

Total Deposition Estimates Using the Measurement Model Fusion (TDep MMF version 2021.01) Approach with Modeled and Monitoring Data

Total deposition maps and the underlying data have been produced using wet deposition measurements from the NADP National Trends Network (NTN) and estimates of dry deposition using a method that combines ambient air monitoring data with output from the Community Multiscale Air Quality (CMAQ) modeling system. This method of estimating dry deposition gives priority to measurement data near the location of the monitor and priority to CMAQ data in areas where monitoring data are not available. Additionally, CMAQ output is used for species such as peroxyacetylnitrate (PAN), dinitrogen pentoxide (N₂O₅), nitric oxide (NO), nitrogen dioxide (NO₂), nitrous acid (HONO) and organic nitrate that are not routinely measured, but likely contribute a significant amount to the total nitrogen budget.

In 2021, the NADP Total Deposition Science committee (TDep) along with the U.S. EPA set out to modernize the TDep Measurement Model Fusion (TDep MMF) model. The scripts were modernized to a single scripting language (Python 3.6.2 using ArcPy; ArcGIS Pro 2.4) and the process streamlined. Several improvements to the product including more translatable grid formats (e.g. a CMAQ datum transformation, NAD1983 projection, and a 4 x 4 km grid cell size), a new bias correction method, and the use of a new CMAQ dataset time-series (the EPA’s Air Quality Time Series (EQUATES)) using CMAQ v5.3 were used. The modifications and improvements, while designed to preserve functionality and consistency, led to differences in the grid product that will be described in Beachley et al., in preparation. This product has been vetted by the TDep committee, but please note that this product is dynamic and will be updated as new monitoring and modeling data become available and as improvements to the methodology are implemented. Therefore, it is critical to note the version number associated with the data. The version number consists of a 4-digit year and a 2-digit release number. The data described below is denoted as version 2021.01.

The sections below provide details on the monitoring and modeling data and methodology. In the final section, notes and caveats are provided that discuss limitations of the data.

Monitoring Data

Data from the Clean Air Status and Trends Network (CASTNET) and National Atmospheric Deposition Program’s (NADP) National Trends Network (NTN) were used in the study. Table 1 provides information on the measurement data used from each network.

Table 1. Summary of data from monitoring networks used in the methodology (p denotes particulate species).

Network	Measurement	Website
CASTNET	Air Concentration: HNO ₃ , SO ₂ , pSO ₄ , pNO ₃ , pNH ₄ , pCa, pCl, pK, pMg, pNa	http://epa.gov/castnet
NTN	Precipitation concentration: SO ₄ , NO ₃ , NH ₄ , Ca, Cl, K, Mg, Na Precipitation amount	https://nadp.slh.wisc.edu/networks/national-trends-network/
MDN	Precipitation amount	https://nadp.slh.wisc.edu/networks/mercury-deposition-network/

CMAQ Model Data

CMAQ is an advanced regional air quality model that simulates the complex physics and chemistry of the atmosphere to predict the simultaneous transport, transformation, and deposition of pollutants (<https://www.epa.gov/cmaq>). The EPA’s Air Quality Time Series (EQUATES) project includes 2002-2017 air quality

modeling using CMAQv5.3.2 (Appel et al., 2021) for the CONUS domain using a 12 km horizontal grid spacing. EQUATES utilized consistent methods for developing boundary conditions, emissions and meteorology inputs for the sixteen years of CMAQ simulations. Emissions inputs for 2017 were based on the 2017 National Emissions Inventory. Emissions for earlier years were processed using the same methods as the 2017 year, or were estimated by scaling the 2017 emissions with scaling factors based on activity surrogates. The CMAQ simulations also included online emissions processing including biogenics and bidirectional exchange of NH₃ using fertilizer emissions from the Environmental Policy Integrated Climate (EPIC) model (<http://epicapex.tamu.edu/>). Meteorological inputs were based on year specific meteorology from the Weather Research and Forecasting (WRF) model version 4.1.1 (Skamarock et al., 2008). Additional information on the CMAQ input data and model configuration can be found here: <https://doi.org/10.15139/S3/F2KJSK>

Methodology

This section summarizes the step-by-step procedure used to create the underlying data and total deposition maps.

