# THE GLOBAL N<sub>2</sub>O MODEL INTERCOMPARISON PROJECT

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The  $N_2O$  Model Intercomparison Project (NMIP) aims at understanding and quantifying the budgets of global and regional terrestrial  $N_2O$  fluxes, environmental controls, and uncertainties associated with input data, model structure, and parameters.

gas (GHG), and the time-integrated radiative  $\frac{1}{100}$   $\frac{1}{10$ itrous oxide (N2O) is an important greenhouse forcing resulting from a mass unit of N2O is 265-298 times larger than that from carbon dioxide (CO<sub>2</sub>) emissions for a 100-yr time horizon (Ciais et al. 2013; Myhre et al. 2013). Multiple lines of evidence indicate that human activities [e.g., industrial N, fixation by the Haber-Bosch process or by fossil fuel combustion and manure nitrogen (N) application] play an increasingly significant role in the perturbation of the global N cycle (Galloway et al. 2008; Gruber and Galloway 2008; Fowler et al. 2015), which has led to an increase in atmospheric N<sub>2</sub>O concentration by ~21%, from 271 ppb at preindustrial level to 329 ppb in 2015 (MacFarling Meure et al. 2006; Prather et al. 2012, 2015; Thompson et al. 2014; www.esrl.noaa .gov/). The anthropogenic N<sub>2</sub>O emissions are estimated to have increased from 0.7 Tg N yr<sup>-1</sup> in 1860 to 6.9 Tg N yr<sup>-1</sup> in 2006, ~60% of which was ascribed to agricultural activities (Ciais et al. 2013; Davidson and Kanter 2014). The increased N<sub>2</sub>O emissions have significantly contributed to climate warming. During the 2000s, the warming effect of N<sub>2</sub>O emissions from the terrestrial biosphere counteracted more than half of the cooling effect of the global land CO, sink (Tian et al. 2016), and anthropogenic N<sub>2</sub>O emissions are

projected to lead to further global warming during the twenty-first century and beyond (Stocker et al. 2013).

In terrestrial ecosystems, N<sub>2</sub>O is mainly produced in soils via nitrification and denitrification processes (Smith and Arah 1990; Wrage et al. 2001; Schmidt et al. 2004). All these processes are regulated by microbial activities under various soil microenvironments such as soil temperature, moisture and aeration, clay content, pH, and carbon (C) and N availability (Firestone and Davidson 1989; Goldberg and Gebauer 2009; Butterbach-Bahl et al. 2013; Brotto et al. 2015; Rowlings et al. 2015). In addition, N<sub>2</sub>O emissions from terrestrial ecosystems can be regulated by both natural disturbances and human management such as synthetic N fertilizer use, manure N application, irrigation, tillage, and the choice of crop varieties (Davidson 2009; Lu and Tian 2007; Rice and Smith 1982; Cai et al. 1997; Ding et al. 2010). However, our understanding of the mechanisms responsible for terrestrial N<sub>2</sub>O emissions is still limited, which contributes to large uncertainties in estimating both preindustrial and contemporary N<sub>2</sub>O emissions. For example, estimates of global terrestrial N<sub>2</sub>O emissions from natural sources vary by up to a factor of 3 and range between 3.3 and 9.0 Tg N yr<sup>-1</sup> (Ciais et al. 2013). Human-induced biogenic N<sub>2</sub>O emissions from the land biosphere have not yet been investigated well (Tian et al. 2016). Therefore, a major international and multidisciplinary effort is required to assess information from different research disciplines and approaches in order to constrain current knowledge on the  $\rm N_2O$  budget and drivers and to identify research gaps.

Process-based modeling is an essential tool in assessing and predicting the terrestrial N cycle and N<sub>2</sub>O fluxes in response to multifactor global changes. Several process-based models have been used to estimate N<sub>2</sub>O emissions from natural and agricultural soils at various spatiotemporal scales. The conceptual model of "hole in the pipe" (Firestone and Davidson 1989) was first incorporated in the Carnegie-Ames-Stanford Approach (CASA) biosphere model (Potter et al. 1993) to estimate N trace gas emissions at the global scale (Potter et al. 1996). The daily version of the CENTURY model (DAYCENT) was linked to atmospheric models to better estimate N<sub>2</sub>O fluxes from different ecosystems (Parton et al. 1998). The Denitrification Decomposition Model (DNDC; Li et al. 1992) was developed to study the impacts of various agricultural practices on N<sub>2</sub>O emissions. In the Dynamic Land Ecosystem Model (DLEM), Tian et al. (2011, 2015) considered the biotic and abiotic processes (e.g., plant N uptake and N leaching loss)

that regulate N<sub>2</sub>O fluxes in natural and managed soils. In recent years, multiple C-N coupled models, such as Dynamic Nitrogen–Lund–Potsdam–Jena (DyN-LPJ; Xu-Ri and Prentice 2008), Organizing Carbon and Hydrology in Dynamic Ecosystems (ORCHIDEE) with N cycle (O-CN; Zaehle and Friend 2010, 2011), Land Surface Processes and Exchanges Model of the University of Bern (LPX-Bern 1.0; Stocker et al. 2013), Community Land Model with prognostic carbon and nitrogen (CLMCN)-N2O (Saikawa et al. 2014), and Land Model 3V-N (LM3V-N; Huang and Gerber 2015) have been developed by integrating a prognostic N cycle into different land surface models and simulate N<sub>2</sub>O emissions from land ecosystems. Unsurprisingly, these models generated divergent estimates of global terrestrial N<sub>2</sub>O budgets and spatiotemporal patterns mainly owing to differences in model input datasets, model structure, and parameterization schemes. What are the major contributing factors responsible for the changing patterns of terrestrial N<sub>2</sub>O emissions? How can we narrow down the model-estimated bias or uncertainties? What are the knowledge gaps in fully accounting for the N<sub>2</sub>O processes? Here, we attempt to answer these questions through the establishment and designing of the global N<sub>2</sub>O Model Intercomparison Project (NMIP).

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During the past two decades, carbon-related model intercomparison projects (MIPs) have been established to evaluate model uncertainties in simulating the terrestrial carbon dynamics. For example, the Vegetation-Ecosystem Modeling and Analysis Project (VEMAP) was a pioneer MIP activity, driven by a common model input database, and was established to provide multimodel ensemble estimates of carbon fluxes and storage in response to changing climate and atmospheric CO<sub>2</sub> (Melillo et al. 1995; Schimel et al. 2000). More recently, a number of CO<sub>2</sub>-oriented MIPs and synthesis activities were implemented, such as the North American Carbon Program site and regional synthesis (NACP; Schwalm et al. 2010; Richardson et al. 2012; Schaefer et al. 2012) and its extended Multi-Scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP; Huntzinger et al. 2013; Wei et al. 2014), the Trends and Drivers of the Regional Scale Sources and Sinks of Carbon Dioxide (TRENDY) Project (Le Quéré et al. 2016; Sitch et al. 2015), the Inter-Sectoral Impact Model Intercomparison Project (ISI-MIP; Warszawski et al. 2014; Ito et al. 2016), and the Multi-Model Data Synthesis of Terrestrial Carbon Cycles in Asia (Asia-MIP; Ichii et al. 2013). These MIPs enhanced our understanding of model uncertainties and provided insight into future directions of model improvement.

Following the CO<sub>2</sub>-related MIPs, global methane (CH<sub>4</sub>) MIPs and synthesis activities were implemented in recent years, for example, the Wetland and Wetland CH<sub>4</sub> Intercomparison of Models Project

(WETCHIMP; Melton et al. 2013; Wania et al. 2013) and Global Carbon Project (GCP) global CH budget synthesis (Saunois et al. 2016; Poulter et al. 2017). Although terrestrial biogenic N<sub>2</sub>O emissions significantly contribute to climate warming, the model development for simulating N cycle and N2O fluxes remains far behind the CO<sub>2</sub>- and CH<sub>4</sub>-related activities. The relatively sparse and short-term observations limited our understanding of N cycling in terrestrial ecosystems. Comparing with CO, and CH<sub>4</sub>, lower N<sub>2</sub>O concentration in the atmosphere and the varying magnitudes of soil N<sub>2</sub>O emissions across observation sites and periods make it more difficult to quantify the N<sub>2</sub>O budget at a large scale. Another important uncertainty comes from the differences in model representation and parameterization schemes of N processes and the influence of biophysical and environmental factors on N<sub>2</sub>O dynamics (see appendix). Similar to the purposes of the CO<sub>2</sub>- and CH<sub>4</sub>-related MIPs, there is a need to initialize an MIP for the N models to assess the global N<sub>2</sub>O budget. Under the umbrella of the GCP and the International Nitrogen Initiative (INI), we initiated the NMIP to investigate the uncertainty sources in N<sub>2</sub>O estimates and provide multimodel N<sub>2</sub>O emissions estimates from natural and agricultural soils. This paper describes the detailed NMIP protocol, input data, model structure, and some preliminary simulation results.

