Northern Hemisphere over the "108NHEMI" 108-km domain. The datasets are publicly available through EPA's Amazon Web Services (AWS) Open Data Sponsorship Program (ODP), EPA's Remote Sensing Information Gateway (RSIG) and the CMAS Data Warehouse (consisting of a Google Drive and AWS ODP) to support numerous human health and ecological modeling endpoints, as well as model evaluation and development. The following sections describe the datasets, including the target audience for the data, the file type, data dictionary (when applicable), and the location of the files on the EPA AWS Storage, EPA RSIG, CMAS Google Drive, and CMAS AWS Storage.

How to Cite EQUATES Data

DOI: https://doi.org/10.15139/S3/F2KJSK

Website: https://www.epa.gov/cmaq/EQUATES

Reference for EQUATES emissions: https://doi.org/10.1016/j.dib.2023.109022

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EQUATES Modeling Domains

Figure 1. 108NHEMI Domain over the Northern Hemisphere: 187 rows × 187 columns × 44 layers

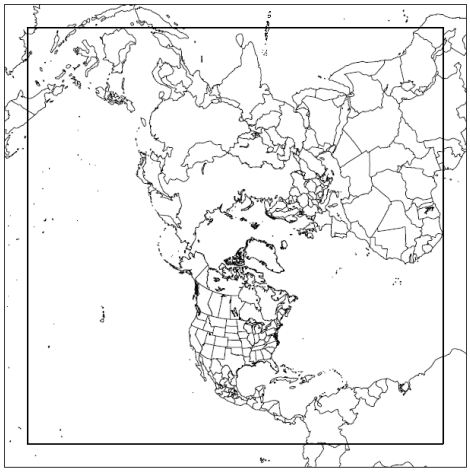
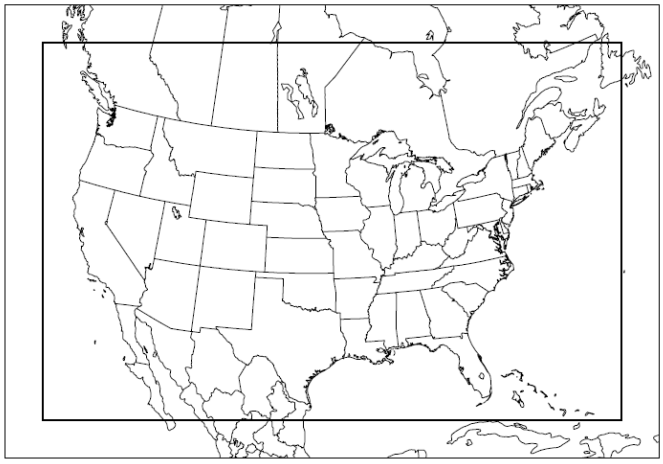


Figure 2. 12US1 Domain over the CONUS: 299 rows × 459 columns × 35 layers



Note: CMAQ output data from EPA can be on different modeling domains. The '12US1' domain above that was used for the EQUATES project is larger than another standard EPA modeling domain referred to as '12US2' which covers less of Canada and Mexico and has dimension 396 rows x 246 columns.

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EQUATES Inventory Emissions for CONUS (12US1 domain)

Purpose: For users who want to run SMOKE using EQUATES emissions files.
Location of Meta Data: EQUATES/SMOKE_INPUT/README_EQUATES_<date of last update>.txt
Units: All emissions data are in US tons.

Table 1

Data description	**File type (File size for all years)**	**Location on CMAS Data Warehouse (File paths relative to this top-level folder: CMAS Google Drive Link)**
Year specific inventory emissions for 2002–2019	tarred and zipped netCDF files (880 GB)	SMOKE_INPUT/< year>[1]/ EQUATES_INV_<year>_version1.0.tar.gz
Ancillary files needed for all years	tarred and zipped netCDF files (11GB)	SMOKE_INPUT/ancillary_data.tar.gz
Files and scripts for applying the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) speciation to EQUATES onroad emissions	zipped .txt and .csh files (486K)	SMOKE_INPUT/ EQUATES_2018_onroad_inv_CRACMM_addendum.zip Meta data: SMOKE_INPUT/README_ EQUATES_2018_onroad_inv_CRACMM_addendum.txt

[1] Four-digit year

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EQUATES Model-Ready Inputs for CONUS (12US1 domain)

Purpose: For users who want to run CMAQ using EQUATES input data. 2002-2019 data are available on the CMAS Google Drive. 2017 data are also available on CMAS AWS Open Data Storage.
Location of Meta Data: EQUATES/CMAQ_12US1/INPUT/README_EQUATES_v1.0_modelready.txt
Units: Units for each variable are included in the meteorology, emissions, and CMAQ netCDF files.

