

Total Deposition Estimates Using a Hybrid 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. 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. 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 2016.01.

Monitoring Data

Data from the Clean Air Status and Trends Network (CASTNET), Atmospheric Integrated Research Monitoring Network (AIRMoN), Southeastern Aerosol Research and Characterization (SEARCH) network (rural sites only), and the 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
SEARCH	Air Concentration: HNO ₃ , SO ₂ , pSO ₄ , pNO ₃ , pNH ₄	http://www.atmospheric-research.com/studies/SEARCH/
NTN	Precipitation concentration: SO ₄ , NO ₃ , NH ₄ , Ca, Cl, K, Mg, Na Precipitation amount	http://nadp.sws.uiuc.edu/NTN/
AIRMoN	Precipitation concentration: SO ₄ , NO ₃ , NH ₄ , Ca, Cl, K, Mg, Na Precipitation amount	http://nadp.sws.uiuc.edu/AIRMoN/
MDN	Precipitation amount	http://nadp.sws.uiuc.edu/MDN/

CMAQ Model Data

CMAQ (Byun and Schere, 2006) 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 (<http://www.cmaq-model.org/>). CMAQ (v5.0.2) was run by the US EPA for the CONUS domain using a 12 km X 12 km grid size for the years 2002-2012. The runs utilized a consistent modeling platform which included the bidirectional NH₃ module, fertilizer emissions from the Environmental Policy Integrated Climate (EPIC) model (<http://epicapex.tamu.edu/>), inline biogenic emissions, and year specific meteorology from the Weather Research and Forecasting (WRF) model (Skamarock et al., 2008). Details of the model runs can be found in Foley et al (in preparation) and a summary is provided in Table 2.

Table 2. Summary of CMAQ model runs used in the methodology.

Year	CMAQ Model Version (Grid Resolution)	NEI	Major Point sources (EGUs)	Mobile Sources (Model)	Fires	Land use Classification
2002	5.0.2 (12km)	2002 v3	2002	MOVES 2010b 2002 emissions factors and activity data	2002 NEI	NLCD 2001 (version 2006)
2003	5.0.2 (12km)	2002 v3	2003	MOVES 2010b 2002 emission factors and activity data	SMARTFIRE v1	NLCD 2001 (version 2006)
2004	5.0.2 (12km)	2005 v3	2004	Interpolated between 2002 and 2005 values	SMARTFIRE v1	NLCD 2001 (version 2006)
2005	5.0.2 (12km)	2005 v3	2005	MOVES 2010b 2005 emissions factors and activity data	SMARTFIRE v1	NLCD 2001 (version 2006)
2006	5.0.2 (12km)	2008 v3	2006	MOVES 2010b Emission factors from 2005 and activity data from 2006	SMARTFIRE v2	NLCD 2006 (version 2006)
2007	5.0.2 (12km)	2008 v3	2007	MOVES 2010b 2007 emissions factors and activity data	SMARTFIRE v2	NLCD 2006 (version 2006)
2008	5.0.2 (12km)	2008 v3	2008	MOVES 2010b 2008 emissions factors and activity data	SMARTFIRE v2	NLCD 2006 (version 2006)
2009	5.0.2 (12km)	2008 v3	2009	MOVES 2010b 2009 emissions factors and activity data	SMARTFIRE v2	NLCD 2006 (version 2006)
2010	5.0.2 (12km)	2008 v3	2010	MOVES 2010b 2009 emission factors and 2010 activity data	SMARTFIRE v2	NLCD 2006 (version 2006)
2011	5.0.2 (12km)	2011 v1	2011	MOVES 2010b 2011 emissions factors and	SMARTFIRE v2	NLCD 2006 (version 2006)

				activity data		
2012	5.0.2 (12km)	2011 v1	2012	MOVES 2010b 2011 emissions factors and 2012 activity data	SMARTFIRE v2	NLCD 2006 (version 2006)

NEI = National Emissions Inventory (<https://www.epa.gov/air-emissions-inventories/national-emissions-inventory>)

MOVES = Motor Vehicle Emissions Simulator (<https://www3.epa.gov/otag/models/moves/index.htm>)

SMARTFIRE = Satellite Mapping Automated Reanalysis Tool for Fire (<http://www.airfire.org/smartfire/>)

NLCD = National Land Cover Database (<http://www.mrlc.gov/nlcd2006.php>)

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 by combining the concentration data from CASTNET and SEARCH. The weekly schedule is determined by the standard CASTNET Tuesday-to-Tuesday week and all other observations were converted to this schedule. Observed concentrations were interpolated into 12 km grids using inverse distance weighting (IDW) and clipped to the CMAQ CONUS 12 km grid. The distances used in the inverse weighting 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 3) and used in the IDW.

