BDSNP Module for Improved Soil NO Emission Estimates for CMAQ Model, Conterminous USA

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Documentation Revision Date: 2016-11-15

Data Set Version: V1

Summary

This model product provides: (1) the source code for the updated Berkeley-Dalhousie Soil Nitric Oxide (NO) Parameterization module (BDSNP, Version 1.0) as implemented with the Community Multi-scale Air Quality model (CMAQ, Version 5.0.2), (2) module input data from historical and new sources of maps for soil biome type, fertilizer, and arid and non-arid climates, and (3) sample CMAQ simulation outputs for three BDSNP module NO parameterizations (standard, historical, and newer inputs). The simulations use a 12-km spatial grid resolution for CMAQ modeling covering the conterminous United States for July 2011.

The updated BDSNP module helps to improve the timing and spatial distribution of estimates of soil NO emissions through better parameterization of soils, meteorology, land use, and mineral nitrogen availability from both fertilization and deposition. The three sets of outputs represent three different applications of the CMAQ model as described in Rasool et al. (2016).

There are five Fortran source code (*.F) files, 53 input data files and six output files for a total of 59 spatial data files in NetCDF (*.nc) file format included in this data set.

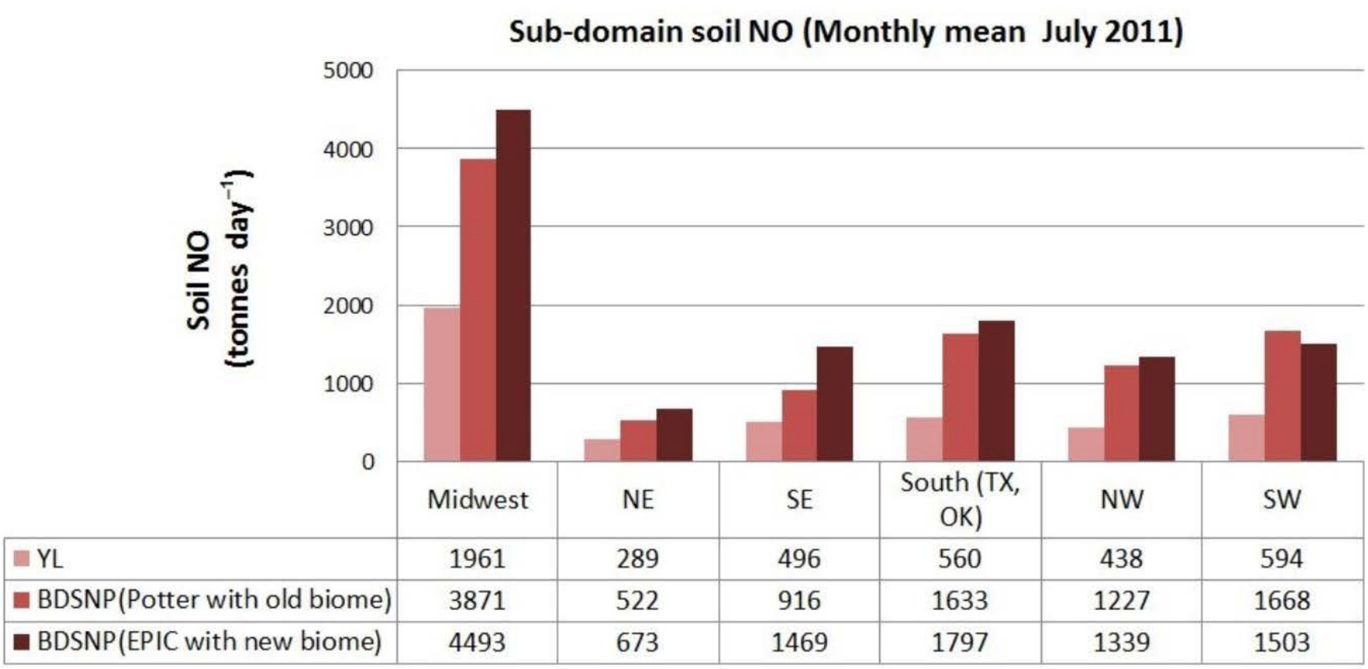

Fig 1. Soil nitric oxide emissions (tonnes/day) from three CMAQ parameterizations (from Rasool et al., 2016)