Table 2

Data description	Data location	File type (File size for all years)	Location on CMAS Data Warehouse (File paths relative to the top-level Google Drive or AWS link provided.)
CMAQ-ready meteorology inputs for 2013–2019[2] (see row 5 for more met inputs)	**CMAS Google Drive**	tarred netCDF files (17 TB)	CMAQ_12US1/INPUT/<year>/met/mcip_v51_wrf_v411_noltng/<month>[3]
CMAQ-ready emissions inputs for 2002–2019	**CMAS Google Drive**	tarred netCDF files (6.6 TB)	CMAQ_12US1/INPUT/<year>/emis
CMAQ boundary condition files for 2002–2019 (monthly files of hourly data at all 12US1 boundary grid cells[4])	**CMAS Google Drive**	netCDF (8.1 TB)	CMAQ_12US1/INPUT/<year>/icbc/BCON_CONC_12US1_CMAQv53_TS_108NHEMI_regrid_<year><month>.nc
CMAQ initial condition files for 2002–2019 are based on EQUATES restart files for the 1st and 15th day of each month. If using these restart files for a new modeling application, users are strongly encouraged to use a 2-4 week 'spin-up' period.	**CMAS Google Drive**	netCDF (885 GB)	CMAQ_12US1/INPUT/<year>/icbc/CCTM_<file_type>[5]_v532_cb6r3_ae7_aq_WR413_MYR_STAGE_<year>_12US1_<year><month><day>[6].nc
CMAQ-ready meteorology inputs for 2002-2017	**CMAS AWS S3 Bucket**	tarred netCDF files (45 TB)	CMAQ_12US1/INPUT/<year>/met/mcip_v51_wrf_v411_noltng/<month>
CMAQ-ready emissions inputs for 2017	**CMAS AWS S3 Bucket**	tarred netCDF files (6.6 TB)	CMAQ_12US1/INPUT/2017/emis
CMAQ boundary condition files for 2017 (monthly files of hourly data at all 12US1 boundary grid cells)	**CMAS AWS S3 Bucket**	netCDF (8.1 TB)	CMAQ_12US1/INPUT/2017/icbc/BCON_CONC_12US1_CMAQv53_TS_108NHEMI_regrid_<year><month>.nc

[2] Only 7 years of MCIP data are being shared due to storage space limitations/cost on the Google Drive.
[3] Two-digit month
[4] https://www.cmascenter.org/ioapi/documentation/all_versions/html/BDY.jpg
[5] Initial condition (restart) file type: CGRID, MEDIA_CONC, SOILOUT
[6] Two-digit day

CMAQ initial condition files for 2017 are based on EQUATES restart files for the 1st and 15th day of each month. If using these restart files for a new modeling application, users are strongly encouraged to use a 2-4 week 'spin-up' period.		netCDF (885 GB)	CMAQ_12US1/INPUT/2017/icbc/CCTM_<file_type>[7]_v532_cb6r3_ae7_aq_WR413_MYR_STAGE_<year>_12US1_<year><month><day>[8].nc

[7] Initial condition (restart) file type: CGRID, MEDIA_CONC, SOILOUT
[8] Two-digit day

EQUATES Anthropogenic Emissions Summary Files for CONUS (12US1 domain)

Purpose: For users who want to investigate spatial and temporal trends in the EQUATES anthropogenic emissions inputs.
Location of Data: These datasets are available from the CMAS Center Dataverse Repository for EQUATES (i.e., they are not saved on the CMAS Google Drive): https://doi.org/10.15139/S3/F2KJSK
Location of Meta Data: The Dataverse repository entry for EQUATES includes a meta data file, README_EQUATES_v1.0_emissions_summaries.txt
Units: All emissions data are in US tons.

Figure 3: EQUATES 12US1 modeling domain is shown as the bold rectangle. The grey shading indicates grid cells that are considered in the CONUS, including federal waters, when calculating the emissions totals in the summary files below.

