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Simulating microbial denitrification with EPIC: Model description and evaluation

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ABSTRACT

Microbial denitrification occurs in anaerobic soil microsites and aquatic environments leading to production of N_2O and N_2 gases, which eventually escape to the atmosphere. Atmospheric concentrations of N_2O have been on the rise since the beginning of the industrial revolution due to large-scale manipulations of the N cycle in managed ecosystems, especially the use of synthetic nitrogenous fertilizer. Here we document and test a microbial denitrification model identified as IMWJ and implemented as a submodel in the EPIC terrestrial ecosystem model. The IMWJ model is resolved on an hourly time step using the concept that C oxidation releases electrons that drive a demand for electron acceptors such as O_2 and oxides of N (NO_3^-, NO_2^-, and N_2O). A spherical diffusion approach is used to describe O_2 transport to microbial surfaces while a cylindrical diffusion method is employed to depict O_2 transport to root surfaces. Oxygen uptake by microbes and roots is described with Michaelis-Menten kinetic equations. If insufficient O_2 is present to accept all electrons generated, the deficit for electron acceptors may be met by oxides of nitrogen, if available. The movement of O_2, CO_2 and N_2O through the soil profile is modeled using the gas transport equation solved on hourly or sub-hourly time steps. Bubbling equations also move N_2O and N_2 through the liquid phase to the soil surface under highly anaerobic conditions. We used results from a 2-yr field experiment conducted in 2007 and 2008 at a field site in southwest Michigan to test the ability of EPIC, with the IMWJ option, to capture the non-linear response of N_2O fluxes as a function of increasing rates of N application to maize [*Zea mays* L.]. Nitrous oxide flux, soil inorganic N, and ancillary data from 2007 were used for EPIC calibration while 2008 data were used for independent model validation. Overall, EPIC reproduced well the timing and magnitude of N_2O fluxes and NO_3^- mass in surficial soil layers after N fertilization. Although similar in magnitude, daily and cumulative simulated N_2O fluxes followed a linear trend instead of the observed exponential trend. Further model testing of EPIC + IMWJ, alone or in ensembles with other models, using data from comprehensive experiments will be essential to discover areas of model improvement and increase the accuracy of N_2O predictions under a wide range of environmental conditions.

1. Introduction

Denitrification is the biological reduction of NO_3^- or NO_2^- to the gases N_2O and N_2 (Saggar et al., 2013; Robertson and Groffman, 2015). Although reduction of NO_3^- to NO_2^- has been reported to occur in oxic environments (Roco et al., 2016) denitrification is

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typically a respiratory process in which NO_3^- (or NO_2^-) replaces oxygen as terminal electron acceptor in facultative anaerobes. Such organisms are capable of extracting energy for their metabolism by coupling oxidation of reduced C or reduced S to reduction of oxides of N (e.g., NO_3^-, NO_2^-) yielding variable proportions of N_2O and N_2 (Conrad, 1996; Saggar et al., 2013). Nitrous oxide is a potent greenhouse gas (Rodhe, 1990) that also depletes the protective layer of stratospheric O_3 (Crutzen, 1970). Atmospheric concentrations of N_2O have been rising since the beginning of the industrial revolution due to large-scale manipulations of the N cycle in managed ecosystems, especially due to use of synthetic nitrogenous fertilizer (Davidson, 2009; Khalil et al., 2002).

Current atmospheric N_2O concentrations of 330 ppb are ~20% larger than those present in the pre-industrial era and during the last decades have been increasing at an annual rate of 0.73 ± 0.03 ppb yr^{-1} (Ciais et al., 2014). Soils produce ~70% of the N_2O flux to the atmosphere mainly through microbial denitrification under anaerobic conditions and, to a lesser extent, through ammonia oxidation and nitrifier denitrification that occur during nitrification under partially anaerobic conditions (Conrad, 1996; Kool et al., 2011; Robertson and Tiedje, 1987; Zhu et al., 2013). Many biophysical factors control the production of N_2O in soils including those directly affected by management such as levels of NO_3^-, O_2 availability, soil water content, and soil temperature (Mosier et al., 1996).

There is a need—and significant potential—to reduce N_2O emissions from managed ecosystems (Khalil et al., 2002; Mosier et al., 1996; Robertson et al., 2000; Smith et al., 2008). Reduced N_2O emissions can be achieved through improved N management by combining organic and inorganic sources, optimizing rate, time, and placement of fertilizer application, and—in some cases—by using nitrification inhibitors (Smith et al., 2008). In order to evaluate N_2O emissions reductions from managed soils, the Intergovernmental Panel on Climate Change (IPCC) has developed a 3-tier approach that includes both direct and indirect emissions of N_2O (De Klein et al., 2006). Following this approach, direct N_2O emissions primarily arise from application of synthetic N fertilizers, organic N amendments, and management of organic soils. In managed soils, indirect N_2O emissions arise from N lost to downwind and downstream ecosystems as NH_3 and NO_x, redeposited as NH_4^+ and NO_3^-, and as N lost via leaching and runoff (Robertson et al., 2013).