THE NMIP FRAMEWORK, OBJECTIVES, AND TASKS. Motivated by large uncertainties

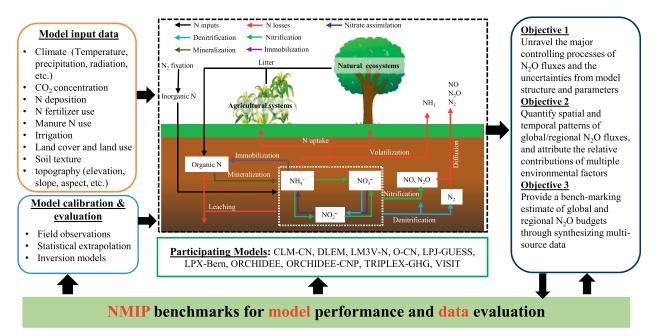


Fig. I. The framework of NMIP.

and increasing data availability, the NMIP is developed to establish a research network for providing a multimodel ensemble estimate on the global/regional  $\rm N_2O$  budgets and to identify major uncertainties associated with model structure, parameters, and input data (Fig. 1). This project was first proposed at the Regional Carbon Cycle Assessment and Processes (RECCAP) workshop, the Fourth International Workshop on Asian Greenhouse Gases, by JAMSTEC, in Yokohama, Japan, 8–10 April 2014. The NMIP was launched at a side meeting during the 2015 American Geophysical Union Fall Meeting and began work in the fall of 2016.

Specific objectives of NMIP are to 1) unravel the major N cycling processes controlling N2O fluxes in each model and identify the uncertainty sources from modeling structure, input data, and parameters; 2) quantify the magnitude and spatial and temporal patterns of global and regional N2O fluxes during 1860-2015 and attribute the relative contributions of multiple environmental factors to N2O dynamics; and 3) provide a benchmark estimate of global/ regional N<sub>2</sub>O fluxes through synthesizing the multimodel simulation results and existing estimates from ground-based observations, inventories, and statistical/empirical extrapolations. To achieve these objectives, the NMIP group members have collectively developed a model simulation protocol as outlined in Fig. 1.

There are five key tasks or progressing stages in the protocol: 1) development and delivery of spatiotemporal model driving forces; 2) individual model calibration and evaluation; 3) model simulations and delivery of results; 4) quality control and analysis of model results; and 5) synthesis and uncertainty analysis.

KEY MODEL INPUT DATASETS. To minimize the uncertainty that results from input datasets, the NMIP provided consistent model driving datasets for all modeling groups. The datasets include potential vegetation, climate, atmospheric CO<sub>2</sub> concentration, atmospheric N deposition, synthetic N fertilizer applications in cropland and pasture, manure N production and applications in cropland and pasture, and historical distribution of cropland at a spatial resolution of 0.5° by 0.5° latitude–longitude (Table 1). Half-degree resolution is appropriate for studies at a global scale, considering that most of the model input data are available and many previous MIPs at a global scale were conducted at this resolution. Here we briefly describe these input datasets and their sources.

Climate. Climatic Research Unit–National Centers for Environmental Prediction (CRU–NCEP) climate version 7 is a fusion of the CRU and NCEP–NCAR reanalysis climate datasets between 1901 and 2015, which was reconstructed by the Laboratoire des Sciences du Climat et l'Environnement, Paris, France (https://vesg.ipsl.upmc.fr). Major climate variables include longwave and shortwave radiation, air pressure, humidity, temperature, precipitation, and wind speed at 6-hourly temporal resolution. Monthly magnitude of climate variables in the CRU–NCEP dataset was

TABLE I. Summary of the NMIP driving forces. Note that detailed descriptions of the major NMIP model input datasets have been provided in previous publications or online documents. Here we only provide a brief description of sources and spatiotemporal patterns of these datasets.

Data name	Period	Temporal resolution	Spatial resolution	Sources	Variables
Climate	1901–2015	6-hourly	0.5°	CRU-NCEP	Incoming longwave/shortwave radiation, air humidity, pressure, precipitation, temperature, and wind speed
CO <sub>2</sub>	1860–2015	Monthly	0.5°	NCAR	CO <sub>2</sub> concentration
N deposition	1860–2015	Yearly	0.5°	Eyring et al. (2013)	NH <sub>x</sub> -N and NO <sub>y</sub> -N deposition
N fertilizer use	1860–2014	Yearly	0.5°	Lu and Tian (2017)	N fertilizer use rate in cropland
Manure N input	1860–2014	Yearly	0.5°	B. Zhang et al. (2017)	Manure N production
Potential vegetation	One time	One time	0.5°	SYNMAP	Fraction of natural vegetation types
Cropland	1860–2015	Yearly	0.5°	HYDE 3.2	Cropland fraction

forced to be consistent with the observation-based CRU datasets.

Atmospheric CO<sub>2</sub>. Monthly atmospheric CO<sub>2</sub> concentration from 1860 to 2015 was obtained from the NOAA GLOBALVIEW-CO<sub>2</sub> dataset derived from atmospheric and ice core measurements (www.esrl.noaa.gov).

Vegetation. Potential vegetation map was acquired from the Synergetic Land Cover Product (SYNMAP; ftp://ftp.bgc-jena.mpg.de/pub/outgoing/mjung /SYNMAP/), which merged multiple global-satellite land-cover maps into a desired classification approach (Jung et al. 2006). Each 0.5° grid cell includes the area fractions for a maximum of 47 land-cover types. Vegetation in SYNMAP is classified according to its life form, leaf type, and leaf longevity. Barren ground, permanent snow, and ice are also included in this dataset. Based on this SYNMAP dataset, participating model groups could create vegetated land fraction and reorganize the vegetation types to generate the corresponding plant functional type and fractions for their models. Annual cropland area from 1860 to 2015 was acquired from the History Database of the Global Environment, version 3.2 (HYDE 3.2), datasets (ftp://ftp.pbl.nl/hyde/), which reconstructed time-dependent land use by historical population and allocation algorithms with weighting maps (Klein Goldewijk et al. 2017). This dataset shows that global cropland area increased from 5.9 million km<sup>2</sup> in 1850 to 15.2 million km2 in 2015.

Atmospheric N deposition onto land surface. The monthly atmospheric N depositions (NH<sub>2</sub>-N and NO,-N) during 1860-2014 were from the International Global Atmospheric Chemistry (IGAC)/Stratospheric Processes and Their Role in Climate (SPARC) Chemistry-Climate Model Initiative (CCMI) N deposition fields. CCMI models explicitly considered N emissions from natural biogenic sources, lightning, anthropogenic and biofuel sources, and biomass burning (Eyring et al. 2013). The transport of N gases was simulated by the chemical transport module in CCMI models. These data were recommended by the Coupled Model Intercomparison Project (CMIP) and used as the official products for CMIP6 models that lack interactive chemistry components (https://blogs.reading.ac.uk/ccmi /forcing-databases-in-support-of-cmip6/).

N fertilizer application. Spatially explicit synthetic N fertilizer use data were specifically developed

in this project. We reconstructed the annual synthetic/mineral N fertilizer dataset from 1960 to 2014 for the global cropland, matched with HYDE 3.2 cropland distribution maps (Lu and Tian 2017; https://doi.pangaea.de/10.1594 /PANGAEA.863323). Data on national-level cropspecific fertilizer use amount were collected from the International Fertilizer Industry Association (IFA) and the Food and Agriculture Organization of the United Nations (FAO). This N fertilizer dataset shows that the global total N fertilizer consumption increased from 11 Tg N yr<sup>-1</sup> in 1960 to 110 Tg N yr<sup>-1</sup> in 2014, and N fertilizer use rate per unit cropland area increased by about 8 times over this period. N fertilizer application rate before 1960 was linearly reduced to the zero in the 1900s.

Manure N production and application. Gridded annual manure N production in the period of 1860-2014 was developed by integrating the Global Livestock Impact Mapping System (GLIMS), the countrylevel livestock population from FAO, and N excretion rates of different livestock categories according to Intergovernmental Panel on Climate Change (IPCC) 2006 Tier I (B. Zhang et al. 2017; https://doi .org/10.1594/PANGAEA.871980). This annual dataset shows that manure N production increased by more than 6 times from 21 Tg N yr<sup>-1</sup> in 1860 to 131 Tg N yr<sup>-1</sup> in 2014, and the application rate of manure N to cropland is less than 20% of the total production. In this project, we consider the manure N application in cropland and pasture area. Manure N production and application rates in 2015 were assumed to be same as that in 2014.