1. Create grids of weekly observed atmospheric concentrations. Create 12 km grids of observed weekly average concentration of sulfur dioxide (SO₂), nitric acid (HNO₃), particulate sulfate (pSO₄), particulate nitrate (pNO₃), and particulate ammonium (pNH₄), for each year from CASTNET concentration data. The weekly schedule is determined by the standard CASTNET Tuesday-to-Tuesday weekly sampling schedule and all other observations were converted to fit this schedule. Observed concentrations were interpolated into 12 km grids using inverse distance weighting (IDW). The IDW method used has a weighting power of 3 and a limit of 12 sampling points found within maximum radius distances. The distances used in the IDW were determined from examining the spatial correlation in the CMAQ gridded average seasonal concentration data using a variogram analysis. For each chemical and season, we plotted the sample variogram and then fitted an exponential covariance model with three parameters (nugget, sill, and range) using a nonlinear least squares algorithm. The covariance model was then normalized and plotted against distance. Distances corresponding to a covariance of 0.7 were determined for each chemical species for each season (Table 2) and used in the IDW.

Table 2. Maximum radius used in the inverse distance weighting to produce concentration grids and distance-weighting grids.

Chemical Species	Maximum Radius (km)			
	Winter	Spring	Summer	Fall
HNO ₃	339	415	278	340
NH ₃	25	96	104	62
SO ₂	302	278	260	304
pNO ₃	501	588	239	302
pNH ₄	386	515	504	484
pSO ₄	769	1322	506	770

2. Create weekly averages and aggregates of hourly CMAQ data. The hourly CMAQ data for concentrations and deposition velocities were averaged and for dry deposition was summed over the standard CASTNET Tuesday-to-Tuesday weekly sampling schedule.
3. Create weekly concentration-weighted deposition velocity grids from the CMAQ data. The hourly CMAQ deposition velocity values were weighted by the concentration to account for the cross-correlation between concentration and deposition velocity. The resulting weighted values were then summed to the CASTNET weekly schedule.

4. Create weekly average dry deposition grids for each measured species from observed concentrations (Step 1) and modeled deposition velocities (Step 2). CMAQ uses a modal aerosol model with three modes (Aitken (I), accumulation (J), and coarse (K)); however, the CASTNET filterpack does not have specific size cut for particulate species. We used the CMAQ concentration ratios of the model size bins for each grid cell to apportion the measurement concentrations into the model size bins and their corresponding weekly average deposition velocity. For the years 2002-2017, the year-specific weekly average concentration was multiplied by the year-specific weekly average deposition velocity. For the years 2000-2001 and 2018-2020, modeled deposition velocities were not available. Therefore, for the years 2000-2001, the year-specific weekly average concentration was multiplied by the weekly average deposition velocities determined from the 2002 model year. Similarly, for the years 2018-2020, the year-specific weekly average concentration was multiplied by weekly average deposition velocities determined from the 2017 model year.
5. Create average seasonal bias adjustment surface for each measured species. A bias adjustment ratio was determined for each monitoring site by dividing the within year seasonal median (i.e. median of 13 weeks for season) CMAQ-modeled concentration for the grid cell containing the site location by that for seasonal median observed concentration. The bias ratio was transformed to a log scale and fitted to a surface using IDW with a weighting power of 2 and a maximum distance of 1000 km. The surface was then smoothed using the arcpy function FocalStatistics using a mean over a radius of 60 km (equivalent to 5 grids). The smoothed surface was then transformed back to the normal scale from the log scale.
6. Create bias-adjusted grids of weekly average CMAQ deposition for measured species. Dry CMAQ deposition grids were averaged to the CASTNET weekly schedule to obtain weekly average values. CMAQ deposition values for measured species were bias corrected by dividing the CMAQ value by the ratio obtained in step 4 for the corresponding week.
7. Merge observed deposition grid with CMAQ bias-adjusted grid for measured species. First, a grid was constructed that contained the distance from the grid cell to the nearest monitor. Next, a distance weight grid was calculated:

$$W_{obs} = 1 - \frac{\text{distance to nearest monitor}}{\text{maximum radius}}$$

where the maximum radius was determined for each chemical species based on the variogram analysis described in Step 1.

The observed deposition grid from Step 4 was multiplied by this distance weighting grid to get weighted observed deposition values. The weighting grid for the modeled values was constructed as $1 - W_{obs}$. The modeled deposition grid for the measured species was multiplied by its weighting grid to get weighted modeled values. The two weighted grids were then summed to get the final deposition grid for each measured species.