Citation

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1. Data Set Overview

This model product contains the source code for the updated Berkeley-Dalhousie Soil NOx Parameterization (BDSNP) module implementation with the Community Multiscale Air Quality (CMAQ) model. The update incorporates dynamic representation of the soil nitrogen pool on a day to day basis from the Environmental Policy Integrated Climate (EPIC) biogeochemical model. Sample input data and three sets of model outputs covering the conterminous United States are included with this data set. The three sets of outputs represent three different applications of the CMAQ as described in Rasool et al. (2016). The BDSNP module helps to improve the timing and spatial distribution of estimates of soil nitric oxide (NO) emissions through parameterization of soils, meteorology, land use, and mineral nitrogen availability from both fertilization and deposition. The simulations use a 12 km spatial grid resolution for CMAQ modeling for July 2011.

Related Publication:

Rasool, Q.Z., R. Zhang, B. Lash, D.S. Cohan, E.J. Cooter, J.O. Bash, and L.N. Lamsal. 2016. Enhanced representation of soil NO emissions in the Community Multiscale Air Quality (CMAQ) model version 5.0.2. *Geosci. Model Dev.*, 9: 3177-3197. doi:10.5194/gmd-9-3177-2016

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2. Data Characteristics

Spatial Coverage: CMAQ model domain for Continental United States and portions of northern Mexico and southern Canada

Spatial Resolution: 12- by 12-km grid

Temporal Coverage: Input fertilizer data: 20110101 - 20120101; Outputs: 20110621 - 20110622

Temporal Resolution: Hourly

Study Area:

Site	Westernmost Longitude	Easternmost Longitude	Northernmost Latitude	Southernmost Latitude
CONUS	-129.79	-65.00	51.76	22.75

Data File Information

This data set is comprised of model source files, sample inputs, and sample outputs. There are five Fortran source code (*.F) files, 53 input data files and six output files for a total of 59 spatial data files in NetCDF (*.nc) file format.

A companion file named ***BDSNPmodule_UserGuide_GMD_Supplement.pdf*** provides detailed instructions for building and executing the BDSNP module in-line with the CMAQ model.

<u>Source files</u>

The 5 Fortran source (*.F) files included in this data set are described in Table 1. See section 2.2 of the companion file for instructions on how to build and run the BDSNP module with CMAQ (***BDSNPmodule_Userguide_GMD_Supplement.pdf***).

Table 1. Fortran source files

Filename	Description
BDSNP_MOD_EPIC.F	Gives soil NO parameterization as given by Hudman et al. (2012) with options of enhancement in terms of 'new' soil biome (NLCD40 for 2006) and dynamic fertilizer nitrogen pool from EPIC (Cooter et al., 2012; see Data Acquisition, Materials, and Methods)

canopy_nox_mod.F	Source code for incorporating canopy reduction of soil NO as proposed by Hudman et al. (2012)
cldproc_acm.F* and *vdiffacm2.F	Two source code files for obtaining total mass of nitrogen per unit area deposited to the ground from the atmosphere through wet (*cldproc_acm.F*) and dry (*vdiffacm2.F*) deposition.
tmpbeis.F	Source code to create model-ready biogenic emissions from gridded land use data with emissions inputs in moles/second; in this implementation, *tmpbeis.F* has been modified to give the option to calculate soil NO emission either from Yienger and Levy (1995) parameterization or from BDSNP (see Data Acquisition, Materials, and Methods)

Input and output files in NetCDF (*.nc) file format

Spatial Reference Properties

Type: Projected
Geographic Coordinate Reference: WGS_1984
Projection: Lambert Conformal Conic
Projection units: meters
Datum (spheroid): WGS_84
1st standard parallel: 33 deg
2nd standard parallel: 45 deg
Central meridian: -96 deg
Latitude of origin: 39 deg
False easting: 0
False northing: 0

Input files

There are two groups of sample input files that are used for the 'old' and 'new' implementation schemes of the BDSNP module.