All the input datasets were delivered to the modeling groups in Network Common Data Form (netCDF). To fit with individual modeling requirements for input datasets, the modeling groups could either use a subset of these datasets or add some additional datasets. For example, the participating model DLEM used all these environmental factors as inputs, while the model O-CN did not use manure N as an input. (See Table 3 for model input requirements in each model.) Figure 2 illustrates the interannual variations of the major input datasets at the global level during different available time periods. Figure 3 shows the spatial patterns of atmospheric N deposition, N fertilizer use, and manure N production in 1860, 1900, 1950, and 2015.

MODEL RESULT BENCHMARKING AND EVALUATION. Except for bottom-up model

simulations, the NMIP also plans to synthesize multiple sources of terrestrial soil N<sub>2</sub>O emission data to provide a benchmark for evaluating model estimates. Four types of data will be collected or developed to serve as a potential benchmark: 1) site-level N cycling processes and N<sub>2</sub>O emission measurements through chamber or eddy-flux tower across biomes; 2) N<sub>2</sub>O flux measurement data from a national or global based measurement network [e.g., Long-Term Ecological Research Network, Long-Term Agroecosystem Research Network, Greenhouse Gas Reduction through Agriculture Carbon Enhancement Network, or the N<sub>2</sub>O Network (www.n2o.net .au)]; 3) other spatialized datasets, including statistical extrapolation (e.g., Xu et al. 2008; Kurokawa

et al. 2013; Zhuang et al. 2012); 4)  $\rm N_2O$  fluxes from other-than-terrestrial ecosystem sources to allow for a global budget (industrial, combustion, waste water and water bodies, and marine and oceanic sources) (e.g., Battaglia and Joos 2018; Davidson and Kanter 2014; Galloway et al. 2004; Fowler et al. 2013; Winiwarter et al. 2017); and 5) atmospheric inversions (e.g., Saikawa et al. 2014; Thompson et al. 2014) in conjunction with atmospheric  $\rm N_2O$  measurements from tall towers. We also call for more observation-derived studies to provide regional and global  $\rm N_2O$  emission estimates through advanced computational techniques, such as machine learning, multitree ensemble (MTE), and remote sensing products. We anticipate that through multiple constraints, a process-based

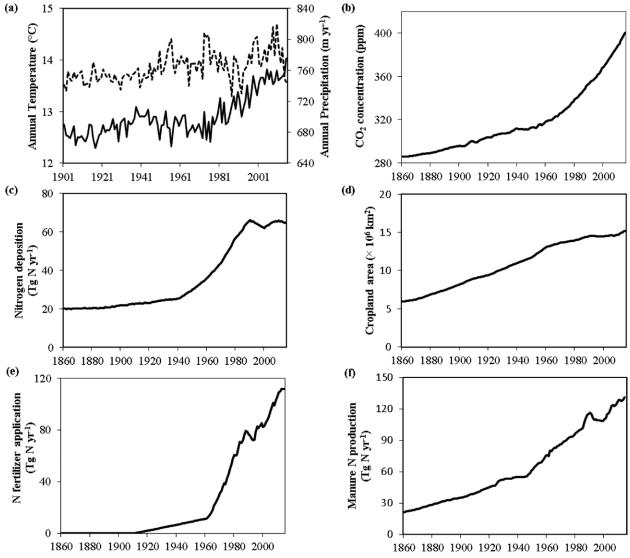


Fig. 2. Evolution of the major driving factors at the global level during 1901–2016. (a) Annual temperature (°C; solid line) and annual precipitation (mm; dashed line), (b) atmospheric CO<sub>2</sub> concentration (ppm), (c) N deposition (Tg N yr<sup>-1</sup>), (d) cropland area (million km<sup>2</sup>), (e) N fertilizer application (Tg N yr<sup>-1</sup>), and (f) manure N production (Tg N yr<sup>-1</sup>).

modeling approach can be more effective and reliable in estimating magnitude and spatial and temporal patterns of terrestrial  $\rm N_2O$  emissions and quantifying relative contributions of environmental drivers to  $\rm N_2O$  dynamics.

MAJOR CHARACTERISTICS OF PARTICI-**PATING MODELS.** The N cycle in the Earth system involves complex biogeochemical processes, in which N is transformed into various chemical forms and circulates among the atmosphere, terrestrial, and aquatic ecosystems. Important terrestrial processes in the N cycle include biological N fixation (BNF), mineralization (conversion of organic N to inorganic N during the processes of organic matter decomposition), immobilization (transformation of soil inorganic N to organic N), volatilization (transformation of soil ammonium N to ammonia gas), nitrification (transformation of ammonium N to nitrate and nitrite N), denitrification (the process of nitrate/nitrite reduction by microbial activities), plant uptake from soil, resorption by living plant organs, adsorption and desorption by

soil mineral particles, and N leaching from soil to aquatic systems. The modeled N processes include N transformation between organic and inorganic forms and movements among atmosphere, vegetation, soil, and riverine systems. Although N processes are tightly coupled with carbon processes in soil and vegetation, the greater variability in N processes compared to C processes makes it more difficult to simulate N cycling. At the current stage, the NMIP has included 10 ecosystem models with explicit terrestrial N cycling processes (Table 2; Fig. 1). Nine models [DLEM, LM3V-N, ORCHIDEE, ORCHIDEE with nitrogen and phosphorous cycles (ORCHIDEE-CNP), O-CN, Lund-Potsdam-Jena General Ecosystem Simulator (LPJ-GUESS), LPX-Bern, TRIPLEX-GHG, and vegetation-integrated simulator for trace gases (VISIT)] are capable of simulating N<sub>2</sub>O emissions from both natural and agriculture ecosystems, while one model (CLM-CN) only simulates N2O emissions from natural vegetation. The biophysical processes (such as canopy structure, albedo, and evapotranspiration), biogeochemical processes (such as decomposition and denitrification), and N input

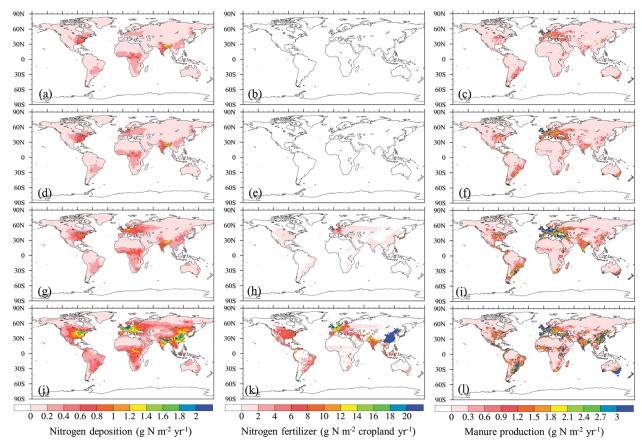


Fig. 3. Spatial distribution of (a),(d),(g),(j) N deposition (g N m<sup>-2</sup> yr<sup>-1</sup>); (b),(e),(h),(k) N fertilizer application (g N m<sup>-2</sup> cropland yr<sup>-1</sup>); and (c),(f),(i),(l) manure N production (g N m<sup>-2</sup> yr<sup>-1</sup>) in (first row) 1860, (second row) 1900, (third row) 1950, and (fourth row) 2015.

for cropland are significantly different from those for natural vegetation. For example, temperature in cropland was found to be lower than that in natural forest owing to the higher albedo and evapotranspiration (Bonan 2001). These differences could lead to different magnitude and timing of  $\rm N_2O$  emissions from cropland. Therefore, biophysical characteristics and management practices in cropland, such as crop cultivation, fertilizer uses, irrigation, and harvesting, are required to be explicitly represented by the models with crop module.

To assess the uncertainty from model structure, each participating model was asked to complete a detailed survey specifying the modeling mechanisms in exogenous N inputs (e.g., N deposition, synthetic N fertilizer and manure N application, and BNF) and N transformation processes. The summarized survey results are shown in Table 3. In general,  $N_2$ O emissions from soil are regulated at two levels, which are the rates of nitrification and denitrification in the soil and soil physical factors regulating the ratio of  $N_2$ O to other nitrous gases (Davidson et al. 2000).

