Mechanistic Module for Soil Nitrogen Emissions for CMAQ Model, North America, 2011

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Documentation Revision Date: 2019-04-25

Dataset Version: 1

Summary

This model product provides source code, input data files, and example model outputs for a new mechanistic soil nitrogen (N) module in-line with the Community Multiscale Air Quality (CMAQ) model 5.1 to simulate nitric oxide (NO), nitrous acid (HONO), nitrous oxide (N2O), and ammonia (NH3) soil emissions. The modeling domain covers the continental USA plus portions of northern Mexico and southern Canada, extending from 25 degrees north to 52 degrees north.The simulations use a 12-km spatial grid resolution. Input data are from high-quality reference sources for year 2011. Example model output data are provided for one day, April 21, 2011.

The mechanistic approach helps to improve the timing and spatial distribution of estimates of soil N emissions by accounting for actual biogeochemical processes that generate these emissions under varied soil conditions and vegetation types so that nitrification and denitrification can be represented. For non-agricultural biomes, the new mechanistic scheme uses a global soil nutrient dataset in an updated C and N mineralization framework. This enables the model to track the conversion of organic soil N to NH4 and NO3 pools on a daily scale for non-agricultural soils.

There are eight data files with this dataset. This includes one compressed file (.zip) with seven Fortran source codes (*.F), five input data files in NetCDF (.nc) format and two output files in NetCDF (.nc) format. A companion file is provided which contains instructions on how to build and run the new mechanistic soil nitrogen (N) module in-line with CMAQ version 5.1.

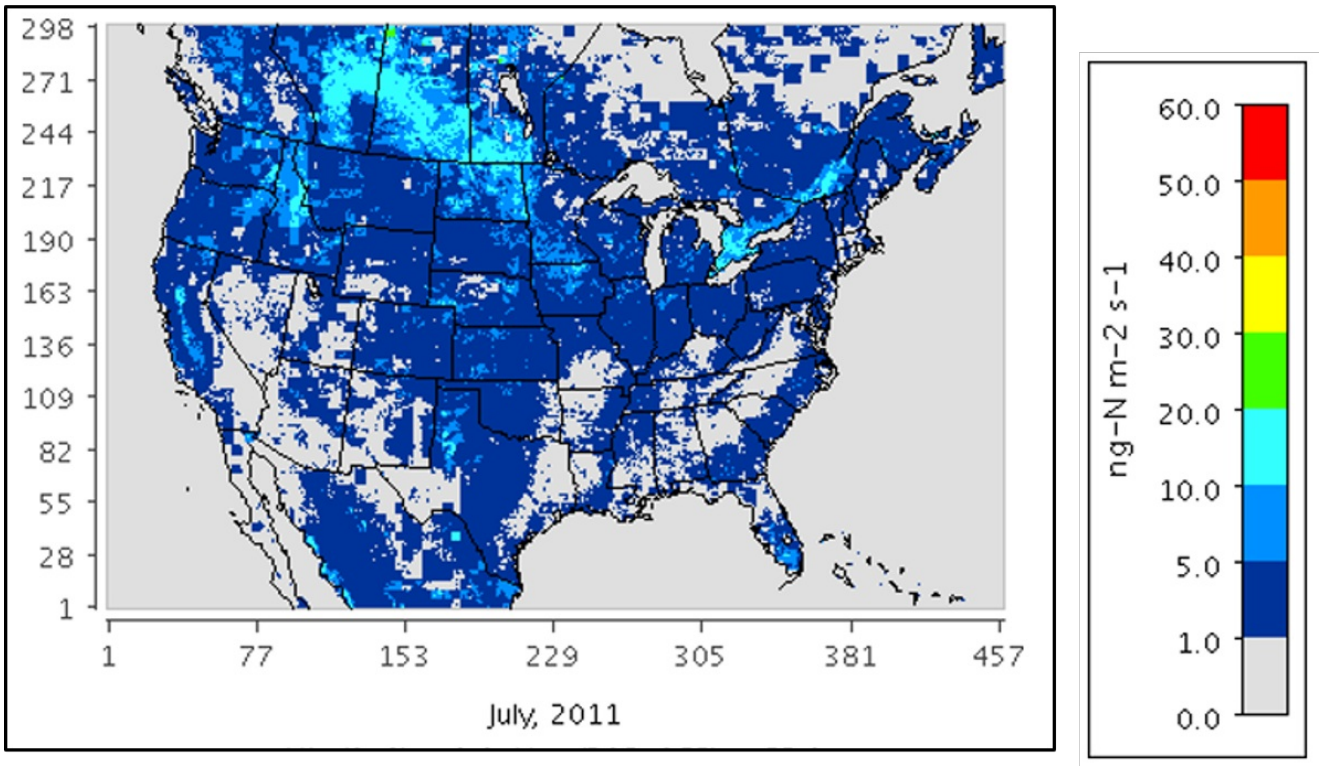

Figure 1. Soil N2O emissions on a monthly average basis for July 2011 estimated with mechanistic scheme. From Rasool et al. (2019).