The three tiers range in complexity (De Klein et al., 2006). In Tier 1, a fertilizer-based emission factor is used to estimate direct N_2O emissions from managed soils. In Tier 2, more detailed—country specific—emission factors are used to estimate N_2O emissions. Finally, the Tier 3 method is based on modeling or measurement approaches. Process-based field-scale N_2O simulation models are deemed useful in the Tier 3 approach because they can help identify the soil and environmental variables responsible for N_2O emissions and allow for the projection of these N_2O emissions to regional and country scales (Chen et al., 2008). Simulation of N_2O emissions, however, carry uncertainties associated with model structure, model parameterization, accuracy of input data, and resolution of spatial and temporal scales. For example, Nol et al. (2010) used Monte Carlo uncertainty propagation analysis to quantify uncertainties of modeled N_2O emissions caused by model input uncertainty at point and landscape scales. Nitrous oxide emission at landscape scale averaged 20.5 ± 10.7 kg N_2O-N ha^{-1} yr^{-1}, producing a relative uncertainty of 52%. At point scale, the relative error averaged 78%, suggesting that upscaling decreases uncertainty. The results confirmed the influence of spatial scale on the uncertainty of modeled results.

Several terrestrial ecosystem models are available to estimate N_2O emissions from managed and unmanaged ecosystems at site, regional, and national scales. They vary in level of resolution, degree of connection to the C cycle and connection between the biological and physical components of the system being modeled (Chen et al., 2008). Three examples of such models include DNDC (Li et al., 1992, 1996), *ecosys* (Grant et al., 1993a, 1993b; Grant and Pattey, 1999), and DayCent (Del Grosso et al., 2000, 2006; Parton et al., 1996). Comparisons of N_2O dynamics (Frolking et al., 1998; Li et al., 2005) and simulation approaches (Chen et al., 2008) employed by N_2O models emphasize the importance of accurate simulation of soil water content and its appropriate linking with denitrification and N_2O flux.

Modeling soil water dynamics is a strength of the Environmental Policy Integrated Climate (EPIC) terrestrial ecosystem model (Williams et al., 1984). Developed originally to model the relationship between erosion and soil productivity, the EPIC model has evolved into a comprehensive and widely used terrestrial ecosystem model (Williams et al., 2008). Our objectives here are to: (a) document a process-based microbial denitrification submodel implemented in EPIC thus adding to two other empirically-based (EPIC-specific) options to simulate denitrification (Williams, 1990); and, (b) test the new microbial denitrification model for its ability to reproduce experimental data (Hoben et al., 2011) exhibiting a non-linear response of N_2O fluxes to incremental rates of N application.

The process-based microbial denitrification model documented and tested here —IMWJ— quantifies microbial denitrification in soils under O_2-limiting conditions. Daily C oxidation quantified in the C model of EPIC (Izaurralde et al., 2006) releases electrons, which are accepted by O_2 under aerobic conditions. Oxygen uptake by microbes and roots is described with Michaelis-Menten kinetic equations. If O_2 is insufficient, then the deficit for electron acceptors may be met by oxides of N (NO_3^-, NO_2^-, and N_2O). When denitrification occurs, there is an adjustment of C decomposition based on the ratio of actual vs. potential electrons accepted by O_2 and oxides of N. The movement of O_2, CO_2, and N_2O through the soil profile is modeled using the gas transport equation solved with an adaptive variable time step.

2. Description of the denitrification submodel in EPIC

2.1. Conceptual framework and model overview

The version of EPIC containing the denitrification submodel described and tested herein is identified as EPIC1704. The denitrification model presented here is identified as the IMWJ (Izaurralde, McGill, Williams, and Jones) denitrification option in EPIC. The connection between main IMWJ subroutines and relevant EPIC subroutines is shown in Appendix 6.1. Microbial decomposition of soil organic matter and respiration by plant roots results in oxidation of C (Fig. 1). Such oxidation produces electrons, typically carried within the cell as $NADH + H^+$, for which there must be an acceptor to allow decomposition or respiration to produce CO_2. Normally O_2 is the acceptor but in cases of O_2 deficiency electrons are transferred to N in NO_3^- to yield NO_2^- and thence N_2O and N_2 through denitrification as shown in the following equations:

$$5\,CH_2O + 5\,HOH \rightarrow 5\,CO_2 + 20\,H^+ + 20\,e^-$$

$$4\,NO_3^- + 8\,H^+ + 8\,e^- \rightarrow 4\,NO_2^- + 4\,HOH$$

$$4\,NO_2^- + 12\,H^+ + 8\,e^- \rightarrow 2\,N_2O + 6\,HOH$$

$$2\,N_2O + 4\,H^+ + 4\,e^- \rightarrow 2\,N_2 + 2\,HOH$$

Overall: $5\,CH_2O + 4\,NO_3^- + 4\,H^+ \rightarrow 5\,CO_2 + 2\,N_2 + 7\,HOH + \text{energy}$

The potential supply of electrons is calculated based on moisture content and temperature coupled with the nature and supply