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Key Points:
- The development of the new TRIPLEX-GHG model resulted from coupling N_2O-related processes into a DGVM model to simulate N_2O emissions
- The calibration and validation results showed the model can reasonably estimate N_2O emissions from global forests and grasslands
- The model would contribute to the scientific modeling community by accounting for N_2O budgets at both regional and global scales

Supporting Information:
- Supporting Information S1
- Figure S1

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Process-based TRIPLEX-GHG model for simulating N_2O emissions from global forests and grasslands: Model development and evaluation

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Abstract The development of the new process-based TRIPLEX-GHG model derives from the Integrated Biosphere Simulator (IBIS), which couples nitrification and denitrification processes to quantify nitrous oxide (N_2O) emissions from natural forests and grasslands. Sensitivity analysis indicates that the nitrification rate coefficient (COE_{NR}) is the most sensitive parameter to simulate N_2O emissions. Accordingly, we calibrated this parameter using data from 29 global forest sites (across different latitudes) and grassland sites. The average nitrification rate coefficient gradually increases in the order of tropical forest to grassland to temperate forest to boreal forest, and giving means of 0.009, 0.03, 0.04, and 0.09, respectively. This study validated the mean value for each ecosystem at 52 sites globally. Calibration results both indicate the good performance of the model and its suitability in capturing seasonal variation and magnitude of N_2O flux; however, it is limited in modeling N_2O uptake and increments during periods of snowmelt. Additionally, validation results indicate that simulated and observed annual or seasonal N_2O fluxes are highly correlated ($R^2 = 0.75$; $P < 0.01$). Consequently, our results suggest that the model is suitable in simulating N_2O emissions from different forest and grassland land types under varying environmental conditions on a global scale.

1. Introduction

Nitrous oxide (N_2O) is a long-lived trace gas. It reached a level of 325.9 ppb in 2013, which exceeded preindustrial levels (270 ppb) by approximately 21% [*Tarasova et al.*, 2015]. Moreover, its global atmospheric warming potential is greater by a factor of 298 compared to CO_2 [*Ciais et al.*, 2014]. Furthermore, N_2O can also release active chemicals that destroy stratospheric ozone via processes catalyzed by chlorine (Cl) or nitrogen oxides [*Crutzen*, 1970]. Substantial research has focused on the abundance of atmospheric N_2O generated by anthropogenic activities, especially from agricultural activities, such as fertilizer use, animal manure generation, and land cultivation [*Tian et al.*, 2013]. However, emissions from natural soils (~8 Tg N_2O N yr^{-1}) still account for a large proportion (~55–60%) of total land biogenic N_2O sources [*Tian et al.*, 2016], with tropical, temperate, and boreal forest, and grassland ecosystems being the main contributors to global N_2O budgets [*Breuer et al.*, 2000; *Dalal and Allen*, 2008; *Kesik et al.*, 2005; *Merbold et al.*, 2014; *Stange et al.*, 2013].

N_2O primarily derives as an intermediate product of microbial nitrification and denitrification, which are controlled by a variety of factors. Factors within the soil microenvironment, including soil temperature, soil water content, soil pH, and interspecific and intraspecific substrate competition, affect the production and consumption of N_2O by influencing the metabolic activity of microorganisms and plants, soil aeration, and substrate availability and redistribution [*Kiese and Butterbach-Bahl*, 2002; *Luo et al.*, 2013; *Verchot et al.*, 1999]. Under a background of global change, alterations in N_2O emissions are caused by atmospheric nitrogen (N) deposition, global climate change, land use change, and tropospheric O_3 pollution [*Tian et al.*, 2010]. Due to the dynamic and variable characteristics of N_2O emissions, which are caused by a multitude of interactive factors, such emissions have strong spatial and temporal variability. Thus, up-scaling N_2O budgets to global and regional scales is difficult, and current site scale estimations remain highly variable

[*Blagodatsky et al*., 2011; *Butterbach-Bahl et al*., 2013; *Del Grosso et al*., 2005, 2010; *Haas et al*., 2013; *Li et al*., 2005]. Therefore, modeling site scale N_2O emissions is the logical next step in providing global estimates.