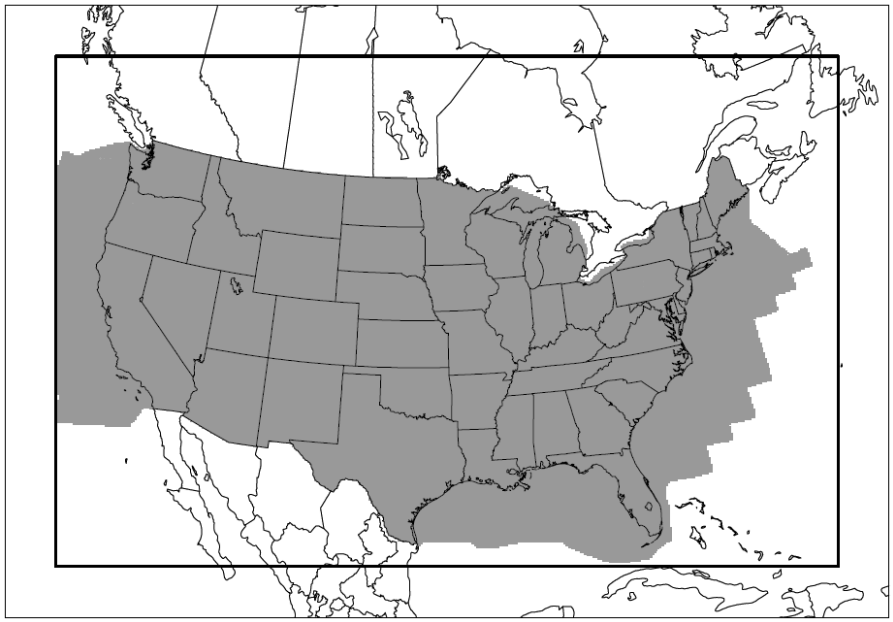

Table 3

Data description	File type (File size)	Files are attached to the EQUATES Dataverse repository
Annual total emissions for CONUS (not including offshore sources) for NO_X, SO_2, CO, $PM_{2.5}$, PM_{10}, VOC_regulatory[9], NH_3_nofert[10], NH_3_fert[11] for 2002-2017 based on the inventory (INV) emissions files	Zipped ASCII file (1.5KB)	EQUATESv1.0_INV_emissions_annual_totals_by_pollutant.csv.gz
Annual total emissions summed over all grid cells overlapping CONUS including federal waters for NO_X, SO_2, CO, $PM_{2.5}$, POC, PEC, VOC_regulatory, NMOG, NH_3_nofert, NH3_fert for 2002-2017 based on the model ready (MR) emissions files	Zipped ASCII file (1.8KB)	EQUATESv1.0_MR_emissions_annual_totals_by_pollutant.csv.gz
Annual total emissions summed over all grid cells overlapping CONUS including federal waters for NO_X, SO_2, CO, $PM_{2.5}$, POC, PEC, VOC_regulatory, NMOG, NH_3_nofert, NH3_fert for 2002-2017 by source category based on the MR emissions files	Zipped ASCII file (28KB)	EQUATESv1.0_MR_emissions_annual_totals_by_source_and_pollutant.csv
CMAQ 12US1 grid information including row/column, Lambert conformal projected x/y coordinates for grid cell centers, and longitude/latitude for the lower left and upper right corner of each grid cell	Zipped ASCII file (5.4MB)	EQUATES_CMAQ_12US1_grid_coordinates.csv.gz
Annual total gridded emissions for the 12US1 domain for 2002-2017 based on the MR emissions files for <pollutant> = NO_X, SO_2, CO, $PM_{2.5}$, POC, PEC, VOC_regulatory, NMOG, NH_3[12]	Zipped ASCII files (17MB per file)	EQUATESv1.0_<pollutant>_12US1_annual_emissions_2002-2017.csv.gz
Monthly total gridded emissions for the 12US1 domain for 2002-2017 based on the MR emissions files for <pollutant> = NO_X, SO_2, CO, $PM_{2.5}$, OC, EC, VOC_regulatory, NMOG, NH_3	Zipped ASCII files (190MB per file)	EQUATESv1.0_<pollutant>_12US1_monthly_emissions_2002-2017.csv.gz

[9] Regulatory volatile organic compounds defined as in the Code of Federal Regulations, 40 CFR 51.100
[10] Anthropogenic NH_3 emissions excluding emissions from fertilizer which were calculated online in CMAQ
[11] NH_3 fertilizer emissions from agriculture, calculated online in CMAQ and post-processed to be included in these summary files
[12] Total anthropogenic NH3 emissions including emissions from fertilizer

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EQUATES Surface Layer Model Output for CONUS (12US1 domain)

Purpose: For users who want to use WRF meteorology and/or CMAQ air quality estimates for regulatory or research applications (e.g., epidemiological studies, critical loads analysis), or model evaluation and development applications (e.g., diagnostic evaluation, reference data for sensitivity studies). CMAQ 3D and vertical column air quality data can be used to evaluate the modeling system, create model-observed 'fused' surfaces, and to analyze spatial and temporal changes in air quality in the upper atmosphere, e.g., https://doi.org/10.1016/j.envint.2019.104909; https://doi.org/10.5194/acp-17-12449-2017; https://doi.org/10.1029/2006JD008085; https://doi.org/10.5194/acp-15-9997-2015.