Citation

Rasool, Q.Z., J.O. Bash, and D.S. Cohan. 2019. Mechanistic Module for Soil Nitrogen Emissions for CMAQ Model, North America, 2011. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1661

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1. Dataset Overview

This model product provides source code, input data files, and example model outputs for a new mechanistic soil nitrogen (N) module in-line with the Community Multiscale Air Quality (CMAQ) model 5.1 to simulate nitric oxide (NO), nitrous acid (HONO), nitrous oxide (N2O), and ammonia (NH3) soil emissions. The modeling domain covers the continental USA plus portions of northern Mexico and southern Canada, extending from 25° N to 52° N. The simulations use a 12-km spatial grid resolution. Input data are from high-quality reference sources for year 2011. Example model output data are provided for one day, April 21, 2011.

The mechanistic approach helps to improve the timing and spatial distribution of estimates of soil N emissions by accounting for actual biogeochemical processes that generate these emissions under varied soil conditions and vegetation types so that nitrification and denitrification can be represented. For non-agricultural biomes, the new mechanistic scheme uses a global soil nutrient dataset in an updated C and N mineralization framework. This enables the model to track the conversion of organic soil N to NH4 and NO3 pools on a daily scale for non-agricultural soils.

Related Dataset:

Rasool, Q.Z., R. Zhang, D.S. Cohan, E.J. Cooter, L.N. Lamsal, J.O. Bash, and B. Lash. 2016. BDSNP Module for Improved Soil NO Emission Estimates for CMAQ Model, Conterminous USA. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1351

Related Publication:

Rasool, Q.Z., Bash, J.O. and Cohan, D.S., 2019. Mechanistic representation of soil nitrogen emissions in the Community Multiscale Air Quality (CMAQ) model v 5.1. *Geoscientific Model Development*, *12*(2), pp.849-878. https://doi.org/10.5194/gmd-12-849-2019.

Acknowledgements:

This research was funded by a NASA ROSES (Research Opportunities in Earth and Space Science) grant, number NNX15AN63G.

2. Data Characteristics

Spatial Coverage: Continental US, portions of northern Mexico and southern Canada

Spatial Resolution: 12 x 12 km grid

Temporal Coverage: Input data are from high-quality reference sources for year 2011. Example model output data are provided for one day, April 21, 2011.

Temporal Resolution: Model run and data aggregation specific per user needs.

Study Area (coordinates in decimal degrees)

Site	Westernmost Longitude	Easternmost Longitude	Northernmost Latitude	Southernmost Latitude
Continental US, portions of northern Mexico and southern Canada	-128.7422132	-59.13283825	51.55248055	25.06967334

Data File Information

There are eight data files with this dataset. This includes one compressed file (.zip) with seven Fortran source codes (*.F), five input data files in NetCDF (.nc) format and two output files in NetCDF (.nc) format.

The companion file **Mechanistic_Soil_N_Module_UserGuide.pdf** provides instructions on how to build and run the new mechanistic soil nitrogen (N) module in-line with CMAQ version 5.1.

Table 1. Data file descriptions

Filename	Description
Model source code files	
cmaq-n-module-source.zip	A compressed file which provides the seven source code files
Ncycling.F	Addresses soil N emissions
vdiffacmx.F	The original code for dry and wet deposition, vdiffacm2.F and cldproc_acm.F respectively modified to obtain total mass of N per area deposited to the ground from atmosphere
CNnonAgcycling.F	Addresses soil N emissions for non-agricultural biome
cldproc_acm.F	The original code for dry and wet deposition, vdiffacm2.F and cldproc_acm.F respectively modified to obtain total mass of N per area deposited to the ground from atmosphere
canopy_nox_mod.F	Canopy reduction factor for incorporating canopy reduction of soil NO as proposed by Hudman et al. (2012)
BIOG_EMIS.F	Biogenic emissions
BDSNP_MOD_EPIC.F	Used to call the new Ncycling.F and CNnonAgcycling.F to pass the computed soil

