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Review

A review on parameterization and uncertainty in modeling greenhouse gas emissions from soil

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A R T I C L E I N F O

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A B S T R A C T

The efficacy of mathematical modeling as a tool for estimating greenhouse gas (GHG) emissions from soil depends on the uncertainty. Systematic evaluation of various sources of uncertainties in GHG emission models is limited. This paper reviews the state-of-the-art knowledge on the parameterization and uncertainty analysis of soil GHG emission models. Major recommendations and conclusions from this work include: (a) uncertainties due to model parameters and structure can be quantified by combining the Bayesian theorem and the Markov Chain Monte Carlo (MCMC) method; (b) uncertainty due to event-based model input may also be assessed by regarding each event as a latent variable; however, the necessity of the simultaneous evaluation of uncertainties from model input, parameters, and structure might be negotiable because strong correlations may exist between input errors and model parameters; (c) uncertainty analysis is essential for a successful model parameterization by reducing both the number of undetermined parameters and the parameter space; and (d) model parameterization (calibration) should be conducted on multiple sites towards multiple objectives. Case studies were presented for comparing the model uncertainties of the denitrification components of four models, DAYCENT, DNDC, ECOSYS, and COMP. The methods discussed in this paper can help to evaluate model uncertainties and performances, and to offer a critical guidance for model selection and parameterization.

Contents

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1. Introduction

Greenhouse gas (GHG) emission has become major concern due to its impact on global warming (Desjardins et al., 2007). The atmospheric concentrations of three particular GHGs, carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O), have kept growing steadily (Haile-Mariam et al., 2008). Although GHGs from agricultural soils account for only 20% of the world's global radiative forcing from CO_2, CH_4, and N_2O (Haile-Mariam et al., 2008), they contribute approximately 52% and 84% of global anthropogenic CH_4 and N_2O emissions, respectively (Smith et al., 2007). Due to the highly temporal and spatial variations in GHG emissions, it is impractical to estimate these emissions only by field measurements. Computer simulation models are effective and supplementary tools that extend quantitative calculations beyond limited observations in time and space. Additionally, computer models can provide scenario analyses and decision supports for policy makers. Comprehensive modeling techniques of the three major GHGs from agroecosystem have been widely developed since the 1970s (Shaffer et al., 2001). CO_2 is released mainly from microbial decay or burning of plant litter and soil organic matter (SOM). N_2O primarily comes from the microbial transformation of nitrogen in soils and manures. Microbial denitrification of fertilizer and biomass burning are considered to contribute significantly to anthropogenic N_2O emissions (IPCC, 2006). CH_4 is generated by the decomposition of SOM under anaerobic conditions, especially by fermentative digestion in ruminant livestock, stored manures and rice grown under flooded conditions (Smith et al., 2008). Emission of GHGs is one of the processes considered in models of carbon and nitrogen dynamics.

Several reviews on models of carbon and nitrogen processes have been published (Chen et al., 2008; Ma and Shaffer, 2001; Smith et al., 1997; Wu and McGechan, 1998). The performances of nine SOM models (RothC, CANDY, DNDC, CENTURY, DAISY, NCSOIL, SOMM, ITE and Verberne) were assessed using 12 datasets from seven long-term experiments (Smith et al., 1997). Models were tested with real experimental datasets after being briefly reviewed. A comparison of the results indicated that no one model was better than the others for all datasets. However, the performance of one group (SOMM, ITE and Verberne) was significantly lower than the other models tested. Differences in model performance were due to the differences in the capacity of model application to certain land use types and the utilization of site-specific calibration (Smith et al., 1997).

Four European soil nitrogen dynamics models were reviewed by Wu and McGechan (1998): SOLIN, ANIMO, DAISY and SUNDIAL. The major processes examined in their review include decomposition, mineralization and immobilization, nitrification and denitrification, and nitrate leaching and uptake by plants. The review also analyzed the response functions of temperature and soil water content. Wu and McGechan's review was informative because the general values of many transformation rate coefficients were compared and listed in the paper.

Chen et al. (2008) conducted a specific review on the development, limitations and applications of N_2O emissions models, and classified them into three categories: laboratory, field and regional/global levels, among which the process-based field scale models (e.g., DNDC and DAYCENT) were the most widely used. Field scale models, taking into account both water dynamics and C–N cycling, served as a link between the laboratory level and regional/global level.

A comprehensive review was presented on carbon and nitrogen processes in nine U.S. soil nitrogen dynamics models: NTRM, NLEAP, RZWQM, CENTURY, CERES, GLEAMS, LEACHM, NCSOIL, and EPIC (Ma and Shaffer, 2001). The review involved the partitioning of surface residue and SOM pools, mineralization and immobilization processes, nitrification and denitrification processes, urea hydrolysis, ammonia volatilization, plant nitrogen uptake, soil horizon differentiation, and parameterization and application of these models. The authors concluded that these nine models were originated from a general understanding of the heterogeneity of SOM and residues, and the mathematical expressions of the models were supported by limited experimental data. Therefore, they were unable to distinguish which method and equation used in the models were better or more reasonable and concluded that the most important feature for a good model was to provide a step-by-step instruction on parameterization.

Previous studies on model comparisons and testing via experimental data indicate that on one hand, in-depth studies via lab and field experiments on the physical, chemical, and biological mechanisms for each process are still needed; on the other hand, significant knowledge gaps exist in the development of reasonable models and the application of appropriate models: (a) limited temporal and spatial experimental data is available for model calibration and verification; (b) multiple processes and complex model structure engender great challenges in model parameterization; and (c) a lack of information on uncertainties from different sources brings difficulty in model selections and applications.

The aforementioned reviews suggest that the performances of most of the models are not significantly different; hence it is crucial for a user to apply a model within its capacity and to select appropriate parameter values. However, one important issue—uncertainty, especially the evaluation method of uncertainty, was seldom mentioned in these reviews and the earlier studies on carbon and nitrogen dynamic models. Uncertainty plays an important role in model parameterization and model assessment (Refsgaard et al., 2007). Usually the uncertainties come from (a) spatial and temporal variability of measured data, including both input data and output data; (b) non-uniqueness of model parameters; (c) interaction among different parameters and various processes; and (d) imperfect model structure (e.g., processes description and equations) (Refsgaard et al., 2007; Thorsen et al., 2001).

This paper focuses on model parameterization and uncertainty and is organized as follows. Section **2** and Section **3** introduced the existing studies on soil GHG emission model parameterization and model uncertainty, respectively. Section **4** addressed the gaps and challenges in model parameterization and uncertainty analysis and proposed the general strategies for model parameterization and a framework for uncertainty assessment. A case study on comparison of four denitrification models from the perspective of uncertainty was subsequently presented in Section **5**.

2. Existing studies on parameterization of soil greenhouse gas emission models

Process-oriented models have led to a better understanding of carbon and nitrogen transformation processes, and resulted in complexity and difficulty in model parameterization. A highly mechanistic-based model might be so complex compared with other models that it is difficult for researchers to use (Chen et al., 2008; Grant, 2001). There are three categories of model parameters controlling carbon and nitrogen processes: (a) experimentally measurable parameters (e.g., weather data, topographic and soil data, management practices); (b) internal parameters that cannot be directly measured (e.g., nitrification/denitrification rate constant); and