Data are available on the CMAS Google Drive and the EPA AWS Open Data Storage, as indicated in the table.

Meta Data (including units): See Tables 6-11. See also meta data on AWS.

CMAQ Source Code: The EQUATES 12US1 air quality modeling is based on CMAQv5.3.2.1 (CMAQv5.3.2 with some bugfixes later released in v5.3.3). The build directory for the 12US1 CMAQ simulations is available from the EQUATES Dataverse DOI: https://doi.org/10.15139/S3/F2KJSK

Table 4a

Data description	Data Location	File type (File size for all years)	File paths relative to the Data Location link
matched WRF output with meteorological surface observations for 4 variables (Table 6) 2002–2019	**CMAS Google Drive**	ASCII (5.3 GB)	WRF_12US1/PAIRED_MODEL_OBS/<year>
CMAQ daily average surface concentrations for 14 species (Table 7) for 2002–2019	**CMAS Google Drive**	netCDF (48.6 GB) and ASCII (102.9 GB)	CMAQ_12US1/output/daily_average_surface_output/<year>
CMAQ annual total deposition for 22 species (Table 8) for 2002–2019	**CMAS Google Drive**	GeoTIFF (244.8 MB)	CMAQ_12US1/output/annual_total_deposition/<year>
Precipitation and bias-adjusted CMAQ annual wet and total deposition for 15 species (Table 9) for 2002–2019	**CMAS Google Drive**	GeoTIFF (66.6 MB)	CMAQ_12US1/output/annual_total_adjusted_wet_deposition/<year>
CMAQ hourly 3D concentrations for 35 layers and 27 species (Table 10) for 2019	**EPA AWS S3 Bucket**	netCDF (4.3 TB)	CMAQ_12US1/OUTPUT/CONC3D/COMBINE_CONC3D_v532_cb6r3_ae7_aq_WR413_MYR_STAGE_2019_12US1_2019<month>.nc
CMAQ hourly column totals 7 species (Table 11) for 2019	**EPA AWS S3 Bucket**	netCDF (32.4 GB)	CMAQ_12US1/OUTPUT/COLUMN/COMBINE_COLUMN_v532_cb6r3_ae7_aq_WR413_MYR_STAGE_2019_12US1_2019<month>.nc

EQUATES 3D Model Output for CONUS (12US1 domain)

Purpose: For users who want to use access 3D hourly CMAQ output. Data are available on EPA's Remote Sensing Information Gateway (RSIG). The RSIG3D interface can be used to subset EQUATES data to a smaller spatial bounding box and select hours/days of interest and save the data in various formats.
Meta Data (including units): Metadata are provided within the RSID3D interface.
CMAQ Source Code: The EQUATES 12US1 air quality modeling is based on CMAQv5.3.2.1 (CMAQv5.3.2 with some bugfixes later released in v5.3.3). The build directory for the 12US1 CMAQ simulations is available from the EQUATES Dataverse DOI: https://doi.org/10.15139/S3/F2KJSK

Table 4b

Data description	Data Location	File type (File size for all years)	File paths relative to the Data Location link
CMAQ hourly 3D concentrations for 44 layers for all model output species for 2002-2019	**EPA RSIG**	EQUATES data can be saved in various formats	Directions for accessing EQUATES data on RSIG

EQUATES 3D Output for Northern Hemisphere (108NHemi domain)