For N input to land ecosystems, all 10 models considered the atmospheric N deposition and biological fixation, 9 models with a crop  $\rm N_2O$  module included N fertilizer use, but only 6 models considered manure as N input. For vegetation processes, all models included dynamic algorithms in simulating N allocation to different living tissues and vegetation N turnover and simulated plant N

uptake using the "demand and supply–driven" approach. For soil N processes, all 10 models simulated N leaching according to water runoff rate; however, the models differ in representing nitrification and denitrification processes and the impacts of soil chemical and physical factors. The differences in simulating nitrification and denitrification processes are one of the major uncertainties in estimating N<sub>2</sub>O emissions. Algorithms associated with N<sub>2</sub>O emissions in each participating model are briefly described in the appendix.

#### THE NMIP MODEL SIMULATION METHODS AND EXPERIMENTAL

**DESIGNS.** Model initialization. The model simulations were divided into two stages: 1) spinup and 2) transient runs (Fig. 4). During the spinup run, models were driven by the repeated climate data from 1901-20 and by other driving forces in 1860 [i.e., atmospheric CO<sub>2</sub> concentration, N deposition, N fertilizer use, manure N application, and land-cover and land-use change (LCLU)]. The N fertilizer use was assumed to be zero in 1860. Each model group could determine the spinup running years according to the model's specific requirement. For example, the DLEM assumed that a model reaches the equilibrium status when the differences of grid-level C, N, and water stocks were less than 0.5 g C m<sup>-2</sup>, 0.5 g N m<sup>-2</sup>, and 0.5 mm in two consecutive 50 years. When these thresholds were met, the spinup run stopped and the model reached an equilibrium state.

Table 2. Participating models.				
Model	Contact	Affiliation	Citation	
CLM-CN	E. Saikawa	Emory University	Saikawa et al. (2013)	
DLEM	H. Tian	Auburn University	Tian et al. (2015); Xu et al. (2017)	
LM3V-N	S. Gerber	University of Florida	Huang and Gerber (2015)	
LPJ-GUESS	S. Olin/A. Arneth	Lund University, Sweden/Karlsruhe Institute of Technology, Germany	Olin et al. (2015); Xu-Ri and Prentice (2008)	
LPX-Bern	S. Lienert/F. Joos	Institute for Climate and Environmental Physics, University of Bern, Switzerland	Stocker et al. (2013); Xu-Ri and Prentice (2008)	
O-CN	S. Zaehle	Max Planck Institute for Biogeochemistry	Zaehle et al. (2011)	
ORCHIDEE	N. Vuichard	L'Institut Pierre-Simon Laplace—Laboratoire des Sciences du Climat et de l'Environnement (IPSL-LSCE), France	N. Vuichard et al. (2018, unpublished manuscript)	
ORCHIDEE-CNP	J. Chang/D. Goll	IPSL-LSCE, France	Goll et al. 2017	
TRIPLEX-GHG	C. Peng	University of Quebec at Montreal, Canada	Zhu et al. (2014); K. Zhang et al. (2017)	
VISIT	A. Ito	National Institute for Environmental Studies, Japan	Inatomi et al. (2010); Ito and Inatomi (2012)	

TABLE 3. Mode	l characteris	tics in simula	ting major N c)	TABLE 3. Model characteristics in simulating major N cycling processes.	Š					
	CLM-CN	DLEM	LM3V-N	LPJ -GUESS	LPX-Bern	N O	ORCHIDEE	ORCHIDEE- CNP	TRIPLEX- GHG	VISIT
Open N cycle <sup>a</sup>	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
C-N coupling	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
N pools <sup>b</sup>	(13, 3, 4)	(6, 6, 8)	(6, 4, 3)	(5, 6, 11)	(4,3,8)	(9, 6, 9)	(6, 6, 9)	(9, 6, 9)	(3, 9, 4)	(4, 1, 4)
Demand and supply-driven plant N uptake	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
N allocation <sup>c</sup>	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic
Nitrification	f(T, SWC)	f(T, SWC, C <sub>NH4</sub> )	f(T, SWC, C <sub>NH4</sub> )	f(T, SWC, C <sub>NH4</sub> )	f(T, SWC, C <sub>NH4</sub> )	f(T, SWC, pH, C <sub>NH4</sub> )	f(T, SWC, pH, C <sub>NH4</sub> )	f(T, SWC, pH, C <sub>NH4</sub> )	f(pH, C <sub>NH4</sub> , T, SWC)	f(T, SWC, pH, C <sub>NH4</sub> )
Denitrification	f(T, SWC, C <sub>NO3</sub> )	f(T clay, rh, C <sub>NO3</sub> )	f(T <sub>soil</sub> , rh, SWC, C <sub>NH4</sub> , C <sub>NO3</sub>	f(T, rh, SWC, C <sub>NO3</sub> )	f(T, SWC, R <sub>mb</sub> , C <sub>NO3</sub> )	f(T, SWC, pH, R <sub>mb</sub> , C <sub>NO3</sub> )	f(T, SWC, pH, denitrifier, $C_{NO_3}$ )	f(T, SWC, pH, R <sub>mb</sub> , C <sub>NO3</sub> )	f(DOC, C <sub>NO3</sub> , pH, T <sub>soll</sub> )	f(SWC, rh, C <sub>NO3</sub> )
Mineralization, immobilization	f(C:N)	f(C:N)	f(C <sub>NO3</sub> , C <sub>NH4</sub> )	f(C:N)	f(C:N)	f(C:N)	f(C:N)	f(C:N)	f(C:N)	f(C:N)
N leaching	f(runoff)	f(runoff)	f(runoff)	f(runoff)	f(runoff)	f(runoff, clay)	f(runoff)	f(runoff)	f(runoff)	f(runoff)
NH <sub>3</sub> volatilization	f(C <sub>NH4</sub> )	f(pH, T, SWC, C <sub>NH4</sub> )	f(pH, Τ, SWC, C <sub>NH4</sub> )	f(pH, Τ, SWC, C <sub>NH4</sub> )	f(pH, T, SWC, C <sub>NH4</sub> )	f(pH, C <sub>NH4</sub> )	f(рН, С <sub>NН4</sub> )	f(рН, С <sub>ин4</sub> )	f(pH, C <sub>NH4</sub> )	f(pH, T, SWC, C <sub>NH4</sub> )
Plant N turnover <sup>d</sup>	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic	Dynamic
N resorption	f(C:N)	f(C:N)	Fixed	Crop: dynamic, the rest: fixed	$f(N_{lea^f})$	Fixed	$f(N_{leaf})$	Fixed	f(C:N)	Fixed
N fixation	f(NPP)	Fixed	f(C <sub>NH4</sub> , C <sub>NO3</sub> , light, plant demand)	f(ET)	Implied by mass balance	f(C <sub>cost</sub> , C <sub>root</sub> )	f(ET)	f(NPP)	f(biomass)	f(ET)
N fertilizer use	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Manure N use	٥ Z	Yes	Yes	Yes	°Z	°Z	Yes	Yes	°N	Yes
N deposition	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
"Open" denotes that excess N can be leached from the system.	that excess N	can be leached fr	rom the system.							

<sup>&</sup>quot;Open" denotes that excess N can be leached from the system.

<sup>&</sup>lt;sup>b</sup> Numbers of N pools (vegetation pools, litter pools, soil pools).

<sup>&</sup>lt;sup>c</sup> Dynamic denotes time-varied N allocation ratio to different N pools.

d Turnover time for various vegetation nitrogen pools: soil temperature (Τ); soil clay fraction (denoted as clay); evapotranspiration (ΕΤ); vegetation carbon (denoted as biomass); NPP; leaf N concentration (N<sub>[cat</sub>); soil surface and drainage runoff (denoted as runoff); carbon cost during N<sub>2</sub> fixation (C<sub>cost</sub>); SWC; denitrifier: soil denitrifier biomass; soil heterogeneous respiration (rh).

Model simulation experiments. During the transient run, seven experiments were designed to simulate global terrestrial N<sub>2</sub>O emissions. All the model experiments started with the equilibrium carbon, water, and N status in 1860, which is obtained from the spinup run, and transiently ran through the period during 1860-2015 (Fig. 4). For the period of 1860-1900 when CRU-NCEP climate data are not available, the 20-yr average climate data between 1901 and 1920 were used. In the NMIP, we applied the progressively reducing factor experimental scheme (i.e., first experiment includes all factors and then reduce one factor each time; the effect of this factor is equal to the difference between the previous and current experiment) to simulate the impacts of individual environmental factors on N<sub>2</sub>O fluxes. In total, seven experiments (from S0 to S6) were designed (Fig. 4). The S0 reference (baseline) run was designed to track the model internal fluctuation and model drift. The S1 experiment included the temporal variations of all time-varying driving forces. "Best estimates" of N<sub>2</sub>O emissions were acquired from either the S1 experiment (for models considering manure as input) or S2 experiment (for models without considering manure). The overall effect of all environmental factors was calculated as S1 - S0. The effects of manure N use (MANN), N fertilizer use (NFER), N deposition (NDEP), LCLU, atmospheric CO<sub>2</sub> (CO<sub>2</sub>), and climate (CLIM) were calculated as S1 - S2, S2 - S3, S3 - S4, S4 - S5, S5 - S6, and S6 - S0, respectively.