	NO, HONO and N_2O into the biogenic emission outpus (B3GTS_S)
Input files	
SMNRESFILE.nc	Soil organic nitrogen data used to drive the C and N cycling based on Schimel and Weintraub (2003) for non-agricultural regions, where EPIC is not applicable
SMCRESFILE.nc	Soil organic carbon data used to drive the C and N cycling based on Schimel and Weintraub (2003) for non-agricultural regions, where EPIC is not applicable
PHTOPSOILFILE.nc	Soil pH, gridded for the CONUS domain
LANDFRACFILE.nc	Soil biome types. CMAQ by default uses 40-category NLCD Land Use classification (NLCD40) with sub-grid fractions for different land use
CNRATIOFILE.nc	Microbial C:N ratio
Output files	
N2O_EMIS_SOILINP_CMAQ51_FILE_20110421.nc	Soil N2O emission estimates and relevant diagnostics calculated for 20110421
NOandHONO_B3GTS_S_CMAQv51_FILE_20110421.nc	Soil NO and HONO emissions estimates calculated for 20110421 along with other biogenic emissions that act as input to CMAQ's chemical transport model unlike the diagnostic N2O estimates

NetCDF file properties

All *.nc files are in Lambert Conformal Conic Projection:

```
OGC WKT :
PROJCS["unnamed",
  GEOGCS["unnamed ellipse",
    DATUM["unknown",
      SPHEROID["unnamed",6370000,0]],
    PRIMEM["Greenwich",0],
    UNIT["degree",0.0174532925199433]],
  PROJECTION["Lambert_Conformal_Conic_2SP"],
  PARAMETER["standard_parallel_1",33],
  PARAMETER["standard_parallel_2",45],
  PARAMETER["latitude_of_origin",40],
  PARAMETER["central_meridian",-97],
  PARAMETER["false_easting",0],
  PARAMETER["false_northing",0],
  UNIT["Meter",1]]
```

Resolution: 12- by 12-km grid

No data value: -2147483647

Table 2. Variables in the Input Files

Filename	Variable	Units/format	Description
SMNRESFILE.nc	SMN30cm	g N/m2	Soil organic nitrogen data used to drive the C and N cycling
SMCRESFILE.nc	SMC30cm	g C/m2	Soil organic carbon data used to drive the C and N cycling
PHTOPSOILFILE.nc	pHsl	n/a	Soil pH
LANDFRACFILE.nc	LANDFRAC	n/a	BIOME Classification based on NLCD40
CNRATIOFILE.nc	CN30cm	percent	Carbon to nitrogen ratio

Variables in the Output Files

Table 3. N2O_EMIS_SOILINP_CMAQ51_FILE_20110421.nc

* Denotes diagnostic parameters

Variable	Units/format	Description
DENITR_rate	kg/ha/s	Denitrification rate from Ncycling routine*
N2O_EMIS	g N/hr	N2O emission from Ncycling routine*

NH4_Pool	kg N/ha	NH4 Pool from Ncycling routine*
NITR_Rate	kg/ha/s	Nitrification rate from Ncycling routine*
NO3_Pool	kg N/ha	NO3 Pool from Ncycling routine*
PFACTOR	0-1	NO emission current pulse factor
DRYPERIOD	hr	Length of the dry period
NDEPRES	g N/m^2	Soil N reservoir from deposition
SOILMPREV	m^3/m^3	Soil moisture ratio for previous time step
THETA_DIAG	0-1	Moisture water-filled pore space *
WET_TERM_DIAG	0-1	Moisture scale factor *
TEMP_DIAG	K	Temperature in last simulation hour *
TEMP_TERM_DIAG		Temperature scale factor*
A_DIAG	0-1	Base emission factor from soil biome type *
NRES_FERT_DIAG	0-1	NRES fertilizer only *
AFERT_DIAG	0-1	Fertilizer emission factor *
NDEPRATE_DIAG	gm/s	Daily average N deposition rate *
CRFAVG	0-1	Daily average canopy reduction factor *
PULSEAVG	0-1	Daily average pulse factor *

Table 4. NOandHONO_B3GTS_S_CMAQv51_FILE_20110421.nc

Units are grams per second for a 12- by 12-km grid cell.

Variable	Units/format	Description
ALDX	gm/s	Propionaldehyde and higher aldehydes
ALD2	gm/s	Acetylaldehyde
BPIN	gm/s	b-PINENE
APIN	gm/s	a-PINENE
CO	gm/s	Carbon monoxide
ETH	gm/s	Ethene
ETHA	gm/s	Ethane
ETOH	gm/s	Ethanol
FORM	gm/s	Formaldehyde
HONO	gm/s	Nitrous acid
IOLE	gm/s	Internal olefin carbon bond (R-C=C-R)
ISOP	gm/s	Isoprene
MEOH	gm/s	Methanol
NO	gm/s	Nitric oxide
OLE	gm/s	Terminal olefin carbon bond (R-C=C)
PAR	gm/s	Paraffin carbon bond (C-C)
SESQ	gm/s	Sesquiterpene
TERP	gm/s	Terpene

3. Application and Derivation

The mechanistic module helps to improve the timing and spatial distribution of estimates of soil N oxide emissions by accounting for actual mechanistic process that generate these emissions under varied soil conditions, nutrient availability and meteorology regional model.

