Supplement of Geosci. Model Dev., 9, 3177–3197, 2016
http://www.geosci-model-dev.net/9/3177/2016/
doi:10.5194/gmd-9-3177-2016-supplement
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Supplement of

Enhanced representation of soil NO emissions in the Community Multiscale Air Quality (CMAQ) model version 5.0.2

Quazi Z. Rasool et al.

Correspondence to: Daniel S. Cohan (cohan@rice.edu)

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Table S1 List of key I/O environment variables in BDSNP model

Environment Variable	Description	Note (*new)
SOILBIOME	[Input file]: soil biome map for model domain, 24 category based on GEOS-Chem and Köppen climate zone	*can be replaced by 24 category based on NLCD2006 and re-gridded Köppen climate zone, see section 2.3
SOILCLIMATE	[Input file]: arid and non-arid region in model domain	
NFERT	[Input file]: fertilizer map for model domain	*can be replaced by EPIC results, see section 2.4
NDEP	[Input file]: nitrogen deposition from previous CMAQ simulations	*currently uses 2005 CMAQ results on 12km CONUS domains (for offline), see section 2.5
GRIDDESC	[Input file]: set the domain size and projection information	
METCRO2D	[Input file]: meteorology fields in NetCDF format from MCIP for model domain, which include the parameters: (1) TMEP2-surface temperature (2) RGRND-solar radiation (3) PRSFC-surface pressure (4) SOIM1-soil moisture (5) SOIT1-soil temperature (6) SNOCOV-snow cover (7) WSPD10-10m wind speed (8) CFRAC-cloud fraction (9) LAI-leaf area index	*soil condition including moisture and temperature must be diagnosed by choosing Pleim-Xiu LSM model (2003) in WRF runs
SOILINSTATE	[Input file]: restart file provides the pulsing factor, dry period, soil moisture and deposition for continuous run as well as other model diagnostic parameters	
BDSNPOUT	[Output file]: hourly soil NO emission flux in 'g/s' or 'mol/s' simulated from BDSNP module	
SOILOUT	[Output file]: same format as 'SOILINSTATE'	

S.2 Stand-alone soil NO module

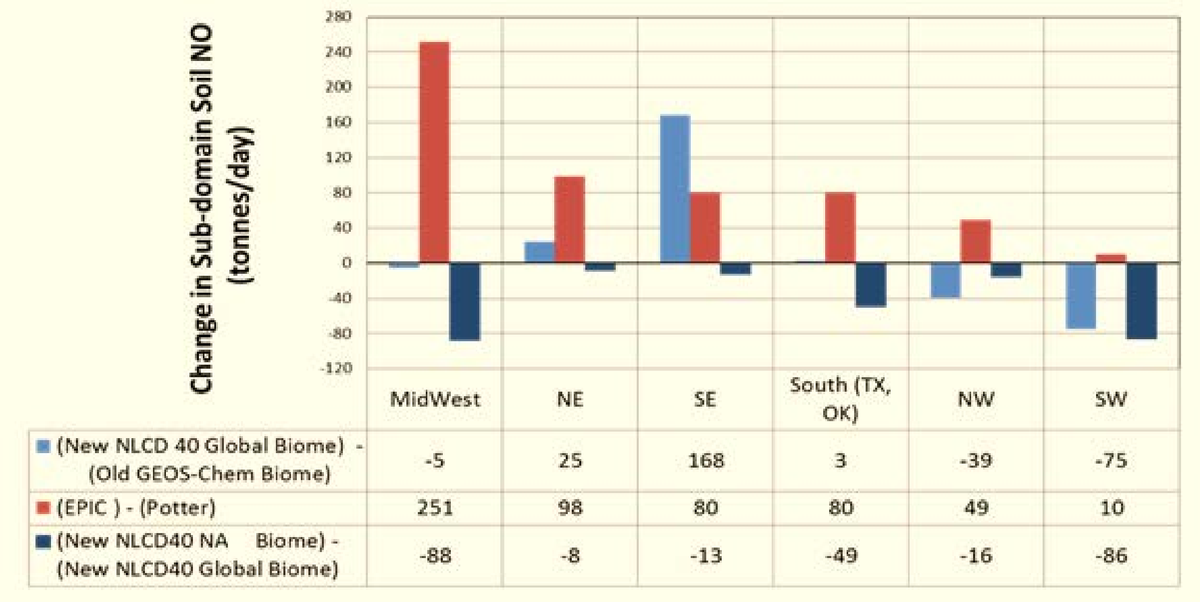
The major difference between our in-line (with CMAQ) and offline implementations is the approach to deal with nitrogen deposition. For the in-line BDSNP model, dry or wet deposition process considered in CMAQ will continuously update the available nitrogen from the atmosphere to the ground. For the stand-alone module, the nitrogen available from wet or dry deposition cannot be calculated instantaneously through the air quality model but needs to be determined from offline, pre-computed files. For the stand-alone model, soil condition from the last hour of previous day's run and the generic daily nitrogen pool from archived deposition fields are used. Since the soil N pool needs a long time to reach the quasi-steady state in the model, a new series of inputs are needed in the stand-alone model to provide the generic daily variation of N deposition. Hence, we performed a full year CMAQ simulation over the 12 km continental U.S. domain using the emission and meteorology files for provided by EPA. We recorded daily data on amount of soil N reservoir resulting from deposition from the simulation. These deposition fields were archived as the restart files for the 2011 run. Simulating soil NO emissions for a region outside North America or for a period with sharply different N deposition rates from 2005 will require development of new deposition fields by this or other means.