**MODEL OUTPUTS, QUALITY CONTROL, AND DATA AVAILABILITY.** All participating model groups are requested to provide the gridded

simulations of N<sub>2</sub>O fluxes from global terrestrial ecosystems and other relevant variables that can be used for understanding C-N coupling and key N processes simulated by each individual model (Table 4). Modeling groups will submit annual simulation results during 1860-2015 and monthly simulation results during 1980-2015. In addition to modeling estimates of grid-level fluxes and pool sizes, modeling groups will submit biome-level results to facilitate biome-level N<sub>2</sub>O emission analysis and split contributions of global N<sub>2</sub>O dynamics to primary biome types. The model output from each modeling group is sent to the core team led by Dr. Hanqin Tian for data quality checking and preliminary analysis. The quality control is conducted to check if the individual model results are reasonable and to avoid the obvious errors during model simulations. After the quality control process, model output is transferred to a data-sharing website.

The model input and output datasets are made available to all model groups for further analyses. Model input data and model results will be made available to the broader research community once the results of the first NMIP are published. A data-use and authorship policy has been established.

# **RESULT ANALYSIS AND SYNTHESIS.** Based on model results, the NMIP team will provide multimodel ensemble estimates for terrestrial N<sub>2</sub>O fluxes at various scales from country, sector, continental, to global and also assess differences and uncertainties among participating models. Through the seven simulation experiments, the magnitudes and spatiotemporal variations in terrestrial N<sub>2</sub>O emissions will

be attributed to changes in different environmental factors at both regional and global scales. The global and regional N<sub>2</sub>O flux data derived from other sources, including atmospheric inversion, statistical extrapolation, and inventory approaches [e.g., the N<sub>2</sub>O emission data collected in Tian et al. (2016)], will be compared and integrated with the NMIP modeled results. Through these syntheses and evaluations of modeled versus fieldobserved N<sub>2</sub>O dynamics, we will further identify the

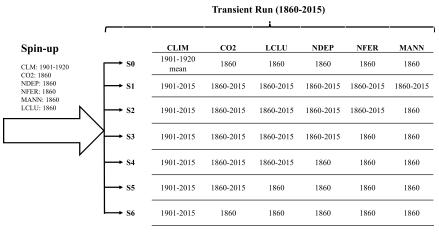


Fig. 4. Model simulation experimental designs [S0, reference (baseline); S1, climate (CLIM) +  $CO_2$  + LCLU + NDEP + NFER + MANN; S2, CLIM +  $CO_2$  + LCLU + NDEP + NFER; S3, CLIM +  $CO_2$  + LCLU + NDEP; S4, CLIM +  $CO_2$  + LCLU; S5, CLIM +  $CO_2$ ; S6, CLIM).  $CO_2$  refers to atmospheric  $CO_2$ .

TABLE 4. List of nitrogen and carbon variables provided by NMIP models.				
Name of variables	Unit	Frequency		
Nitrogen fluxes				
N <sub>2</sub> O flux, biological N fixation, plant N uptake (sum of ammonium and nitrate), net N mineralization, nitrification rate, denitrification rate, N leaching (Dissolved Inorganic Nitrogen, Dissolved Organic Nitrogen, Particulate Organic Nitrogen, or total N leaching), NH <sub>3</sub> volatilization	kg N m $^{-2}$ s $^{-1}$	Monthly (1980–2015) Annual (1860–2015)		
Nitrogen pools				
N in vegetation, N in above-ground litter pool, N in soil (including below-ground litter), N in products pools	$kg N m^{-2}$	Annual (1860–2015)		
Carbon fluxes				
Gross primary production, autotrophic (plant) respiration, net primary production, heterotrophic respiration	kg C $\mathrm{m}^{-2}$ $\mathrm{s}^{-1}$	Monthly (1980–2015) Annual (1860–2015)		
Carbon pools				
C in vegetation, C in above-ground litter pool, C in soil (including below-ground litter), C in products pools, C in vegetation	kg C m <sup>-2</sup>	Annual (1860–2015)		

gaps in our understanding to estimate  $N_2O$  fluxes and put forward potential strategies to improve the models. In the following sections, we provide an initial analysis of simulated terrestrial  $N_2O$  emissions from the three models (DLEM, O-CN, and VISIT) that simulate both natural and agricultural emissions.

As indicated by the model ensemble, the global N<sub>2</sub>O emission has significantly increased, especially since the 1960s with more rapidly rising exogenous N inputs to terrestrial ecosystems (Fig. 5). Natural soils were the largest source across the entire period. Cropland is the single largest contributor to the increasing trend in N<sub>2</sub>O emissions during 1860–2015. Despite the same input datasets, the interannual variations among the three models were different because of the differences in model structure and parameters. The estimated N<sub>2</sub>O emissions from VISIT were consistently higher than those from the other two models during 1860–2015; N<sub>2</sub>O emissions from DLEM and O-CN were similar in magnitude. The increasing trends of N<sub>2</sub>O emissions before the end of the 1960s were similar among the three models, while the largest increasing trend was found from O-CN, followed by DLEM, and the least from VISIT. The ultimate global terrestrial N<sub>2</sub>O budgets, interannual variations, and attributions of the differences among models will be further analyzed in more detail after modeling results from all 10 models are included.

The terrestrial N<sub>2</sub>O emissions showed substantial spatial variations across the global land surface since

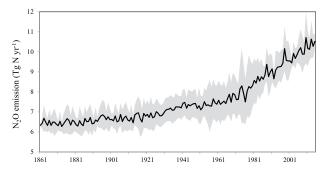


Fig. 5. Long-term trend and variations in  $N_2$ O emissions from global terrestrial ecosystems during 1861–2015 as estimated by the average of three process-based models (DLEM, O-CN, and VISIT). The gray shades denote  $\pm 1$  standard deviation.

1860 (Fig. 6). The highest emission was from the tropical area during all four periods (i.e., the 1860s, 1900s, 1950s, and 2001–15) (Fig. 6), primarily owing to higher soil N transformation rates and soil N contents in tropical ecosystems. The latitudinal distribution patterns were slightly different from the 1860s to 2001–15, showing an increasing importance and the emerging second peak of N<sub>2</sub>O emissions in the temperate climatic zone of the Northern Hemisphere. Temperate regions were another hot spot for N<sub>2</sub>O emissions owing to the high N fertilizer use and N deposition rates in China, India, Europe, and the contiguous United States. Of all 14 examined regions as defined by GCP CH<sub>4</sub> budget synthesis (Saunois

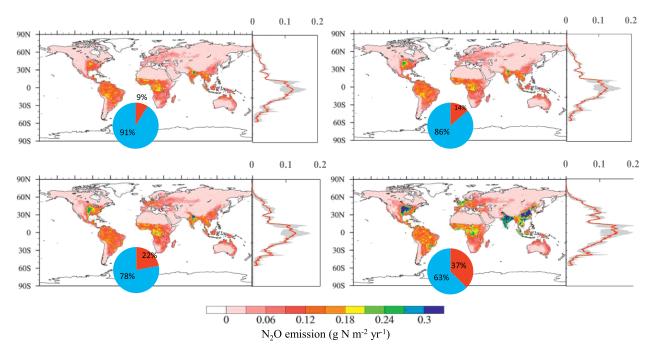


Fig. 6. Spatial patterns and the latitudinal variations of mean annual N<sub>2</sub>O emissions as represented by the mean estimates from DLEM, VISIT, and O-CN models in the (top left) 1860s, (top right) 1900s, (bottom left) 1950s, and (bottom right) 2001–15. The pie charts indicate the relative contributions of natural vegetation (blue) and cropland (red) to the total N<sub>2</sub>O emissions. The gray shades denote ±1 standard deviation.

et al. 2016), tropical South America had the largest N<sub>2</sub>O emissions throughout the study period, contributing to about 20% of the global total emission (Fig. 7). China and the contiguous United States were characterized by the most rapid N<sub>2</sub>O increasing rates increase. In the recent three decades, China, India, and western Europe were the only three regions with higher N<sub>2</sub>O emissions from cropland than that from natural ecosystems. It is noteworthy that the estimated cropland N<sub>2</sub>O emissions in these three regions have large uncertainty ranges due to varied model representation and parameterization methods of the impacts from agricultural management. Larger uncertainty ranges for N<sub>2</sub>O emissions from natural ecosystems were found in Russia, northern Africa, boreal North America, Southeast Asia, and the contiguous United States.