- The old scheme (Hudman et al. 2012) uses the global fertilizer database from Potter et al. (2010) and soil biome type map based on the GEOS-Chem land surface model.
- The new scheme uses dynamic fertilizer fields from the EPIC fertilizer model (Cooter et al. 2012; see Data Acquisition, Materials, and Methods) and soil biome type map based on the NLCD40 (Fry et al., 2011).

The input maps for soil biome type, fertilizer, and arid and non-arid climates have an individual set of inputs for each of the two implementation schemes.

Soil biome type maps

Two soil biome type maps are included as sample inputs for the old and new implementations of the module.

CCTM_V5g_Linux2_x86_64ifort_SOILLANDFRAC12US2.CONUS.nc is the sample input for the old implementation.
BIOME_CMAQ_LANDFRAC_FINAL.nc is the sample input for the new implementation. Data variables are listed in Table 2.

Table 2. Data variables in soil biome type maps

Variable	Description	Units
LANDFRAC	Biome classification *	
TFLAG	Timestep **	
x	Synthesized coordinate from XORIG XCELL ***	km
y	Synthesized coordinate from YORIG YCELL ***	km

* Biome classification for the old implementation of BDSNP module based on soil biome data from the GEOS-Chem, with emission factors for each biome under dry/wet conditions taken from Steinkamp and Lawrence (2011). Classification for the new implementation scheme is based on the NLCD40 for 2006. See Appendix A of Rasool et al. (2016), Tables A1 and A2 for soil biome classifications for the two implementation schemes.

** No data for this variable. All values are 0.

*** See *BDSNPmodule_UserGuide_GMD_Supplement.pdf* companion file for model grid description.

Arid/non-arid climate maps

Separate sample map inputs for both module implementation schemes are included for arid and non-arid climates as 4 NetCDF (*.nc) files. Data variables are listed in Table 3.

SOILCLIMATE.ARID.nc and ***CCTM_V5g_Linux2_x86_64ifort_SOILCLIMA12US2.CONUS.nc*** are the classification maps for arid climates for the new and old module implementation schemes, respectively.

SOILCLIMATE.NONARID.nc and ***CCTM_V5g_Linux2_x86_64ifort_SOILCLIMNA12US2.CONUS.nc*** are the classification maps for non-arid climates for the new and old module implementation schemes, respectively.

Table 3. Data variables for NetCDF inputs for soil biome type

Variable	**Description**	**Units**
TFLAG *	Timestep *	
x	Synthesized coordinate from XORIG XCELL **	km
y	Synthesized coordinate from YORIG YCELL **	km
Arid	Arid land climate ***	0/1
NonArid	NonArid land climate ***	0/1

* No data for this variable. All values are 0.

** See *BDSNPmodule_UserGuide_GMD_Supplement.pdf* companion file for model grid description.

*** Arid and NonArid variables only exist in their respective NetCDF files listed above.

Fertilizer maps

There are two groups of fertilizer inputs to the model

The first is a single NetCDF (*.nc) file ***CCTM_V5g_Linux2_x86_64ifort_SOILFERT12US2.CONUS.nc*** that contains inputs from a global fertilizer database (Potter et al., 2010) used in the implementation of the BDSNP module for GEOS-Chem as described in Hudman et al. (2012). Data variables are listed in Table 4.