8. Create annual dry deposition grids. Weekly deposition grids for each species were summed to annual values. For the measured species, the grids constructed in step 7 were summed. For unmeasured species, the weekly CMAQ dry deposition values (step 2) were summed. For the years 2002-2017, the year-specific annual deposition was used. For the years 2000-2001, the annual deposition for 2002 was used. For the years 2018-2020, the annual deposition for 2017 was used. Grid cells outside the CMAQ CONUS 12 km domain were removed.
9. Create annual wet deposition grids. Annual wet deposition grids were calculated from the annual precipitation-weighted concentrations obtained from NADP and a modified version of the annual precipitation estimates obtained from the PRISM Climate Group (<http://www.prism.oregonstate.edu/>). Annual concentration grids were created using IDW interpolation of NADP/NTN annual concentration data that met annual completeness criteria. PRISM 4-km precipitation grids were modified by adjusting the grid to the precipitation amounts measured at NADP monitoring network sites. The adjustment was made proportionally as a distance gradient from 0 to 30 km from the measurement location, similar to the fusion process described in step 4. Where precipitation measurements from the NTN or MDN networks differed, the maximum amount reported by either of the networks was used. Table 3 summarizes the differences between the IDW parameters used by TDEP and NADP.

Table 3. Parameters used in preparation of TDEP and NADP/NTN precipitation grids

Parameter	TDEP	NADP/NTN
Precipitation measurements used to supplement PRISM	NTN, MDN	NTN, MDN
Concentration measurements used in grids	NTN	NTN
Grid cell size	4000 m	2338.383 m
Maximum search distance	500 km	500 km
Minimum number of points	12	0
Weighting power of IDW	3	3
PRISM resampling method	None	Nearest neighbor

10. Create grids of total deposition. The 12 km grids of dry deposition were regridded to the 4 km NTN grid. For each year and species, the dry deposition calculated above was summed with the wet deposition calculated above to determine total deposition. Table 5 describes the output variables available for download.

Table 4. TDEP output variables

Variable ¹	Description	Units
bc_dw	Dry deposition of all base cations	kg/ha
bc_dwpct	Dry deposition of base cations as percent of total (wet + dry) deposition	Percent
bc_tw	Total deposition of all base cations	kg/ha
ca_dw	Dry deposition of calcium	kg-Ca/ha
ca_tw	Total deposition of calcium	kg-Ca/ha
ca_ww	Wet deposition of calcium	kg-Ca/ha
cl_dw	Dry deposition of chlorine	kg-Cl/ha
cl_tw	Total deposition of chlorine	kg-Cl/ha
cl_ww	Wet deposition of chlorine	kg-Cl/ha
hno3_dw	Total deposition of nitric acid	kg-N/ha
k_dw	Dry deposition of potassium	kg-K/ha
k_tw	Total deposition of potassium	kg-K/ha
k_ww	Wet deposition of potassium	kg-K/ha
mg_dw	Dry deposition of magnesium	kg-Mg/ha
mg_tw	Total deposition of magnesium	kg-Mg/ha
mg_ww	Wet deposition of magnesium	kg-Mg/ha
n_dw	Dry deposition of nitrogen	kg-N/ha