**SUMMARY.** Current assessments of terrestrial  $\rm N_2O$  emission at regional and global scales are subject to large uncertainties. The NMIP is attempting to better identify, and eventually reduce, those uncertainties. The activity was initialized in 2015 and currently includes 10 terrestrial biosphere models with N cycling coupled. NMIP is an open initiative, and other models are invited to join the effort. It aims to provide an improved estimate of global and regional terrestrial  $\rm N_2O$  fluxes as a contribution to the larger GCP global  $\rm N_3O$ 

budget synthesis activity. NMIP is being developed with the capacity to update flux estimates at regular intervals and quantify the uncertainties related to model structure, algorithms, and parameters. The NMIP protocol includes seven simulation experiments to quantify and attribute the contribution of environmental factors to the interannual variation and long-term trend of terrestrial N<sub>2</sub>O emissions. In addition, this project intends to identify our knowledge gaps and bring forward potential strategies for improving the predictive capability of N<sub>2</sub>O models in the future. The data products and ensemble estimates of terrestrial N<sub>2</sub>O emissions will be made available and packaged to be relevant for policy makers and nongovernment entities participating in the climate change issues.

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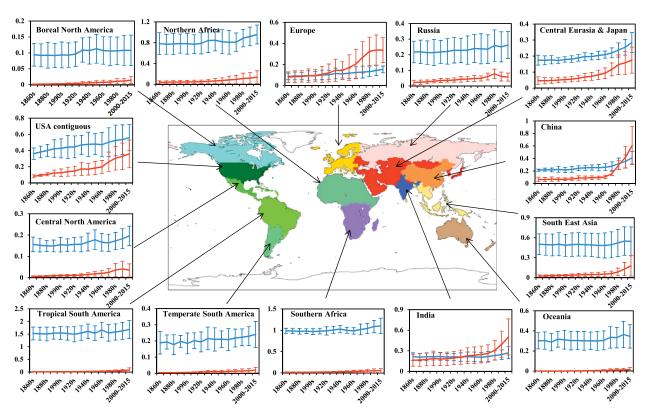


Fig. 7. Decadal N<sub>2</sub>O emissions (Tg N yr<sup>-1</sup>) from the natural ecosystems (blue lines) and cropland (red lines) in 14 regions (region delineation is from the Global Carbon Project global CH<sub>4</sub> budget synthesis; Saunois et al. 2016). N<sub>2</sub>O emissions are represented by the average of DLEM, VISIT, and O-CN model simulations. The error bars denote ±1 standard deviation.

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## APPENDIX: BRIEF DESCRIPTION OF ALGORITHMS ASSOCIATED WITH N<sub>2</sub>O FLUX IN EACH PARTICIPATING MODEL.

CLM-CN- $N_2O$ . CLM-CN- $N_2O$  is based on the DNDC model (Li et al. 1992) implemented in the Community Land Model, version 3.5 (Oleson et al. 2008; Stöckli et al. 2008), with explicit carbon and nitrogen (CN) processes (Thornton et al. 2007; Randerson et al. 2009; Thornton et al. 2009). CLM-CN- $N_2O$  is added to CLM-CN, version 3.5, in a one-way coupling framework and simulates  $N_2O$  emissions during

nitrification and denitrification processes at an hourly time step.

Nitrification  $R_{\text{nit}}$  is temperature and moisture dependent, and N<sub>2</sub>O is computed by the following equation as described in Li et al. (1992):

$$R_{\rm nit} = C_{\rm NH_4} f(\rm T1), \tag{1}$$

where  $C_{\rm NH_4}$  is the NH<sub>4</sub><sup>+</sup>–N content in soil and  $f({\rm T1})$  is the response function of soil temperature to nitrification rate.

Denitrification is also soil temperature and moisture dependent, and it takes place under the anaerobic state. CLM-CN- $N_2O$  specifies the anaerobic state when the water-filled pore space is more than 41.5% in the soil layer. Under this condition,  $N_2O$  is created based on the growth rate of denitrifying bacteria, as well as consumption and assimilation by plants and microbes, following Li et al. (1992). Detailed processes in simulating  $N_2O$  emissions can be found in Saikawa et al. (2013).

DLEM2.0. The nitrogen cycle schemes in DLEM2.0 (Yang et al. 2015; Xu et al. 2017; Pan et al. 2015) are similar as DLEM1.0 (Tian et al. 2010, 2011, 2012; Lu

and Tian 2013; Xu et al. 2012). However, the  $\rm N_2O$  emission schemes in DLEM2.0 (Xu et al. 2017) have been modified based on Chatskikh et al. (2005) and Heinen (2006):

$$R_{\text{nit}} = k_{\text{nit\_max}} f(\text{T1}) f(\text{WFPS}) C_{\text{NH}_4} \text{ and}$$
 (2)

$$R_{\text{den}} = k_{\text{den max}} f(\text{T2}) f(\text{WFPS}) C_{\text{NO}_3}, \tag{3}$$

where  $R_{\rm nit}$  is the daily nitrification rate (g N m<sup>-2</sup> day<sup>-1</sup>);  $R_{\rm den}$  is the daily denitrification rate (g N m<sup>-2</sup> day<sup>-1</sup>);  $f({\rm T1})$  and  $f({\rm T2})$  are the impact function of daily soil temperature on nitrification and denitrification, respectively;  $f({\rm WFPS})$  is the impact function of waterfilled pore space (WFPS) on nitrification, denitrification, and N<sub>2</sub>O diffusion;  $k_{\rm nit\_max}$  is the maximum fraction of NH<sub>4</sub><sup>+</sup>-N that is converted to NO<sub>3</sub><sup>-</sup>-N or gases (0–1);  $k_{\rm den\_max}$  is the maximum fraction of NO<sub>3</sub><sup>-</sup>-N that is converted to gases (0–1); and  $C_{\rm NH_4}$  and  $C_{\rm NO_3}$  are the soil NH<sub>4</sub><sup>+</sup>-N and NO<sub>3</sub><sup>-</sup>-N content (g N m<sup>-2</sup>). N<sub>2</sub>O from denitrification and nitrification processes is calculated as follows:

$$R_{\rm N_2O} = (R_{\rm nit} + R_{\rm den}) f({\rm T3}) [1 - f({\rm WFPS})],$$
 (4)

where  $R_{\rm N_2O}$  is the daily  $\rm N_2O$  emission rate (g N m<sup>-2</sup> day<sup>-1</sup>) and  $f(\rm T3)$  is the impact function of daily soil temperature on  $\rm N_2O$  diffusion rate from soil pores. The calculation methods for these functions and parameters were described in detail in Xu et al. (2017) and Yang et al. (2015).

*LM3V-N*. In LM3V-N, nitrification is proportional to substrate availability (i.e.,  $NH_4^+$ ), modified by functions that account for effects of temperature and WFPS adapted from Parton et al. (1996).

Nitrification-associated  $N_2O$  emission  $R_{nit}$  is evaluated by

$$R_{\text{nit}} = k_{\text{nit base}} f(\text{WFPS}) f(\text{T1}) C_{\text{NH4}} / b_{\text{NH4}}, \tag{5}$$

where  $k_{\text{nit\_base}}$  is the base nitrification rate and  $b_{\text{NH}_4}$  is the buffer parameter for soil NH<sub>4</sub>.

Denitrification is described by a Monod-type equation, where both carbon and nitrate substrate availability can have limiting effects on N gas production following Li et al. (2000). These functions are further modified by temperature (based on Xu-Ri and Prentice 2008) and by WFPS indicating the availability and/or absence of oxygen (adapted from Parton et al. 1996):

$$R_{\text{den}} = k_{\text{den\_base}} f(\text{T2}) f(\text{WFPS}) f_g C_{\text{NO3}} / b_{\text{NO3}}, \quad (6)$$

where  $k_{\rm den\_base}$  is the base denitrification rate,  $f_g$  denotes the impact of labile carbon availability to nitrate on the growth of denitrifies, and  $b_{\rm NO_3}$  is the buffer parameter for soil  ${\rm NO_3}^-$ .

Gaseous losses partitioning between  $NO_x$  and  $N_2O$  during nitrification are parameterized based on air-filled porosity, following Parton et al. (2001). Partitioning between  $N_2O$  and  $N_2$  during denitrification follows the empirical function of Del Grosso et al. (2000), which combines effects of substrate, electron donors (labile C), and water-filled pore space:

$$R_{\rm N_2O} = 0.004 R_{\rm nit} + R_{\rm den} f({\rm WFPS}) f(C_{\rm NO_2}).$$
 (7)

Nitrification and denitrification are treated as fast processes (Shevliakova et al. 2009) and thus updated on subhourly time steps along with updates on soil moisture, soil temperature, and C and N mineralization. Model description including model formulation are detailed in Huang and Gerber (2015).