Table 4. Data variables for *C**CTM_V5g_Linux2_x86_64ifort_SOILFERT12US2.CONUS.nc***

Variable	**Description**	**Units**
FERTDAY(001-366)	Nitrogen from manure and fertilizer for day ### *	ng N/m^2
TFLAG	Timestep **	
x	Synthesized coordinate from XORIG XCELL ***	km
y	Synthesized coordinate from YORIG YCELL ***	km

* 366 variables give the daily fertilizer nitrogen inputs for 20110101 - 20120101.

** No data for this variable. All values are 0.

*** See *BDSNPmodule_UserGuide_GMD_Supplement.pdf* companion file for model grid description.

The second is a group of 44 NetCDF (*.nc) files that contain the daily fertilizer nitrogen inputs from EPIC (see Data Acquisition, Materials, and Methods). They are named as follows:

e.g. ***SOILFERT_EPIC_Potter_2011MMDD.nc***

where *MM* and *DD* indicate the month and day, respectively. Data variables are listed in Table 5.

Table 5. Data variables for ***SOILFERT_EPIC_Potter_2011MMDD.nc***

Variable	**Description**	**Units**
T1_EPIC	Fertilizer nitrogen from EPIC	ng N/m^2
TFLAG	Timestep *	
x	Synthesized coordinate from XORIG XCELL **	km
y	Synthesized coordinate from YORIG YCELL **	km

* No data for this variable. All values are 0.

** See *BDSNPmodule_UserGuide_GMD_Supplement.pdf* companion file for model grid description.

Soil instate/soilout

Restart files generated by the BDSNP module. Contains the previous day's soil moisture, pulsing factor, and dry period information for continuous run as well as several diagnostic variables for further model verification and analysis. Additional information found in section 3.2.7 of the companion file (*BDSNPmodule_UserGuide_GMD_Supplement.pdf*).

CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.SOILINSTATE.20110620.nc

CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.SOILINSTATE.20110621.nc

Table 6. Data variables for soil instate/soilout restart files.

Variable	**Description**	**Units**
PFACTOR	NO emission current pulse factor	0-1
DRYPERIOD	Length of the dry period	hr
NDEPRES	Soil N reservoir from deposition	Ng/m^2
SOILMPREV	Soil moisture ratio for previous time step	m^3/m^3
THETA_DIAG	Moisture water-filled pore space *	0-1
WET_TERM_DIAG	Moisture scale factor *	0-1
TEMP_DIAG	Temperature in last simulation hour *	K
A_DIAG	Base emission factor from soil biome type *	0-1
NRES_FERT_DIAG	NRES fertilizer only *	0-1
AFERT_DIAG	Fertilizer emission factor *	0-1
NDEPRATE_DIAG	Daily average N deposition rate *	gm/s
CRFAVG	Daily average canopy reduction factor *	0-1
PULSEAVG	Daily average pulse factor *	0-1

* Diagnostic parameters

Sample output files

Three sets of sample output files that correspond to the three applications of the CMAQ model with different soil NO emission schemes (standard, historical, and with newer inputs). The three applications are listed below along with corresponding output files. Data variables are described in Table 7.

Note that emissions estimates other than NO remain the same across all three applications.

1. CMAQ with standard Yienger and Levy (1995) soil NO scheme (standard)

CCTM_v502_BDSNP_EPIC_cb05_BDSNP_N.B3GTS_S.20110621_yl.nc
CCTM_v502_BDSNP_EPIC_cb05_BDSNP_N.B3GTS_S.20110622_yl.nc

2. BDSNP-CMAQ with Potter et al. (2010) fertilizer data and old soil biome mappings from GEOS-Chem (historical)

CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.B3GTS_S.20110621_potter.nc
CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.B3GTS_S.20110622_potter.nc

3. BDSNP-CMAQ with EPIC 2011 data and new soil biome mappings from Pleim-Xiu (2003) (newer inputs)

CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.B3GTS_S.20110621_epic.nc
CCTM_v502_BDSNP_EPIC_cb05_BDSNP_Y.B3GTS_S.20110622_epic.nc

Table 7. Data variables for sample output files. Units are grams per second for a 12- by 12-km grid cell.