Variable ¹	Description	Units
n_dwpct	Dry deposition of nitrogen as percent of total (wet + dry) deposition	Percent
n_tw	Total (wet + dry) nitrogen deposition	kg-N/ha
n_ww	Wet deposition of nitrogen	kg-N/ha
n_wwpct	Wet deposition of nitrogen as percent of total (wet + dry) deposition	Percent
na_dw	Dry deposition of sodium	kg-Na/ha
na_tw	Total deposition of sodium	kg-Na/ha
na_ww	Wet deposition of sodium	kg-Na/ha
nh3_dw	Dry deposition of ammonia	kg-N/ha
nh3net_dw	Net deposition of ammonia	kg-N/ha
nh4_dw	Dry deposition of particulate ammonium	kg-N/ha
nh4_ww	Wet deposition of particulate ammonium	kg-N/ha
no3_dw	Dry deposition of particulate nitrate	kg-N/ha
no3_ww	Wet deposition of particulate nitrate	kg-N/ha
nom_dw	Dry deposition of unmeasured nitrogen species, including nitrous acid (HONO), nitrogen pentoxide (N ₂ O ₅), nitric oxide (NO), nitrogen dioxide (NO ₂), organic nitrate (NTR), peroxyacyl nitrate (PAN), aromatic PANs (OPAN), and C ₃ and higher PANs (PANX)	kg-N/ha
nom_dwpct	Dry deposition of unmeasured nitrogen species as percent of total (wet + dry) deposition	Percent
noxi_dw	Dry deposition of oxidized nitrogen	kg-N/ha
noxi_dwpct	Dry deposition of oxidized nitrogen as percent of total (wet + dry) deposition	Percent
noxi_tw	Total (wet + dry) deposition of oxidized nitrogen	kg-N/ha
noxi_twpct	Total (wet + dry) deposition of oxidized nitrogen as percent of total (wet + dry) deposition	Percent
nred_dw	Dry deposition of reduced nitrogen	kg-N/ha
nred_dwpct	Dry deposition of reduced nitrogen as percent of total (wet + dry) deposition	Percent
nred_tw	Total (wet + dry) deposition of reduced nitrogen	kg-N/ha
nred_twpct	Total (wet + dry) deposition of reduced nitrogen as percent of total (wet + dry) deposition	Percent
ns_tw	Total equivalent nitrogen + sulfur deposition	keq/ha
precip_ww	Annual precipitation	cm
s_dw	Dry deposition of sulfur	kg-S/ha
s_dwpct	Dry deposition of sulfur as percent of total (wet + dry) deposition	Percent
s_tw	Total (wet + dry) sulfur deposition	kg-S/ha
s_ww	Wet deposition of sulfur	kg-S/ha
s_wwpct	Wet deposition of sulfur as percent of total (wet + dry) deposition	Percent
so2_dw	Dry deposition of sulfur dioxide	kg-S/ha
so4_dw	Dry deposition of particulate sulfate	kg-S/ha

Variable ¹	Description	Units
tno3_dw	Dry deposition of nitric acid + particulate nitrate	kg-N/ha

¹Note that the variable names have changed from previous versions to indicate that these values are determined using concentration-weighted deposition velocities.

Availability of Files

Images of the above variables for all years are available in PNG format at https://gaftp.epa.gov/castnet/tdep/2021_01_images/.

Gridded data of the above variables are available in GeoTIFF format export files at https://gaftp.epa.gov/castnet/tdep/2021_01_grids/. All available years, including 3-year averages of the first and last three-year periods, are contained in the zip file for the variable. Zip file names are constructed using the convention *[variable]-yyyy.zip* for single year grids, and *[variable]-xxyy.zip* for three-year averages, where *xx* is the last two digits of the beginning year and *yy* is the last two digits of the final year of the period. Table 6 provides the geographic information for the provided grids.

Table 5. Description of TDEP grids

GRID Description	
Cell Size	4000
Data Type	Floating Point
Number of Rows	783
Number of Columns	1200
Boundary Statistics	
Xmin	-2400000.000
Xmax	2400000.000
Ymin	170000.000
Ymax	3302000.000
Coordinate System Description	
Projection	ALBERS
Units	METERS
Spheroid	NAD1983
Parameters:	
1st standard parallel	29.5
2nd standard parallel	45.5
central meridian	-96.0
latitude of projection's origin	23.0
false easting (meters)	0.00000
false northing (meters)	0.00000

Caveats

As additional monitoring and modeling data become available the maps will be adjusted. CMAQ continues to be updated and more recent versions of the model contain new capabilities that will affect the predictions of atmospheric concentration and deposition. Use of a newer version of the CMAQ modeling system would have an effect on the data used in this methodology. The potential effect of some of these changes is summarized below:

- There is likely an incomplete characterization of the wet and dry organic N components resulting in an underestimate of total nitrogen deposition.
- NH₃ data from AMoN is only used for model evaluation and is not included in the development of the concentration surfaces.
- Since the measurement sites used in the method are located in primarily rural areas, deposition in urban areas may not be well represented.
- Interpolation techniques inherently minimize extreme values, so more variability would be expected if more spatially resolved observations were available for use.
- The use of monitoring data is limited to sites and times that meet network completion criteria to ensure that measurements are representative of actual conditions. Discontinuities in temporal and spatial trends at specific locations may occur where monitoring data are intermittent.
- The methodology used to develop the wet deposition grids differs from that used for the NTN grids (<https://nadp.slh.wisc.edu/networks/national-trends-network/>).
- CASTNET did not start measuring chloride as an analyte until mid-2003. This caused a step function between the modeled 2002 and 2003 chloride dry deposition since that data could not be bias-adjusted. For this reason, the adjusted CMAQ chloride dry deposition for 2004 grid was used for the years 2000 through 2003. Revisions to the bias adjustment protocol are underway and will be included in the next version to address this issue.
- A few instances of maximum dry deposition excursions that far exceed typical deposition levels have been identified in isolated areas. Three of these instances have been identified and are described as follows: 1) in 2006, three grid cells in mid-TX have elevated dry deposition of Ca, K, Mg, Na, NO₃⁻, pNH₄, pNO₃, pSO₄; 2) in 2011, a single grid cell Northern MO has elevated dry deposition of pNH₄, pNO₃, pSO₄, and Mg; and 3) in 2016, two grid cells in northeastern NY have elevated dry deposition of K, Mg, pNH₄, pNO₃, pSO₄. These large excursions in estimated dry deposition are the result of isolated and unreasonably high deposition velocity estimates in the modeled CMAQ dataset that occur under conditions where aerosol number concentration estimates are very low. This is a known issue and efforts are underway to limit the impact of this artifact contributing to very large deposition values.