Purpose: Daily average 3D data for all species is suitable for users who want to examine continental-scale air quality trends or who want to create boundary conditions for any subset domain in the Northern Hemisphere. Hourly CMAQ 3D and vertical column air quality data for a subset of species can be used to evaluate the modeling system, create model-observed 'fused' surfaces, and to analyze spatial and temporal changes in air quality in the upper atmosphere, e.g., https://doi.org/10.1016/j.envint.2019.104909; https://doi.org/10.5194/acp-17-12449-2017; https://doi.org/10.1029/2006JD008085; https://doi.org/10.5194/acp-15-9997-2015.
Data are available on the EPA Open Data Storage, EPA RSIG, the CMAS Google Drive and the CMAS AWS Open Data Storage, as indicated in the table.
Location of Meta Data: See the CMAQ IC/BC Tutorial on GitHub:
https://github.com/USEPA/CMAQ/blob/main/DOCS/Users_Guide/Tutorials/CMAQ_UG_tutorial_HCMAQ_IC_BC.md
For hourly data, see tables 11 and 12 for model species. See also AWS meta data.
Units: Units for each variable are included in the CMAQ netCDF files.
CMAQ Source Code: The EQUATES 108NHEMI air quality modeling is based on H-CMAQv5.3.2.1 (v5.3.2 with some bugfixes later released in v5.3.3 and modifications to halogen chemistry and O3-PV scaling). The build directory for the H-CMAQ simulations is available from the EQUATES Dataverse DOI: https://doi.org/10.15139/S3/F2KJSK

Table 5

Data description	Data Location	File type (File size for all years)	File paths relative to the Data Location link

CMAQ daily average 3D output for 44 layers for 260 model variables for 2002–2019[13]	**CMAS Google Drive**	netCDF (10.8 TB)	CMAQ_108NHemi/OUTPUT/<year>/CTM_CONC_v532_intel18.0_CMAQv53_TS_108NHEMI_<year><month>_dailyav.nc
CMAQ daily average 3D output for 44 layers for 260 model variables for 2018–2019[12]	**CMAS AWS S3 Bucket**	netCDF (1.2 TB)	CMAQ_108NHemi/<year>/CTM_CONC_v532_intel18.0_CMAQv53_TS_108NHEMI_<year><month>_dailyav.nc
CMAQ hourly 3D concentrations for 44 layers and 22 species (Table 12) for 2019	**EPA AWS S3 Bucket**	netCDF (1.1 TB)	CMAQ_108NHEMI/OUTPUT/CONC3D/COMBINE_CONC3D_v532_intel18.0_CMAQv53_TS_108NHEMI_2019<month>.nc
CMAQ hourly column totals 7 species (Table 11) for 2019	**EPA AWS S3 Bucket**	netCDF (8.3 GB)	CMAQ_108NHEMI/OUTPUT/COLUMN/COMBINE_COLUMN_v532_intel18.0_CMAQv53_TS_108NHEMI_2019<month>.nc
CMAQ hourly 3D concentrations for 44 layers for all model output species for 2002-2019	**EPA RSIG**	EQUATES data can be saved in various formats	Directions for accessing EQUATES data on RSIG

List of Column Names and Descriptions in 12US1 Paired Model/Obs Files

Table 6: Hourly surface meteorological values for 12US1 from the Weather Research & Forecasting (WRF) model matched in space and time to observations from the Meteorological Assimilation and Data Ingest System of the National Oceanic and Atmospheric Administration.

Column name in .csv file	**Variable description**	**Units**
Date Time	Date and time stamp in UTC	
SiteID	Weather station ID	
Temp Mod (K)	Modeled 2-meter temperature (WRF estimate)	K
Temp Obs (K)	Observed 2-meter temperature	K
Q Mod (g/kg)	Modeled 2-meter water vapor mixing ratio (WRF estimate)	g/kg
Q Obs (g/kg)	Observed 2-meter water vapor mixing ratio	g/kg

[13] can be used to created CMAQ BCs

WS Mod (m/s)	Modeled 10-meter wind speed (WRF estimate)	m/s
WS Obs (m/s)	Observed 10-meter wind speed	m/s
WD Mod (Deg)	Modeled 10-meter wind direction (WRF estimate)	degrees
WD Obs (Deg)	Observed 10-meter wind direction	degrees

List of Available Species in 12US1 Concentration and Deposition Files

Table 7: Daily average surface concentrations for 12US1. The species definition file (SpecDef_cb6r3_ae6_aq.txt) can be found here: https://github.com/USEPA/CMAQ/blob/5.3.2/CCTM/src/MECHS/cb6r3_ae6_aq/SpecDef_cb6r3_ae6_aq.txt