Variable	**Description**	**Units**
ALD2	Acetaldehyde	gm/s
ALDX	Propionaldehyde and higher aldehydes	gm/s

CO	Carbon monoxide	gm/s
ETH	Ethene	gm/s
ETHA	Ethane	gm/s
ETOH	Ethanol	gm/s
FORM	Formaldehyde	gm/s
IOLE	Internal olefin carbon bond (R-C=C-R)	gm/s
ISOP	Isoprene	gm/s
MEOH	Methanol	gm/s
NO	**Nitric oxide**	**gm/s**
OLE	Terminal olefin carbon bond (R-C=C)	gm/s
PAR	Paraffin carbon bond (C-C)	gm/s
SESQ	Sesquiterpene	gm/s
TERP	Terpene	gm/s
time	synthesized coordinate from SDATE, STIME, STEP	seconds since 2011-06-21 01:00:00 UTC
x	synthesized coordinate from XORIG XCELL	km
y	synthesized coordinate from YORIG YCELL	km

3. Application and Derivation

The implementation of the BDSNP module with the CMAQ model as described in Rasool et al. (2016) improves the timing and spatial distribution of soil NO emission estimates by considering soil parameters, meteorology, land use, and mineral nitrogen availability to estimate NO emissions. Compared with the previous usage with the GEOS-Chem model, this implementation with CMAQ incorporates finer-scale representation of its dependence on land use, soil conditions, and nitrogen availability. The finer resolution and updated biome and fertilizer data set resulted in higher sensitivity of soil NO to biome emission factors. These improvements represent crucial advancements toward enhanced representation of soil NO in a regional model.

4. Quality Assessment

No uncertainty estimates are provided with this data set; however, a comparison of CMAQ tropospheric NO_2 column densities to those from NASA's Ozone Monitoring Instrument is detailed in Rasool et al. (2016).

Comparison of the model outputs from the three implementation schemes described in Rasool et al. (2016) indicate that the finer resolution and updated biome and fertilizer data sets used for the BDSNP module in CMAQ resulted in higher sensitivity of soil NO to biome emission factors. The updated BDSNP scheme (EPIC and 'new' biome) predicts slightly higher soil NO than the inputs used in GEOS-Chem, primarily due to the use of daily EPIC fertilizer data and fine resolution NLCD40 biomes. Switching from GEOS-Chem biome data to the 'new' NLCD40 biome data drops soil NO in the northwest and southwest portions of the CONUS due to the finer resolution biome map exhibiting lower emission factors in those regions. Replacing fertilizer data from Potter et al. (2010) with the EPIC data set increased soil NO mostly in the Midwest. The results of this comparison are illustrated in Figure 1.

5. Data Acquisition, Materials, and Methods

Module Description

The Berkeley-Dalhousie Soil NO_x Parameterization (BDSNP) module improves the timing and spatial distribution of soil nitric oxide (NO) emission estimates in the Community Multi-scale Air Quality model (CMAQ version 5.0.2). The parameterization considers soil parameters, meteorology, land use, and mineral nitrogen availability to estimate NO emissions. The BDSNP has been previously implemented in a global chemical transport model (GEOS-Chem) to update soil NO emission estimates (Hudman et al., 2010, 2012). Compared to the soil NO emission module currently coded in biogenic emission models such as BEIS3 and MEGAN (YL95 module; Yienger and Levy 1995), the BDSNP scheme has a more continuous soil temperature/moisture dependence function.

The BDSNP scheme determines soil NO emissions at each modeling grid and time-step using the base emission varied by the biome type as well as available soil nitrogen, soil temperature and moisture response function, soil pulsing after precipitation, and canopy reduction due to resistance. Figure 2 provides the flow chart of the BDSNP scheme implementation. Static input files such as arid/non-arid climate zone, and soil biome type are needed to determine the soil base emission value at each modeling grid.

