Metadata for 2002 – 2012 12km CONUS BiDi-CAFO CMAQv5.0.2 Simulations

Purpose: Provide annual adjusted CMAQ deposition fields for 2002 - 2012, with a bi-directional NH3 formulation and a dynamic CAFO emissions profile for critical loads analyses and as input to other ecological models where the most accurate wet deposition fields are desired (via precipitation and bias adjustments).

Simulation settings and inputs:
Model options and inputs that were common for all of the simulations in the 2002 – 2012 series are listed below. Differences in the simulations are summarized in Table 1.

CMAQ
* Community Multiscale Air Quality (CMAQ) modeling system version 5.0.2 was run with bi-directional NH3 air-surface exchange using Massad formulation, CB05TUCL chemical mechanism, aero6 aerosol module.
* CMAQv5.0.2 simulations are run for the CONUS domain using a 12 km grid size and a Lambert Conformal projection assuming a spherical earth with radius 6370.0 km. There are 35 vertical layers from the surface to the top of the free troposphere with layer 1 nominally 19m tall.

Boundary Condition Inputs
* GeosCHEM Boundary conditions using Geos5 meteorology inputs: See Table 1 below for year-specific details.

Emissions Inputs
* Anthropogenic emissions: See Tables 1 and 2 below for year-specific emissions inventory information.
* CMAQ v5.0.2 lightning NOx adjusted to year-specific lightning strike data.
* Economic Policy Integrated Climate (EPIC) chemical fertilizer application schedule that is year specific with chemical specification of form applied.
* New confined animal feeding operations (CAFO) resistance and thermodynamics-based diurnal profile calculation for NH3 emissions.
* Biogenic Emissions Landuse Database, version 4 (BELD4) crop distributions in EPIC and CMAQ, and biogenic emissions.
* Fire emissions developed using the US Forest Service's BlueSky modeling framework with these components: Area Burned: SmartFirev2 | Fuels = FCCS fuelbeds | Consumption Efficiency = CONSUMEv3 | Emission Factors = FEPS (flaming to smoldering ratio)
Additional details can be found here https://www.airfire.org/wp-content/uploads/2012/08/EIC2012-05-EmissionsProcessingComparisons.pdf

Meteorology Inputs

* Weather Research Forecast model, version 3.4 (WRF v3.4) meteorology simulated for 2002 through 2012. NLCD land cover data used for each simulation is summarized in Table 1 below. Data assimilation was based on version2 four-dimensional data assimilation with no nudging in the planetary boundary layer and used blended 3-hourly reanalysis fields (combination of 6-hour Meteorological Assimilation Data Ingest System (MADIS) data and intermediate North American Mesoscale Model (NAM) 3-hour forecast) organized into 12km NAM Data Assimilation System (NDAS) fields up to 50 hPa.
* WRF v3.4 with Kain-Fritsch Ma and Tan (2009) trigger; with NLCD woody wetlands land use category recognized (wetlands-100); with Pleim-Xiu land-surface model.
* WRF post-processing to create inputs for CMAQ was done with the Meteorology-Chemistry Input Processor (MCIP) v4.1.3. There are 35 vertical layers in the WRF simulations from the surface to the top of the free troposphere with layer 1 nominally 19m tall.

Table 1. Difference in input data that are used for the 2002 through 2012 CMAQv5.0.2 simulations.

Year	Date of CMAQ Simulation	Emissions Inventory Label	Boundary Conditions	NLCD land cover Used in WRF
2002	Oct 2013	2002af	Monthly median values from 2005 simulation of GeosCHEM v9-01-02 with Geos5 meteorology	2001
2003	Aug 2013	2003af	Monthly median values from 2005 simulation of GeosCHEM v9-01-02 with Geos5 meteorology	2001
2004	Jun 2014	2005ct_04	Monthly median values from 2005 simulation of GeosCHEM v9-01-02 with Geos5 meteorology*	2001
2005	Mar 2014	2005ct	Hourly values from 2005 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2001
2006	Sep 2013	2007ed_06	Hourly values from 2006 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2007	Dec 2013	2007rh	Hourly values from 2007 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2008	Feb 2014	2008ab	Hourly values from 2008 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2009	Nov 2013	2009ef	Hourly values from 2009 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2010	Jan 2014	2007ed_10	Hourly values from 2010 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2011	May 2014	2011ed	Hourly values from 2011 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006
2012	Sep 2014	2011ed_12	Hourly values from 2012 simulation of GeosCHEM v8-03-02 with Geos5 meteorology	2006

* The incorrect boundary conditions were used for Jan-June 2004. The error had a large impact on ozone but is not expected to have a large impact on wet deposition or PM predictions.