4. Quality Assessment

The corresponding modeled estimates from the new mechanistic soil N module have been compared to OMI tropospheric NO2 columns, SEARCH campaign NOx concentrations and secondary pollutant concentrations like Ozone and PM2.5 NO3 observed from IMPROVE, AQS, CSN and CASTNET observation networks. Statistical performance of modeled vs observed values was thoroughly analyzed for May and July 2011 for Conterminous US and both improvement and uncertainty in model performance is explained

in Rasool et al. (2019).

5. Data Acquisition, Materials, and Methods

The new mechanistic module has been implemented into the Community Multiscale Air Quality (CMAQ) modeling system v5.1 to produce soil NO, HONO, and N_2O emission estimates using the soil temperature/moisture information from the Pleim-Xiu land surface model (Pleim and Xiu, 2003) in the Weather Research Forecasting (WRF) model v 3.7. The Mechanistic module helps to improve the timing and spatial distribution of estimates of soil N oxide emissions by accounting for actual mechanistic process that generate these emissions under varied soil conditions, nutrient availability and meteorology.

Based on the mechanistic scheme, soil NO, HONO, and N_2O emissions at each modeling grid and time-step are determined by accounting for soil nitrogen (either form the fertilizer application during the growing season or the soil N naturally available in non-agricultural biome or the nitrogen dry/wet deposition from the atmosphere), and the subsequent transformation of soil nitrogen either through nitrification or denitrification depending on variables such as, soil temperature and moisture, availability of soil NH_4 or NO_3, relative availability of NO_3 to C, soil pH, gas diffusivity, the soil pulsing after precipitation, and the canopy reduction due to the resistance (Rasool et al., 2019).

New codes in the mechanistic module

The mechanistic module is simultaneously compiled with other executables of the CMAQ Chemistry-Transport Model (CCTM). CCTM integrates model-ready inputs such as emissions, meteorology, photochemistry, initial and boundary conditions to simulate continuous atmospheric chemical conditions at user-defined time frequency (hourly, daily etc.). Implementation of the mechanistic module in-line with CCTM ensures that soil NO, HONO and N_2O as per newly proposed mechanistic scheme is also accounted for while generating gridded and temporally resolved air pollutant concentrations as output.

Ncycling.F and **CNnonAgcycling.F:**

Ncycling.F and **CNnonAgcycling.F** were added as global attributes in the CCTM source code repository, which basically gives the mechanistic representation of soil NO, HONO, and N2O emissions which are passed into the biogenic emission outputs (Rasool et al., 2019).

Environmental variables specific to mechanistic module

Understanding the environment variables defined in the mechanistic module is crucial for the real case implementation and further model development if needed.

LANDFRACFILE.F:

CMAQ v5.1 has sub-grid scale representation for 40 National Land Cover dataset (NLCD) biomes and was thus utilized rather than the MODIS 24 classification.

SMCRESFILE, SMNRESFILE, CNRATIOFILE, and **PHTOPSOILFILE:**

The input files **SMCRESFILE, SMNRESFILE, CNRATIOFILE** and **PHTOPSOILFILE** provide the soil organic carbon and nitrogen pools, microbial C:N ratio and soil pH respectively over the simulation domain. These inputs are used in the mechanistic module to drive the C and N cycling based on Schimel and Weintraub (2003) for non-agricultural regions. For the modeling grid, non-agricultural grids can be classified from 'LANDFRFILE' and MODIS to NLCD mapping algorithm coded in mechanistic scheme source codes (Rasool et al., 2019).

Refer to the companion file **Mechanistic_Soil_N_Module_UserGuide.pdf** for detailed instructions for building and executing the module in-line with CMAQ version 5.1.

6. Data Access

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

Mechanistic Module for Soil Nitrogen Emissions for CMAQ Model, North America, 2011

Contact for Data Center Access Information:

- E-mail: uso@daac.ornl.gov
- Telephone: +1 (865) 241-3952

7. References

Hudman, R.C., A.R. Russell, L.C. Valin, and R.C. Cohen.: Interannual variability in soil nitric oxide emissions over the United States as viewed from space, Atmos. Chem. Phys., 10, 9943-9952. https://doi.org/10.5194/acp-10-9943-2010

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