S.3 Impact of different BDSNP inputs on soil NO in CONUS

For stand-alone BDSNP, sensitivity of the model in terms of soil NO emissions for different inputs were analyzed for the same test period of July, 2011. Our offline BDSNP module allows us to quantify the sensitivities of soil NO emissions that can occur by switching between the 'old' (Potter and old GEOS-Chem based biome) and 'new' (EPIC and new NLCD40 biome; both global and North American) datasets (refer to Fig. 2). The sensitivity analysis gives a quick diagnostics about the changes in soil NO (on a monthly mean basis for July 2011) to different inputs without being computationally extensive. From Figure S4, for the 3 cases in standalone BDSNP for July 2011: a) Change from old GEOS-Chem biome to new NLCD40 biome (with global geometric mean EF, EF1 Table A2) shows drop in soil NO in north-west and south-west domains by 39 and 75 tonnes/day respectively. These drops are due to the characterization in finer resolution biome map showing lower EF biome type in those regions than what was there in old biome map. b) Shift from Potter et al. (2010) to EPIC 2011 dataset showed an increase in soil

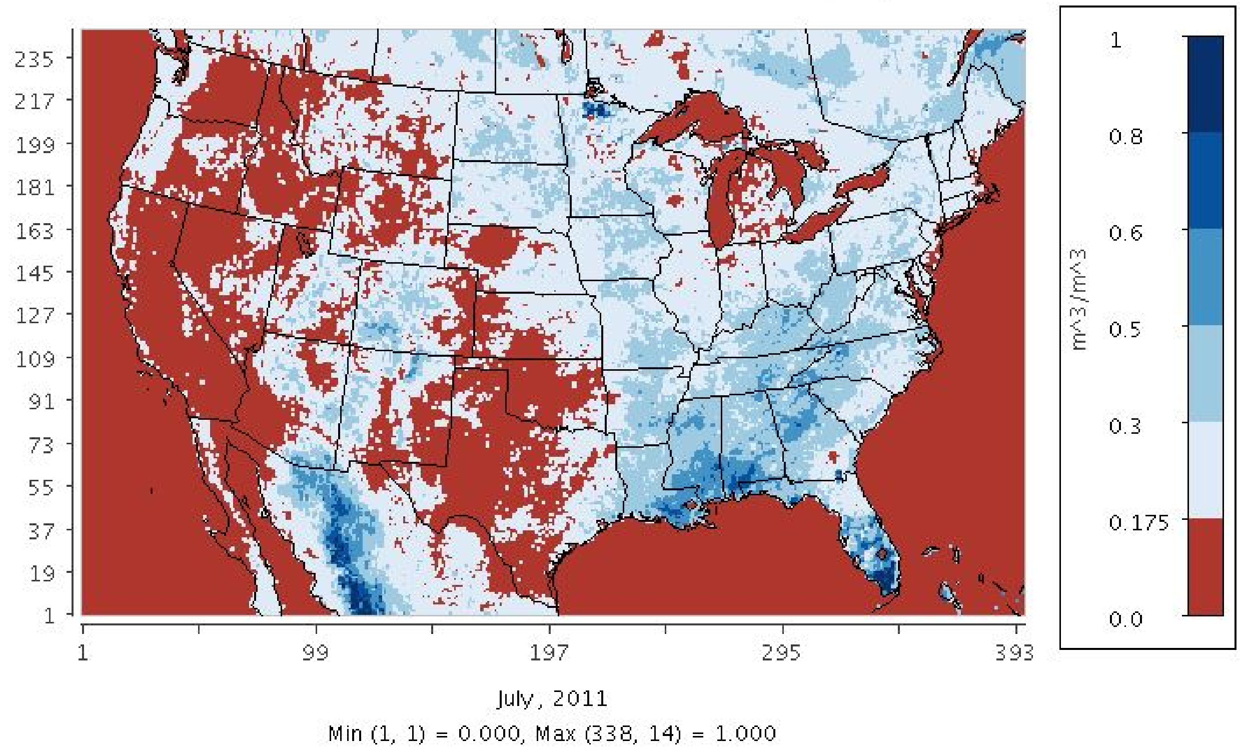
NO for all sub-domains with the mid-west being highest at 251 tonnes/day for July 2011 mean, due to the increased N input in 2011 as exhibited by FEST-C outputs as compared to decade old Potter et al. (2010) data. c) Shift to North American (NA) biome EF from global one (EF1 to EF3, see Table A2) exhibits drops in mid-west and south west for monthly mean soil NO up to 88 and 86 tonnes/day respectively. These drops are attributed to the fact that croplands in North America in mid-west and south-west (Sacramento and San Joaquin valleys in California) have been shown to exhibit lower soil NO emissions than those in Asia or Africa (Stehfest and Bouwman, 2006).

Figure S4 Comparison of the 3 standalone BDSNP cases in terms of impact on soil NO (monthly mean) in tonnes/day due to changes in different input data sets in the test period of July, 2011



	MidWest	NE	SE	South (TX, OK)	NW	SW
🟦 (New NLCD 40 Global Biome) - (Old GEOS-Chem Biome)	-5	25	168	3	-39	-75
🟥 (EPIC) - (Potter)	251	98	80	80	49	10
■ (New NLCD40 NA Biome) - (New NLCD40 Global Biome)	-88	-8	-13	-49	-16	-86

Figure S5 Soil moisture (m^3/m^3) for CONUS on a monthly mean basis (July 2011) for CONUS


235
217
199
181
163
145
127
109
91
73
55
37
19
1
1
99
197
295
393
July, 2011
Min (1, 1) = 0.000, Max (338, 14) = 1.000
m^3/m^3
1
0.8
0.6
0.5
0.3
0.175
0.0