A wide variety of methods have been applied to estimate N_2O fluxes, such as statistical extrapolations and process-based models [*Tian et al*., 2016]. Empirical statistical approaches are common tools in estimating N_2O emissions. Large amounts of sampling data methods related to mathematical statistical analyses that consider various environmental factors have been used to estimate N_2O under natural conditions [*Freibauer and Kaltschmitt*, 2003; *Leppelt et al*., 2014]. For the estimation of agricultural N_2O emissions, a well-known model was selected by the Intergovernmental Panel on Climate Change (IPCC), which is regulated by N input and default emission factors [*Stocker et al*., 2013]. However, such approaches become inaccurate or fail at finer spatial or temporal scales because of data limitations, an inability to describe highly complex and interactive microbial processes [*Butterbach-Bahl et al*., 2013], or large uncertainties when default emission factors are applied at a global scale [*Stocker et al*., 2013]. As an alternative, process-based biogeochemical models have been developed in recent decades, providing a useful instrument for estimating N_2O at different temporal and spatial scales. Most of these models have been developed and applied for specific circumstances, and large divergences or limitations may therefore occur when they are used to simulate N_2O emissions [*Tian et al*., 2016]. The DAYCENT (Daily Century) model, developed by *Parton et al*. [1996], has provided reliable simulations of N_2O flux for cropland [*Del Grosso et al*., 2002, 2009] and pasture [*Abdalla et al*., 2010], although the model does not include a description for oxygen diffusion and consumption processes [*Butterbach-Bahl et al*., 2013]. The Carnegie-Ames-Stanford (CASA) Biosphere model, which was first developed by *Potter et al*. [1993], estimates natural soil N_2O flux based on the "hole in pipe model" concept [*Firestone and Davidson*, 1989]. The expanded version of this model has already been used for global N_2O estimates [*Potter et al*., 1996]; however, the nitrification and denitrification modules are primarily conceptually driven, regardless of the level of detail of microbial processes. The ECOSYS model, developed by *Grant* [2001], is capable of simulating N_2O emissions from soils at any temporal or spatial scale via three-dimensional flux equations; however, its application is limited due to relatively large input data requirements and difficult parameterizations [*Chen et al*., 2008]. The Farm ASSEssment Tool (FASSET) model, developed by *Olesen et al*. [2002], accurately predicts year-round N_2O emissions for European countries [*Chatskikh et al*., 2005]; however, it lacks a specific description for denitrification and uses semiempirical functions instead. The Dynamic Land Ecosystem Model (DLEM), developed by *Tian et al*. [2010], has been successfully applied to simulate N_2O flux from terrestrial ecosystems throughout North America, as well as on a global scale [*Tian et al*., 2013]. However, the daily time step of this model may underestimate N_2O emissions because the possibility of high pulses was not taken into account. The DeNitrification-DeComposition (DNDC) model, first described by *Li et al*. [1992], is a rain event-driven process-based model that has been widely used to model N cycling in croplands and grasslands under a range of management practices [*Congreves et al*., 2016; *Cui et al*., 2014; *Giltrap et al*., 2010; *Kröbel et al*., 2011; *Uzoma et al*., 2015]. Beyond applications to agriculture, PnET-N-DNDC was developed for forests, and involves the simultaneous occurrence of oxic and anoxic sites for nitrification and denitrification processes via the concept of a dynamic anaerobic balloon. This model specifically considers the effect of freezing and thawing on soil moisture [*Kiese et al*., 2005; *Li et al*., 2000]; however, its application is limited due to the detailed growth information (e.g., tree density, tree survival rate, and mean tree height) requirements from sample plots [*Miehle et al*., 2006].

Furthermore, dynamic global vegetation models (DGVM) are commonly used to reproduce complex energy, carbon (C), and water dynamics, including vegetation, land surface, soil biogeochemistry, biogeography, and plant physiology and phenology. These models can also reflect the response of vegetation to climate change [*Olofsson and Hickler*, 2008]. Nevertheless, DGVMs do not model coupled C and N dynamics well and do not consider the processes associated with trace N gases [*Xu and Prentice*, 2008]. Therefore, in recent years, N_2O-related processes based on previous studies have been incorporated into DGVMs. The DyN-LPJ model [*Xu and Prentice*, 2008] was developed by coupling the Dynamic Nitrogen scheme (DyN) into the Lund-Potsdam-Jena (LPJ) model and has been applied to simulate N_2O emissions from natural ecosystems globally. The model compensates for the N cycling shortcomings of the LPJ model; however, it is based on simple semiempirical equations that do not consider complex and subsidiary processes (e.g., plant uptake of organic N, alienated nitrate reduction, and anammox processes), and the coupled model is not anticipated to reproduce daily time series of N_2O emissions [*Xu and Prentice*, 2008; *Xu et al*., 2012]. The