Suggested Citation

The original method (version 2014.01) has been published in Atmospheric Environment (Schwede and Lear, 2014). Updates to the methodology have occurred since the publication of the manuscript. The modernized method (version 2021.01) will be described in Beachley et al., in preparation. Changes are noted below in the Revision History. To cite data or maps from this project, a suggested citation is:

National Atmospheric Deposition Program, 2022. Total Deposition Maps, v2021.01.
<https://nadp.slh.wisc.edu/committees/tdep/>. [date accessed].

Revision History

Version Number	Change Number	Description	Date of Change
2014.01	1	An error was corrected in unit conversion for SO ₂ and HNO ₃ air concentrations from 2007-2009 CMAQ runs. Because these air concentrations are used in the bias corrections for dry deposition from 2007 to 2012, dry and total deposition values for SO ₂ and HNO ₃ and their derivatives were also affected for	4/7/2014
2014.02	1	All network data were updated through 2013	11/3/2014
2014.02	2	SEARCH data for pNH ₄ , pNO ₃ and pSO ₄ was added	11/3/2014

2016.01	1	All CMAQ data were updated to use runs from version 5.0.2	7/11/2016
2016.01	2	All network data were updated through 2014. SEARCH data for aerosols is now included.	7/11/2016
2016.01	3	Deposition velocities are now weighted by concentration to account for the cross-correlation between concentration and deposition velocity. File names have been changed to indicate this change.	7/11/2016
2016.01	4	Total ammonia deposition and net ammonia deposition grids (i.e., total deposition – emission) are now included. Derivative N deposition grids (e.g., dry and total N) use the total ammonia deposition value. Because the relationship between concentration and flux is not linear in this model, ammonia grids	7/11/2016
2016.01	5	Maps of base cations are now provided.	7/11/2016
2016.01	6	The assumption used for the particle size distribution for aerosols is now based on the CMAQ modal concentrations in each grid cell for the relevant model year.	7/11/2016
2016.01	7	Wet deposition grids now include precipitation measurements from NTN, MDN and AIRMoN monitoring sites, whereas previously only measurements from NTN were used.	7/11/2016
2018.01	1	The most recent PRISM model was used for the wet deposition for all years. In previous TDEP versions, the revised PRISM model was used for 2014 and 2015 but prior years used the older PRISM dataset.	4/1/2018
2018.01	2	An SO ₂ concentration artifact from 2015 was corrected by the CASTNET program, resulting in a reduction in dry sulfur deposition for 2015 from TDEPv2016.01	4/1/2018
2018.01	3	All measurements from the SEARCH network were removed because the network ceased operation in late 2015. In previous TDEP versions, 6 rural SEARCH sites in the southeastern US were used.	4/1/2018
2018.02	1	An error was discovered in the aggregation of hourly deposition values for the final week of the CMAQ 2002 model run which resulted in erroneously high values of annual aggregations of ammonia and other non-measured nitrogen-containing variables for the years 2000 through 2002. These grids and their derivative grids of dry, total, and percentages of nitrogen deposition were replaced with corrected grids.	10/5/2018

2021.01	1	The TDep script was modernized as described in the introduction. Improvements include a CMAQ datum transformation, NAD1983 projection, and a 4 x 4 km grid cell size. The modeled CMAQ dataset was updated to the EQUATES time-series and a correction to the 2018.02 base cation CMAQ data was made. A direct comparison of the versions using 2010 data is described in Beachley et al., in preparation.	2/18/2022
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References

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