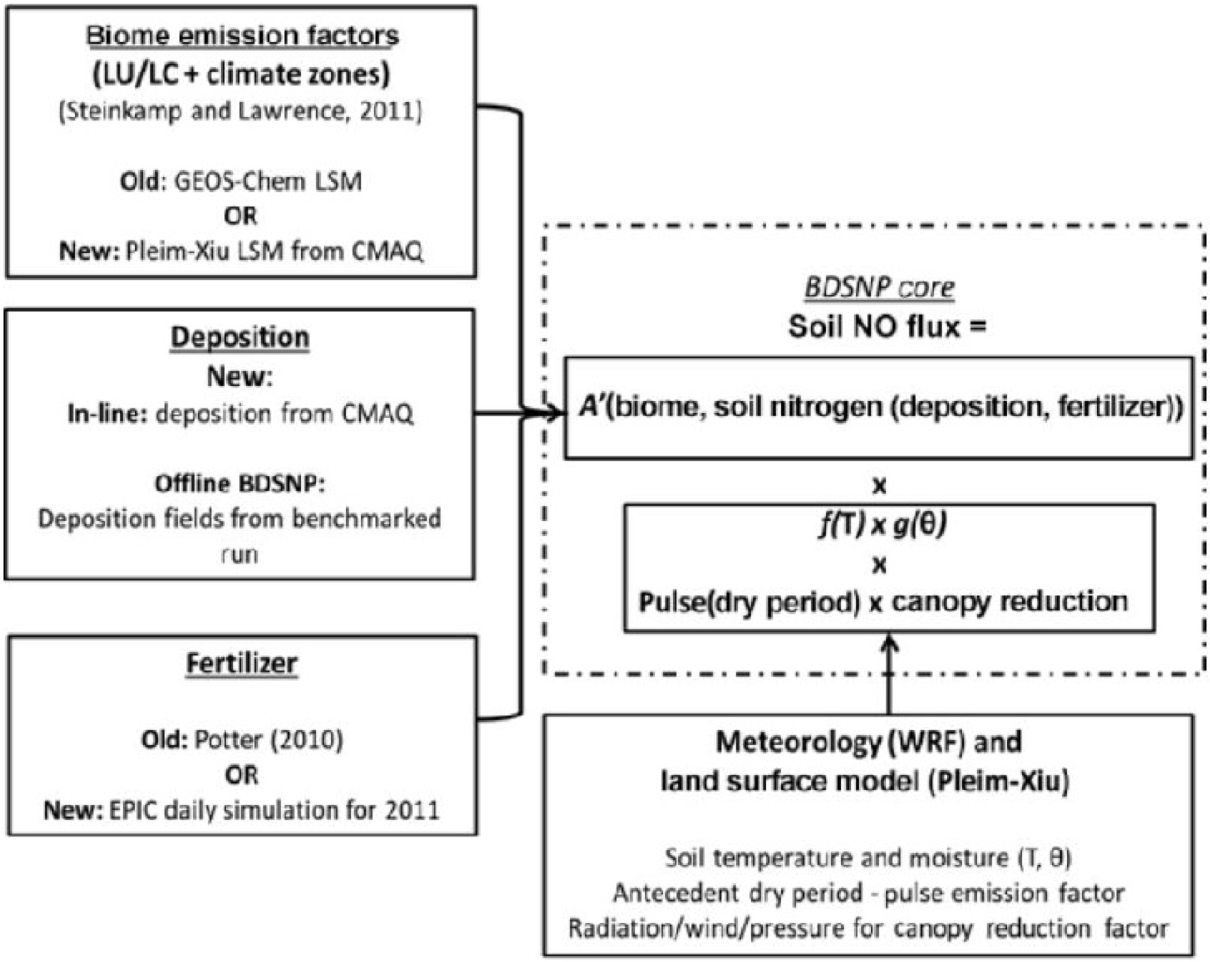

Figure 2. Soil NO emissions modeling framework as implemented in CMAQ (from Rasool et al., 2016)

Soil NO parameterization in CMAQ

The three CMAQ model implementation schemes differed in how fertilizer inputs account for nitrogen deposition.