Variable name in .csv	**Model species defined in SpecDef_cb6r3_ae6_aq.txt**	**Variable description (daily average unless otherwise noted)**	**Units**
column		CMAQ 12US1 grid column number	
row		CMAQ 12US1 grid row number	
longitude		Longitude of grid cell center	degrees
latitude		Latitude of grid cell center	degrees
Lambert_X		Projected x coordinate of grid cell center	meters
LAMBERT_Y		Projected y coordinate of grid cell center	meters
date		Date formatted as YYYY-MM-DD	
CO_AVG	CO	Carbon Monoxide	ppb
NO_AVG	NO	Nitric Oxide	ppb
NO2_AVG	NO2	Nitrogen Dioxide	ppb
CH2O_AVG	FORM	Formaldehyde	ppb
O3_AVG	O3	Ozone	ppb
O3_MDA8	O3	Daily Maximum 8-hr Average Ozone	ppb
SO2_AVG	SO2	Sulfur Dioxide	ppb
PM2.5_AVG	PM25_TOT	Total $PM_{2.5}$ (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$
PM10_AVG	PM10	Particulate Matter up to 10 micrometers in Diameter	$\mu g/m^3$
PM25_NO3_AVG	PM25_NO3	$PM_{2.5}$ Nitrate (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$

PM25_NH4_AVG	PM25_NH4	$PM_{2.5}$ Ammonium (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$
PM25_SO4_AVG	PM25_SO4	$PM_{2.5}$ Sulfate (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$
PM25_OC_AVG	PM25_OC	$PM_{2.5}$ Organic Carbon (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$
PM25_EC_AVG	PM25_EC	$PM_{2.5}$ Elemental Carbon (sharp cutoff computed using modeled size distribution)	$\mu g/m^3$

Table 8: Annual total deposition for 12US1. The species definition file (SpecDef_Dep_cb6r3_ae6_aq.txt) can be found here: https://github.com/USEPA/CMAQ/blob/5.3.2/CCTM/src/MECHS/cb6r3_ae6_aq/SpecDef_Dep_cb6r3_ae6_aq.txt

Variable name for GeoTIFF file	**Model species defined in SpecDef_Dep_cb6r3_ae6_aq.txt**	**Variable description**	**Units**
WETDEP_TNO3_12US1	WDEP_TNO3	Wet Deposition of Total Nitrate (includes HNO_3, NO_3)	kg/ha
WETDEP_NHX_12US1	WDEP_NHX	Wet Deposition of NH_X (includes NH_4, NH_3)	kg/ha
WETDEP_TSO4_12US1	WDEP_TSO4	Wet Deposition of Total Sulfate (includes SO_4, SO_2)	kg/ha
WETDEP_OXN_12US1	WD_OXN_TOT	Wet Deposition of Oxidized Nitrogen (includes NO_X, TNO_3, PANs, Organic Nitrates, N_2O_5, HONO, PNA)	kg-N/ha
WETDEP_REDN_12US1	WD_REDN_TOT	Wet Deposition of Reduced Nitrogen (includes NH_4, NH_3)	kg-N/ha
WETDEP_N_12US1	WETDEP_OXN + WETDEP_REDN	Wet Deposition of Nitrogen	kg-N/ha
WETDEP_S_12US1	WD_S_TOT	Wet Deposition of Sulfur	kg-S/ha
WETDEP_CL_12US1	WDEP_TCL	Wet Deposition of Chloride	kg/ha
WETDEP_NA_12US1	WDEP_ANAJK	Wet Deposition of Sodium	kg/ha
DRYDEP_OXN_12US1	DD_OXN_TOT	Dry Deposition of Oxidized Nitrogen (includes NO_X, TNO_3, PANs, Org N, N_2O_5, HONO, PNA)	kg-N/ha
DRYDEP_REDN_12US1	DD_REDN_T	Dry Deposition of Reduced Nitrogen (includes NH_4, NH_3)	kg-N/ha

DRYDEP_N_12US1	DD_OXN_TOT + DD_REDN_T	Dry Deposition of Nitrogen	kg-N/ha
DRYDEP_S_12US1	DD_S_TOT	Dry Deposition of Sulfur	kg-S/ha
DRYDEP_CL_12US1	DDEP_ACLJK	Dry Deposition of Chloride	kg/ha
DRYDEP_NA_12US1	DDEP_ANAJK	Dry Deposition of Sodium	kg/ha
TOTDEP_OXN_12US1	DD_OXN_TOT + WETDEP_OXN	Total (Dry + Wet) Deposition of Oxidized Nitrogen	kg-N/ha
TOTDEP_REDN_12US1	DD_REDN_T + WETDEP_REDN	Total (Dry + Wet) Deposition of Reduced Nitrogen	kg-N/ha
TOTDEP_N_12US1	TOTDEP_OXN + TOTDEP_REDN	Total (Dry + Wet) Deposition of Nitrogen	kg-N/ha
TOTDEP_S_12US1	DRYDEP_S + WETDEP_S	Total (Dry + Wet) Deposition of Sulfur	kg-S/ha
TOTDEP_CL_12US1	DDEP_CL + WETDEP_CL	Total (Dry + Wet) Deposition of Chloride	kg/ha
TOTDEP_NA_12US1	DDEP_NA + WETDEP_NA	Total (Dry + Wet) Deposition of Sodium	kg/ha
WRF_PRECIP_12US1	RT	WRF Precipitation	cm