*LPJ-GUESS*. The nitrogen cycle scheme in LPJ-GUESS is based on CENTURY (Parton et al. 1996) and Xu-Ri and Prentice (2008). Inorganic soil nitrogen pools in the model are ammonium, nitrite, and nitrate. Nitrification occurs only in the dry part of the soil (fractionated using WFPS); the ratio between  $N_2O$  and  $NO_x$  of the gaseous losses in nitrification is based on the moisture content in the soil [f(WFPS)]:

$$R_{\text{nit}} = k_{\text{nit\_max}} f(\text{WFPS}) C_{\text{NH}_4}. \tag{8}$$

Denitrification occurs in the wet part (based on WFPS) of the soil, and the denitrification rate depends on temperature, soil moisture, and labile carbon (approximated with heterotrophic respiration  $_{rh}$ ). Gaseous losses through denitrification result in  $N_2O$ ,  $N_2$ , and  $NO_x$ :

$$R_{\text{den}} = k_{\text{den\_base}} f(\text{T2}) f(\text{WFPS}) f(\text{rh}) C_{\text{NO}_3}.$$
 (9)

The fractionation between the gaseous N species is modeled using soil moisture and temperature. All losses of gaseous N are modeled. Emissions to the atmosphere from these pools are modeled using rate modifiers that are based on the soil moisture and temperature. No retransformation of these gaseous N species is considered. These processes (N-cycling and gaseous N emissions) are modeled in different landuse classes: natural vegetation, pastures/rangelands, and croplands. On croplands, fertilizers are spread as mineral and/or organic N. Mineral fertilizers are considered as an input to the ammonium and nitrate pools at a fixed ratio (50/50) and manure as an input into the organic nitrogen pool with a fixed C:N ratio (currently set to 30).

*LPX-Bern*. The implementation of nitrogen dynamics in LPX-Bern is based on the work of Xu-Ri and Prentice (2008). Nitrogen uptake by plants is governed

by their demand and the availability of nitrogen in two soil pools representing ammonium and nitrate. Nitrogen from deposition and fertilization are added to these inorganic soil pools. Losses include ammonium volatilization and nitrate leaching as well as  $N_2O$  and NO production during nitrification and  $N_2O$ , NO, and  $N_2$  production during denitrification. Aerobic nitrification of ammonium is dependent on soil temperature  $T_{\rm soil}$  and indirectly on soil water content (SWC) owing to the partitioning of wet and dry soil:

$$R_{\text{nit}} = \max_{\text{nit}} f_1(T_{\text{soil}}) C_{\text{NH4,dry}}, \tag{10}$$

where  $\max_{\text{nit}} = 0.92 \text{ day}^{-1}$  is the daily maximum nitrification rate at 20°C.

Anaerobic denitrification of nitrate in wet soil depends on labile carbon availability and soil temperature:

$$R_{\text{den}} = R_{\text{mb}}/(R_{\text{mb}} + K_{\text{mb}}) f_2(T_{\text{soil}}) C_{\text{NO}_3,\text{wet}}$$
 (11)  
 
$$/(C_{\text{NO}_3,\text{wet}} + K_{\text{n}}).$$

The parameters  $K_{\rm mb}$  and  $K_{\rm n}$  are taken from Xu-Ri and Prentice (2008) and  $R_{\rm mb}$  is the microbiotical soil respiration. The amount of nitrogen lost as N<sub>2</sub>O due to nitrification and denitrification is modeled as a function of soil temperature, water content, and the respective process rate.

O-CN. The treatment of inorganic soil nitrogen dynamics in O-CN largely follows Xu-Ri and Prentice (2008). O-CN (Zaehle and Friend 2010) considers N losses to  $\mathrm{NH_3}$  volatilization,  $\mathrm{NO_x}$ ,  $\mathrm{N_2O}$ , and  $\mathrm{N_2}$  production and emission, as well as  $\mathrm{NH_4}$  and  $\mathrm{NO_3}$  leaching. Inorganic nitrogen dynamics in the soil are tightly coupled to plant uptake and net mineralization. The anaerobic volume fraction of the soil is estimated by an empirical function of the fractional soil moisture content (Zaehle et al. 2011). The fraction of ammonium in the aerobic part of the soil is subject to nitrification, according to

$$R_{\text{nit}} = \text{vmax}_{\text{nit}} f(\text{T1}) f(\text{pH1}) C_{\text{NH}}, \qquad (12)$$

where f(pH1) is the soil pH response functions for nitrification (Li et al. 1992; Xu-Ri and Prentice 2008) and vmax<sub>nit</sub> is the maximum daily nitrification rate under 20°C and favorable pH conditions (Xu-Ri and Prentice 2008).

Gross denitrification of the fraction of nitrate under anoxic conditions is modeled as follows:

$$R_{\rm den} = R_{\rm mb}/(R_{\rm mb} + K_{\rm mb})f({\rm T2})f({\rm pH2})C_{{\rm NO}_3}$$
 (13)  
/( $C_{{\rm NO}_3} + K_n$ ),

where f(pH2) is the soil pH response functions for denitrification (Li et al. 1992; Xu-Ri and Prentice

2008),  $R_{\rm mb}$  is the soil microbial respiration rate, and the  $K_{\rm mb}$  and  $K_n$  parameters are taken from Li et al. (1992).

The N<sub>2</sub>O production from nitrification and denitrification is then calculated as follows:

$$R_{\text{N}_{2}\text{O}} = a_{\text{nit}} f(\text{T1}) R_{\text{nit}} + b_{\text{den}} f(\text{T2}) f(\text{pH3}) R_{\text{den}},$$
 (14)

where  $a_{\rm nit}$  and  $b_{\rm denit}$  are fraction loss constants and  $f({\rm pH3})$  is a pH modifier changing the degree of denitrification producing N<sub>2</sub>O versus NO<sub>x</sub> or N<sub>2</sub> (Zaehle et al. 2011). Emissions of volatile compounds are simulated using the empirical emission of Xu-Ri and Prentice (2008).

ORCHIDEE. Modeling of the mineral N dynamics by the ORCHIDEE model originates from the formulations used in the O-CN (Zaehle and Friend 2010). It is composed of five pools for ammonium/ammoniac, nitrate, NO<sub>x</sub>, nitrous oxide, and dinitrogen forms. N<sub>2</sub>O production in both nitrification and denitrification processes are represented.

The potential daily rate of nitrification  $R_{\rm nit}$  occurs only on the aerobic fraction of the soil and is a function of temperature, pH, and ammonium concentration  $C_{\rm NH,:}$ :

$$R_{\text{nit}} = [1 - f(\text{WFPS})] f(\text{T1}) f(\text{pH1}) k_{\text{nit}} C_{\text{NH4}},$$
 (15)

where  $k_{\text{nit}}$  is the reference potential NO $_3^-$  production per mass unit of ammonium.

 $N_2O$  production by nitrification ( $R_{N_2O,nit}$ , g N-N<sub>2</sub>O m<sup>-2</sup> day<sup>-1</sup>) is expressed as a function of the potential daily rate of nitrification ( $R_{nit}$ , g N-NO $_3^-$  m<sup>-2</sup> day<sup>-1</sup>), temperature, and the water content as shown in Zhang et al. (2002):

$$R_{\text{N}_2\text{O,nit}} = f(\text{WFPS}) f(\text{T1}) R_{\text{nit}} p_{\text{N}_2\text{O,nit}}, \qquad (16)$$

where  $p_{\rm N_2O,nit}$  [g N-N<sub>2</sub>O (g N-NO<sub>3</sub>)<sup>-1</sup>] is the reference N<sub>2</sub>O production per mass unit of NO<sub>3</sub> produced by nitrification. The denitrification occurs on the anaerobic fraction of the soil, which is computed as a function of the water-filled porosity [f(WFPS)] and is controlled by temperature, pH, soil NO concentration, and denitrifier microbial activity ( $a_{\rm microb}$ , g m<sup>-2</sup>) (Li et al. 2000):

 $R_{\rm N_2O,den} = f({\rm WFPS}) f({\rm T2}) f({\rm pH}) f({\rm NO}) p_{\rm N_2O,den} a_{\rm microb},$  (17) where  $f({\rm NO})$  is a Michaelis–Menten shape function and  $p_{\rm N_2O,den}$  is the reference N<sub>2</sub>O production per mass unit of denitrifier microbes.

