



## 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<sub>2</sub>O and N<sub>2</sub> gases, which eventually escape to the atmosphere. Atmospheric concentrations of N<sub>2</sub>O 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<sub>2</sub> and oxides of N (NO<sub>3</sub><sup>-</sup>, NO<sub>2</sub><sup>-</sup>, and N<sub>2</sub>O). A spherical diffusion approach is used to describe O<sub>2</sub> transport to microbial surfaces while a cylindrical diffusion method is employed to depict O<sub>2</sub> transport to root surfaces. Oxygen uptake by microbes and roots is described with Michaelis-Menten kinetic equations. If insufficient O<sub>2</sub> 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<sub>2</sub>, CO<sub>2</sub> and N<sub>2</sub>O through the soil profile is modeled using the gas transport equation solved on hourly or sub-hourly time steps. Bubbling equations also move N<sub>2</sub>O and N<sub>2</sub> 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<sub>2</sub>O 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<sub>2</sub>O fluxes and NO<sub>3</sub><sup>-</sup> mass in surficial soil layers after N fertilization. Although similar in magnitude, daily and cumulative simulated N<sub>2</sub>O 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<sub>2</sub>O predictions under a wide range of environmental conditions.

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### 1. Introduction

Denitrification is the biological reduction of NO<sub>3</sub><sup>-</sup> or NO<sub>2</sub><sup>-</sup> to the gases N<sub>2</sub>O and N<sub>2</sub> (Saggar et al., 2013; Robertson and Groffman, 2015). Although reduction of NO<sub>3</sub><sup>-</sup> to NO<sub>2</sub><sup>-</sup> has been reported to occur in oxic environments (Roco et al., 2016) denitrification is

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typically a respiratory process in which  $\text{NO}_3^-$  (or  $\text{NO}_2^-$ ) 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.,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ) yielding variable proportions of  $\text{N}_2\text{O}$  and  $\text{N}_2$  (Conrad, 1996; Saggart et al., 2013). Nitrous oxide is a potent greenhouse gas (Rodhe, 1990) that also depletes the protective layer of stratospheric  $\text{O}_3$  (Crutzen, 1970). Atmospheric concentrations of  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  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  $0.73 \pm 0.03 \text{ ppb yr}^{-1}$  (Ciais et al., 2014). Soils produce ~70% of the  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  in soils including those directly affected by management such as levels of  $\text{NO}_3^-$ ,  $\text{O}_2$  availability, soil water content, and soil temperature (Mosier et al., 1996).

There is a need—and significant potential—to reduce  $\text{N}_2\text{O}$  emissions from managed ecosystems (Khalil et al., 2002; Mosier et al., 1996; Robertson et al., 2000; Smith et al., 2008). Reduced  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  (De Klein et al., 2006). Following this approach, direct  $\text{N}_2\text{O}$  emissions primarily arise from application of synthetic N fertilizers, organic N amendments, and management of organic soils. In managed soils, indirect  $\text{N}_2\text{O}$  emissions arise from N lost to downwind and downstream ecosystems as  $\text{NH}_3$  and  $\text{NO}_x$ , redeposited as  $\text{NH}_4^+$  and  $\text{NO}_3^-$ , 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  $\text{N}_2\text{O}$  emissions from managed soils. In Tier 2, more detailed—country specific—emission factors are used to estimate  $\text{N}_2\text{O}$  emissions. Finally, the Tier 3 method is based on modeling or measurement approaches. Process-based field-scale  $\text{N}_2\text{O}$  simulation models are deemed useful in the Tier 3 approach because they can help identify the soil and environmental variables responsible for  $\text{N}_2\text{O}$  emissions and allow for the projection of these  $\text{N}_2\text{O}$  emissions to regional and country scales (Chen et al., 2008). Simulation of  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  emissions caused by model input uncertainty at point and landscape scales. Nitrous oxide emission at landscape scale averaged  $20.5 \pm 10.7 \text{ kg N}_2\text{O-N ha}^{-1} \text{ yr}^{-1}$ , 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  $\text{N}_2\text{O}$  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  $\text{N}_2\text{O}$  dynamics (Frolking et al., 1998; Li et al., 2005) and simulation approaches (Chen et al., 2008) employed by  $\text{N}_2\text{O}$  models emphasize the importance of accurate simulation of soil water content and its appropriate linking with denitrification and  $\text{N}_2\text{O}$  flux.

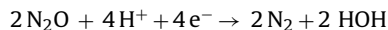
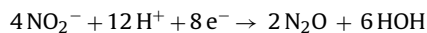
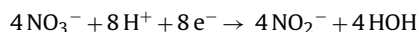
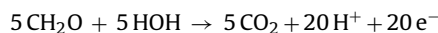
Modeling soil water dynamics is a strength of the Environmental Policy Integrated Climate (EPIC) terrestrial ecosystem model (Williams et al., 1984). Developed originally to model the relationship between erosion and soil productivity, the EPIC model has evolved into a comprehensive and widely used terrestrial 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  $\text{N}_2\text{O}$  fluxes to incremental rates of N application.

The process-based microbial denitrification model documented and tested here —IMWJ— quantifies microbial denitrification in soils under  $\text{O}_2$ -limiting conditions. Daily C oxidation quantified in the C model of EPIC (Izaurralde et al., 2006) releases electrons, which are accepted by  $\text{O}_2$  under aerobic conditions. Oxygen uptake by microbes and roots is described with Michaelis-Menten kinetic equations. If  $\text{O}_2$  is insufficient, then the deficit for electron acceptors may be met by oxides of N ( $\text{NO}_3^-$ ,  $\text{NO}_2^-$ , and  $\text{N}_2\text{O}$ ). When denitrification occurs, there is an adjustment of C decomposition based on the ratio of actual vs. potential electrons accepted by  $\text{O}_2$  and oxides of N. The movement of  $\text{O}_2$ ,  $\text{CO}_2$ , and  $\text{N}_2\text{O}$  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  $\text{NADH} + \text{H}^+$ , for which there must be an acceptor to allow decomposition or respiration to produce  $\text{CO}_2$ . Normally  $\text{O}_2$  is the acceptor but in cases of  $\text{O}_2$  deficiency electrons are transferred to N in  $\text{NO}_3^-$  to yield  $\text{NO}_2^-$  and thence  $\text{N}_2\text{O}$  and  $\text{N}_2$  through denitrification as shown in the following equations:



Overall:  $5 \text{CH}_2\text{O} + 4 \text{NO}_3^- + 4 \text{H}^+ \rightarrow 5 \text{CO}_2 + 2 \text{N}_2 + 7 \text{HOH} + \text{energy}$

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

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