Table 9: Annual total deposition for 12US1 using precipitation and bias-adjusted wet deposition estimates. CMAQ deposition outputs are adjusted using PRISM precipitation data and NADP/NTN wet deposition measurements following the method in **Benish et al. (2022).** Since the PRISM and NTN data are only available for the US, model values in grid cells outside of the Conterminous US (CONUS) are set to missing.

Variable name for GeoTIFF file	**Model species defined in SpecDef_Dep_cb6r3_ae6_aq.txt**	**Variable description**	**Units**
ADJ_WETDEP_TNO3_CONUS	precip_NO3_bias_factor*WDEP_TNO3	Precipitation and Bias Adjusted Wet Deposition of Total Nitrate (includes HNO_3, NO_3)	kg/ha
ADJ_WETDEP_NHX_CONUS	precip_NH4_bias_factor*WDEP_NHX	Precipitation and Bias Adjusted Wet Deposition of NH_X (includes NH_4, NH_3)	kg/ha
ADJ_WETDEP_TSO4_CONUS	precip_SO4_bias_factor*WDEP_TSO4	Precipitation and Bias Adjusted Wet Deposition of Total Sulfate (includes SO_4, SO_2)	kg/ha

ADJ_WETDEP_CL_CONUS	precip_factor*WDEP_TCL	Precipitation Adjusted Wet Deposition of Chloride	kg/ha
ADJ_WETDEP_NA_CONUS	precip_factor*WDEP_ANAJK	Precipitation Adjusted Wet Deposition of Sodium	kg/ha
ADJ_WETDEP_OXN_CONUS	precip_NO3_bias_factor*WD_OXN_TOT	Precipitation and Bias Adjusted Wet Deposition of Oxidized Nitrogen (includes NO_X, TNO_3, PANs, Organic Nitrates, N_2O_5, HONO, PNA)	kg-N/ha
ADJ_WETDEP_REDN_CONUS	precip_NH4_bias_factor*WD_REDN_T	Precipitation and Bias Adjusted Wet Deposition of Reduced Nitrogen (includes NH_4, NH_3)	kg-N/ha
ADJ_WETDEP_N_CONUS	ADJ_WETDEP_OXN + ADJ_WETDEP_REDN	Precipitation and Bias Adjusted Wet Deposition of Nitrogen	kg-N/ha
ADJ_WETDEP_S_CONUS	precip_SO4_bias_factor*WD_S_TOT	Precipitation and Bias Adjusted Wet Deposition of Nitrogen	kg-S/ha
ADJ_TOTDEP_OXN_CONUS	DD_OXN_TOT + ADJ_WETDEP_OXN	Total (Dry + Precip/Bias Adjusted Wet) Deposition of Oxidized Nitrogen	kg-N/ha
ADJ_TOTDEP_REDN_CONUS	DD_REDN_T + ADJ_WETDEP_REDN	Total (Dry + Precip/Bias Adjusted Wet) Deposition of Reduced Nitrogen	kg-N/ha
ADJ_TOTDEP_N_CONUS	TOTDEP_OXN + TOTDEP_REDN	Total (Dry + Precip/Bias Adjusted Wet) Deposition of Nitrogen	kg-N/ha
ADJ_TOTDEP_S_CONUS	DRYDEP_S + ADJ_WETDEP_S	Total (Dry + Precip/Bias Adjusted Wet) Deposition of Sulfur	kg-S/ha
ADJ_TOTDEP_CL_CONUS	DDEP_CL + ADJ_WETDEP_CL	Total (Dry + Precip Adjusted Wet) Deposition of Chloride	kg/ha
ADJ_TOTDEP_NA_CONUS	DDEP_NA + ADJ_WETDEP_NA	Total (Dry + Precip Adjusted Wet) Deposition of Sodium	kg/ha

Table 10: Hourly 3D concentrations for 27 model variables for 12US1 domain.