Table 2: Information about the Emissions Inventories used for 2002 through 2012 CMAQv5.0.2 simulations.

Year	Emission Inventory Label	Description	Link to Platform
2002	2002af	2005 modeling platform version 4.3 with year specific updates for Electric Generating Units (EGUs), fires, mobile sources	https://www.epa.gov/air-emissions-modeling/2005-version-43-platform
2003	2003af	2005 modeling platform version 4.3 with year specific updates for EGUs, fires, mobile sources	https://www.epa.gov/air-emissions-modeling/2005-version-43-platform
2004	2005ct_04	2005 modeling platform version 4.3 with year specific updates for EGUs, fires, mobile sources. Mobile on-road emissions were interpolated between 2002 and 2005 due to lack of 2004 MOVES outputs	https://www.epa.gov/air-emissions-modeling/2005-version-43-platform
2005	2005ct_04	2005 modeling platform version 4.3 with year specific updates for EGUs, fires, mobile sources	https://www.epa.gov/air-emissions-modeling/2005-version-43-platform
2006	2007ed_06	2007/2008 modeling platform based on AQMEII phase 2 emissions *	https://www.epa.gov/air-emissions-modeling/20072008-version-5-air-emissions-modeling-platforms
2007	2007rh	2007/2008 modeling platform version 5	https://www.epa.gov/air-emissions-modeling/20072008-version-5-air-emissions-modeling-platforms
2008	2008ab**	2007/2008 modeling platform version 5	https://www.epa.gov/air-emissions-modeling/20072008-version-5-air-emissions-modeling-platforms
2009	2009ef**	2007/2008 modeling platform with year specific updates for fires, EGUs and mobile sources	https://www.epa.gov/air-emissions-modeling/20072008-version-5-air-emissions-modeling-platforms
2010	2007ed_10**	2007 modeling platform based on AQMEII phase 2 emissions *	https://www.epa.gov/air-emissions-modeling/20072008-version-5-air-emissions-modeling-platforms
2011	2011ed**	2011 modeling platform version 6.0	https://www.epa.gov/air-emissions-modeling/2011-version-60-platform
2012	2011ed_12**	2011 modeling platform version 6.0 with year specific updates for fires, mobile sources, and mobile source	https://www.epa.gov/air-emissions-modeling/2011-version-60-platform

* Additional Reference:

(1) Pouliot, G., H. A. D. van der Gon, J. Kuenen, J. Zhang, M. D. Moran, and P. A. Makar (2015), Analysis of the emission inventories and model-ready emission datasets of Europe and North America for phase 2 of the AQMEII project, Atmospheric Environment, 115, 345-360. https://doi.org/10.1016/j.atmosenv.2014.10.061

** Additional analysis of the fire inventories for 2008-2012 can be found in:

(1) Fann, N., B. Alman, R. A. Broome, G. G. Morgan, F. H. Johnston, G. Pouliot, and A. G. Rappold (2018), The health impacts and economic value of wildland fire episodes in the US: 2008–2012, Science of the Total Environment, 610, 802-809. https://doi.org/10.1016/j.scitotenv.2017.08.024

(2) Rappold, A. G., J. M. Reyes, G. Pouliot, W. E. Cascio, and D. Diaz-Sanchez (2017), Community vulnerability to health impacts of wildland fire smoke exposure, Environmental Science & Technology, 51, 6674-6682. DOI: 10.1021/acs.est.6b06200

Use Constraints: Evaluation of model output has thus far focused on model predicted wet deposition of nitrate, sulfate, ammonium and base cations (K^+, Ca^{2+}, Mg^{2+}) that are measured at NADP/NTN sites. Evaluation of ozone, PM2.5 and other species, including evaluation of spatial and temporal trends, has been extremely limited and biases in the model predictions from these simulations has not yet been documented. Errors in the January through June 2004 simulation are expected to cause errors in ozone predictions and will thus impact the estimation of ozone trends across the time series.

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