ORCHIDEE-CNP. ORCHIDEE-CNP (Goll et al. 2017) is a version with the implementation of the phosphorus cycle into the nitrogen enabled version of

ORCHIDEE (ORCHIDEE-CN; N. Vuichard et al. 2018, unpublished manuscript). The inorganic soil nitrogen dynamics of ORCHIDEE-CNP includes N2O from both nitrification and denitrification processes following the processes of O-CN (Zaehle et al. 2011). One exception is the BNF. In ORCHIDEE-CNP, BNF is a function of net primary production (NPP; Cleveland et al. 1999) and also regulated by soil mineral N concentration. ORCHIDEE-CNP accounts for influence of phosphorus state of vegetation on tissue nutrient concentrations and phosphatase-mediated biochemical mineralization. Changes in nutrient content (quality) of litter affect the carbon use efficiency of decomposition and in return the nutrient availability to vegetation. The model explicitly accounts for root zone depletion of phosphorus as a function of root phosphorus uptake and phosphorus transport from soil to the root surface.

TRIPLEX-GHG. The TRIPLEX-GHG model (Zhu et al. 2014; K. Zhang et al. 2017) is designed to simulate N<sub>2</sub>O emissions by coupling major theoretical foundations for processes of nitrification and denitrification reported by Li et al. (2000). Briefly, the nitrification rate is calculated by the Michaelis-Menten function based on the concentration of NH<sub>4</sub>, and microbial activity of nitrifying bacteria is explicitly involved based on simulating their growth and death; denitrification is expressed in a more complex way by taking into account the chain reaction  $(NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2)$ . Each step of denitrification can be regarded as an independent process, but these steps are linked by competition for DOC between specific denitrifiers during each step. A double substrate-based (DOC and NO<sub>x</sub>) Michaelis-Menten equation was adopted to simulate the growth rates of NO<sub>x</sub> denitrifiers (Li et al. 2000). In addition, the effects of different factors, such as soil temperature, soil moisture, and pH, are also considered. The key equations for nitrification are as follows:

$$R_{\text{nit}} = B_{\text{nit}} \frac{R_{\text{max}} C_{\text{NH}_4}}{(6.18 + C_{\text{NH}_4})} \text{pH},$$
 (18)

$$R_{\text{max}} = \text{COE}_{\text{NR}} \times N_p$$
, and (19)

$$F_{\text{N-N-O}} = \text{FMAX}_{\text{N-O}} R_{\text{nit}} f(\text{T1}) f(\text{WFPS}),$$
 (20)

where  $R_{\rm nit}$  is the nitrification rate (kg N m<sup>-2</sup> day<sup>-1</sup>),  $R_{\rm max}$  is the maximum nitrification rate (day<sup>-1</sup>),  $B_{\rm nit}$  is the biomass concentration of nitrifiers (kg C m<sup>-2</sup>), pH is the soil pH, COE<sub>NR</sub> represents the nitrification coefficient,  $N_p$  represents the nitrification potential

(mg N kg<sup>-1</sup> day<sup>-1</sup>), FMAX<sub>N<sub>2</sub>O</sub> is the maximum N<sub>2</sub>O fraction during nitrification (kg N m<sup>-2</sup> day<sup>-1</sup>), and f(T1) and f(WFPS) are the functions of the effects of soil temperature and soil moisture on N<sub>2</sub>O emissions during nitrification, respectively.

The key equations for denitrification are showed as follows:

$$R_{NO_x} = MUE_{NO_x} \frac{[DOC]}{[DOC] + K_c} \frac{[NO_x]}{[NO_x] + K_n}$$
 and (21)

$$F_{\text{ANNOX}} = \text{COE}_{d\text{NO}_x} B_{\text{denit}}$$

$$\left(\frac{R_{\text{NO}_x}}{\text{EFF}_{\text{NO}_x}} + \frac{\text{MAI}_{\text{NO}_x}[\text{NO}_x]}{[\text{N}]}\right) f_{\text{NO}_x}(\text{pH2}) f(\text{T2}), (22)$$

where MUE<sub>NO<sub>r</sub></sub> is the maximum growth rate of NO<sub>x</sub> denitrifiers (h<sup>-1</sup>); [DOC] and [NO<sub>x</sub>] represent the concentrations of DOC (kg C m<sup>-3</sup> h<sup>-1</sup>) and NO<sub>x</sub> (kg N m<sup>-3</sup> h<sup>-1</sup>), respectively, in the anaerobic balloon; and  $K_c$  (kg C m<sup>-3</sup>) and  $K_n$  (kg N m<sup>-3</sup>) are the half saturation value of C and N oxides, respectively. The  $F_{\text{ANNOX}}$  is the consumption rate of NO<sub>x</sub> (kg N m<sup>-3</sup> h<sup>-1</sup>);  $COE_{dNO_x}$  represents the coefficient of  $NO_x$  consumption;  $B_{\text{denit}}$  is the biomass of denitrifiers (kg C m<sup>-3</sup>);  $R_{NO_x}$  is the NO<sub>x</sub> reduction rate (h<sup>-1</sup>); [NO<sub>x</sub>] and [N] are the concentrations of NO<sub>x</sub> and total N, respectively, in the anaerobic balloon (kg N m<sup>-3</sup>); EFF<sub>NO</sub> is the efficiency parameter for NO<sub>x</sub> denitrifiers (kg C kg  $N^{-1}$ ); MAI<sub>NO</sub>, is the maintenance coefficient of NO<sub>x</sub> (h<sup>-1</sup>); and  $f(t)_{\text{denit}}^{x}$  represents the effect of the soil temperature on the denitrification rate during each step.

*VISIT*. The nitrogen cycle scheme of VISIT is composed of three organic soil nitrogen pools (microbe, litter, and humus), two inorganic soil nitrogen pools (ammonium and nitrate), and vegetation pools. Fertilizer is considered as an input to the ammonium and nitrate pools at a fixed ratio and manure as an input into the litter organic nitrogen pool.  $N_2O$  emissions through nitrification and denitrification are estimated using the scheme developed by Parton et al. (1996). Nitrification-associated  $N_2O$  emission  $R_{\rm nit, \, N_2O}$  is evaluated as follows:

$$R_{\text{nit, N,O}} = f(\text{WFPS}) f(\text{pH1}) f(\text{T1}) [K_{\text{max}} + F_{\text{max}} f(\text{NH}_4)],$$
 (23)

where  $K_{\rm max}$  is the soil-specific turnover coefficient,  $F_{\rm max}$  is the parameter of maximum nitrification gas flux, and  $f({\rm NH_4})$  is the effect of soil ammonium on nitrification. Denitrification-associated N<sub>2</sub>O emission  $R_{\rm den,\,N_2O}$  is evaluated by the following equation:

$$R_{\text{den, N}_2\text{O}} = R_{\text{den}} (1 + R_{\text{N}_2/\text{N}_2\text{O}}) \text{ and}$$
 (24)

$$R_{\text{den}} = \min[f(\text{NO}_3)f(\text{CO}_2)] \times f(\text{WFPS}), \quad (25)$$

where  $R_{\rm N_2/N_2O}$  is the fractionation coefficient, which is also a function of WFPS, soil nitrate, and heterotrophic respiration;  $f({\rm NO_3})$  is the maximum denitrification rate in high soil respiration rate condition;  $f({\rm CO_2})$  is the maximum denitrification rate in high  ${\rm NO_3}^-$  levels; and  $f({\rm WFPS})$  is the effect of WFPS on denitrification rate.

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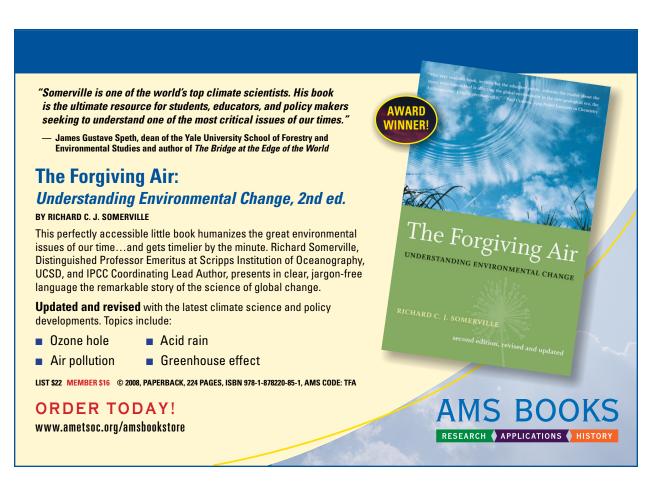
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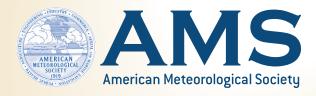
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