- YL95 and Potter et al. (2010) in CMAQ neglect nitrogen deposition, which can result in major underestimation in soil NO_X globally (Hudman et al., 2012).
- EPIC nitrogen pools include nitrogen deposition.

Nitrogen Fertilizer and Depostion input data for corresponding CMAQ simulations,

See Sample Output 1:

YL95 (Yienger and Levy, 1995) in CMAQ assumed a linear correlation between fertilizer application and its induced emissions over the general growing season, rather than peaking near the time of fertilization at the beginning of the local growing season. This likely caused inaccurate temporal representation of fertilizer-driven emissions in certain regions (Hudman et al., 2012).

See Sample Output 2:

The GEOS-Chem implementation of BDSNP applied a long-term average fertilizer application with a decay term after fertilizer is applied. Constant fertilizer emissions neglect an important phenomenon: applying fertilizer during a dry period when neither plants nor bacteria may have the water available to use it may result in a large pulse when the soil is eventually re-wetted (Pilegaard, 2013). This implementation used fertilizer data scaled to global 2006 emissions by Hudman et al. (2012) using a spatial distribution for year 2000 from Potter et al. (2010).

See Sample Output 3:

This implementation of BDSNP into CMAQ uses the Environmental Policy Integrated Climate (EPIC) biogeochemical model for dynamic representation of the soil nitrogen pool on a day-to-day basis. EPIC is a field-scale biogeochemical process model developed by the USDA to represent plant growth, soil hydrology, and soil heat budgets for multiple soil layers of variable thickness, multiple vegetative systems, and crop management practices (Cooter et al, 2012). It is implemented through the Fertilizer Emission Scenario Tool for CMAQ (FEST-C v1.1; http://www.cmascenter.org) to enable updates by subsequent developers to use new year- and location-specific fertilizer data. EPIC simulations for 2011 were used in these CMAQ runs.

Additional Input Data

Land surface model

The 'new' implementation of BDSNP soil NO parameterization in CMAQ (described in Rasool et al. 2016) uses Pleim-Xiu Land Surface Model (Pleim and Xiu, 2003). Compared to the coarser land surface model in GEOS-Chem (Bey et al., 2001), Pleim-Xiu provides finer-scale estimates of soil moisture and soil temperature based on solar radiation, temperature, leaf area index, vegetation coverage, and aerodynamic resistance.

Meteorology

The Meteorology-Chemistry Interface Processor (MCIP; Otte and Pleim, 2010) takes outputs from a meteorological model such as the Weather Research and Forecasting model (WRF; Skamarock et al., 2008) to provide a complete set of meteorological data needed for emissions and air quality simulations within CMAQ.

Canopy reduction factor

The same approach to integrating canopy reduction factor as used in Wang et al. (1998) is used in this implementation of BDSNP for the CMAQ model. Biome categorization is based on Steinkamp and Lawrence (2011) and Köppen climate classes (Kottek et al., 2006) in the soil NO_x parameterization.

Soil biome map over CONUS

A soil biome map was generated from the 30 arc-second NLCD40 (Fry et al., 2011) at 12 km resolution for the CONUS. Additionally, a model resolution compatible Köppen climate zone classification (Kottek et al., 2006) was added to allocate different emission factors for the same biome type, e.g., to account for different altitudes of "grassland" at different locations.

6. Data Access

These data are available through the Oak Ridge National Laboratory (ORNL) Distributed Active Archive Center (DAAC).

BDSNP Module for Improved Soil NO Emission Estimates for CMAQ Model, Conterminous USA

Contact for Data Center Access Information:

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