Table 3. 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	394.6	477.0	229.0	381.5
NH ₃	41.9	109.6	84.6	58.4
SO ₂	288.5	271.5	232.8	305.4
pNO ₃	582.3	583.5	192.5	407.0
pNH ₄	538.8	564.3	425.7	563.0
pSO ₄	538.8	564.3	425.7	563.0

2. Create weekly average 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 averaged to the CASTNET weekly schedule.
3. 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 and the SEARCH data are binned by PM_{2.5} and PM₁₀. 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 2002-2012, the year-specific weekly average concentration was multiplied by the year-specific weekly average deposition velocity. For the years 2000-2001 and 2013-2014, 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 2013-2014, the year-specific weekly average concentration was multiplied by weekly average deposition velocities determined from the 2012 model year.

4. Create average seasonal bias adjustment surface for each measured species. The bias adjustment was determined for each monitor by pairing the 3-week rolling average of the monitored values with the 3-week rolling average CMAQ concentration in the grid cell that contains the site. The bias ratio was transformed to a log scale and fitted to a surface using IDW with a maximum distance of 1000 km. The surface was then smoothed using the ESRI ArcGrid function FocalMean with a radius of 60 km. The smoothed surface was then transformed back to the normal scale from the log scale. Resulting ratios were capped at 10 to eliminate mathematical effects of very small concentrations.
5. Create bias-adjusted grids of weekly average CMAQ deposition for measured species. All 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 multiplying the CMAQ value by the ratio obtained in step 4 for the corresponding week in the center of the 3-week rolling average bias.
6. 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 3 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.

7. Create annual dry deposition grids. Weekly average deposition grids for each species were summed to annual values. For the measured species, the grids constructed in step 6 were summed. For unmeasured species, the weekly average CMAQ values were summed. For the years 2002-2012, the year-specific annual deposition was used. For the years 2000-2001, the annual deposition for 2002 was used. For the years 2013-2014, the annual deposition for 2012 was used.
8. 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 and AIRMoN 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 6. Where precipitation measurements from the NTN or MDN networks differed, the maximum amount reported by either of the networks was used. AIRMoN precipitation amounts were used where neither NTN nor MDN sites were colocated. Table 4 summarizes the differences between the IDW parameters used by TDEP and NADP.

Table 4. Parameters used in preparation of TDEP and NADP/NTN precipitation grids

Parameter	TDEP	NADP/NTN
Precipitation measurements used to supplement PRISM	NTN, MDN, AIRMoN	NTN, MDN
Concentration measurements used in grids	NTN, AIRMoN	NTN
Grid cell size	4134.354 m	2338.383 m
Maximum search distance	500 km	500 km
Minimum number of points	10	0
Weighting power of IDW	3	2
PRISM resampling method	None	Nearest neighbor

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 5. 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_dwpct	Dry deposition of chloride as percent of total (wet + dry) deposition	Percent
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-HNO ₃ /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
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
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 <ftp://ftp.epa.gov/castnet/tdep/images>.

Gridded data of the above variables are available in compressed ESRI ArcGRID export files at <ftp://ftp.epa.gov/castnet/tdep/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. Table 6 provides the geographic information for the provided grids.

Table 6. Description of TDEP grids

GRID DESCRIPTION	
Cell Size	4134.354
Data Type	Floating Point
Number of Rows	775
Number of Columns	1440
BOUNDARY STATISTICS	
Xmin	-2950369.148
Xmax	3003100.612
Ymin	115686.836
Ymax	3319811.186
COORDINATE SYSTEM DESCRIPTION	
Projection	ALBERS
Units	METERS
Spheroid	GRS1980
Parameters:	
1st standard parallel	29 30 0.000
2nd standard parallel	45 30 0.000
central meridian	-96 0 0.000
latitude of projection's origin	23 0 0.000
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.
- CMAQ does not include magnesium from windblown dust; therefore, magnesium values between monitoring locations may be significantly underestimated.
- NH₃ data from AMoN and SEARCH is only used for model evaluation and is not included in the development of the concentrations 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 (<http://nadp.sws.uiuc.edu/ntn/>).

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. Changes are noted below in the Revision History. To cite data or maps from this project, a suggested citation is:

National Atmospheric Deposition Program, 2016. Total Deposition Maps, v2016.01.
<http://nadp.sws.uiuc.edu/committees/tdep/tdepmaps>. [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 those years.	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 were not corrected for bias using monitoring data.	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

References

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- Schwede, D.B. and Lear, G.G., 2014. A novel hybrid approach for estimating total deposition in the United States. *Atmospheric Environment*, 92(0): 207-220.
- Skamarock, W., Klemp, J., Dudhia, J., Gill, D., Barker, D., Wang, W., Huang, X.-y. and Duda, M., 2008. A Description of the Advanced Research WRF Version 3. University Corporation for Atmospheric Research.