Variable name in .ncf file	**Variable description**	**Units**
AIR_DENS	Air Density	kg/m^3
PRESS	Pressure	Pa

TEMP	Temperature	K
QV	Water vapor mixing ratio	kg/kg
ZH	Mid-layer height above ground	m
ZF	Full-layer height above ground	m
CO	Carbon Monoxide	ppbv
FORM	Formaldehyde	ppbv
NH3	Ammonia	ppbv
NO	Nitric Oxide	ppbv
NO2	Nitrogen Dioxide	ppbv
O3	Ozone	ppbv
SO2	Sulfur Dioxide	ppbv
ISOP	Isoprene	ppbv
GLY	Glyoxal	ppbv
ANO3_PPB	Aerosol Nitrate in ppb by volume	ppbv
NTR	Organic Nitrates	ppbv
PANS	Peroxyacylnitrate	ppbv
NOY	All oxides of nitrogen in which the oxidation state of the N atom is +2 or greater, i.e., the sum of all reactive nitrogen oxides including NOX (NO + NO2) and other nitrogen oxides referred to as NOZ.	ppbv
ASOILJ	Soil (accumulation mode[14]) = 2.20*AL+2.49*SI+1.63*CA+2.42*FE+1.94*TI	$\mu g/m^3$
AECIJ	$PM_{2.5}$ Elemental Carbon (Aitken and accumulation modes)	$\mu g/m^3$
ANO3IJ	$PM_{2.5}$ nitrate (Aitken and accumulation modes)	$\mu g/m^3$
ANH4IJ	$PM_{2.5}$ ammonium (Aitken and accumulation modes)	$\mu g/m^3$

[14] https://www.epa.gov/system/files/documents/2022-08/PM_2021.pdf

ASO4IJ	$PM_{2.5}$ sulfate (Aitken and accumulation modes)	µg/m^3
AOCIJ	$PM_{2.5}$ Organic Carbon (Aitken and accumulation modes)	µg/m^3
AOMIJ	$PM_{2.5}$ Organic Matter (Aitken and accumulation modes)	µg/m^3
ATOTIJ	Total $PM_{2.5}$ Mass (Aitken and accumulation modes)	µg/m^3

Table 11: Column totals for 7 model variables for 12US1 or 108NHemi domains.

Variable name in .ncf file	**Variable description**	**Units**
NO2_COLUMN	Nitrogen Dioxide	petamolec/cm^2
CO_COLUMN	Carbon Monoxide	petamolec/cm^2
SO2_COLUMN	Sulfur Dioxide	petamolec/cm^2
HCHO_COLUMN	Formaldehyde	petamolec/cm^2
O3_COLUMN	Ozone Column Total	DU
JNO2_COLUMN	NO2 Photolysis Rate Coefficient	min^{-1}
AOD550	Aerosol Optical Depth at a Wavelength of 550 nm	

Table 12: Hourly 3D concentrations for 22 model variables for 108NHEMI domain.

Variable name in .ncf file	**Variable description**	**Units**
AIR_DENS	Air density	kg/m^3
PRESS	Pressure	Pa
TEMP	Temperature	K
QV	Water vapor mixing ratio	kg/kg
ZH	Mid-layer height above ground	m
ZF	Full-layer height above ground	m
PV	Potential Vorticity	m^2 s^{-1}K kg^{-1}
CO	Carbon Monoxide	ppbv

FORM	Formaldehyde	ppbv
NH3	Ammonia	ppbv
NO2	Nitrogen dioxide	ppbv
O3	Ozone	ppbv
O3PV	Ozone Potential Vorticity[15]	ppbv
SO2	Sulfur Dioxide	ppbv
ASOILJ	Soil (accumulation mode)	$\mu g/m^3$
AECIJ	$PM_{2.5}$ Elemental Carbon (Aitken and accumulation modes)	$\mu g/m^3$
ANO3IJ	$PM_{2.5}$ Nitrate (Aitken and accumulation modes)	$\mu g/m^3$
ANH4IJ	$PM_{2.5}$ Ammonium (Aitken and accumulation modes)	$\mu g/m^3$
ASO4IJ	$PM_{2.5}$ Sulfate (Aitken and accumulation modes)	$\mu g/m^3$
AOCIJ	$PM_{2.5}$ Organic Carbon (Aitken and accumulation modes)	$\mu g/m^3$
AOMIJ	$PM_{2.5}$ Organic Matter (Aitken and accumulation modes)	$\mu g/m^3$
ATOTIJ	Total $PM_{2.5}$ Mass (Aitken and accumulation modes)	$\mu g/m^3$

[15] https://doi.org/10.5194/acp-16-10865-2016