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Nitrogen cycling under urine patches: Model comparison and sensitivity analysis

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Abstract: Agricultural greenhouse gas (GHG) emissions, including nitrous oxide (N_2O), are a major contributor to New Zealand's GHG emissions, and animal excreta deposited onto pastures are a main source of these emissions. Reducing these N_2O emissions requires a better understanding of the factors driving emissions and evaluation of mitigation strategies. Computer simulation models can provide an effective tool for these tasks. We compared two process-based models, APSIM and NZ-DNDC, on results of three experiments on N_2O emissions following urine application to the Horotiu soil in the Waikato region of New Zealand in various seasons and years. Soil ammonium and nitrate concentrations were also determined in the experiments. With default parameter settings, both models predicted the daily pattern of N_2O emissions poorly (Figure 1) with negative model efficiencies. The sensitivity of various model parameters was examined: For APSIM these included the nitrification rate, the optimum soil temperature on nitrification, the fraction of nitrified N emitted as N_2O, the denitrification rate, and the rainfall intensity. For DNDC they were microbial activity, nitrification rate, denitrification rate, plant growth, ammonia volatilisation, rainfall intensity, and fraction of N_2O produced during nitrification were varied. Changing some of the default model parameters improved the model agreement in some cases; e.g. for APSIM when the fraction of nitrified nitrogen emitted as N_2O was increased or the optimum temperature for nitrification was decreased, and for DNDC when microbial activity was decreased or volatilization increased. However, none of the parameters investigated could improve predicted emissions so that they agreed reasonably with all three datasets. A sensitivity analysis which includes more parameters and model functions, as well as changing various parameters simultaneously is needed.

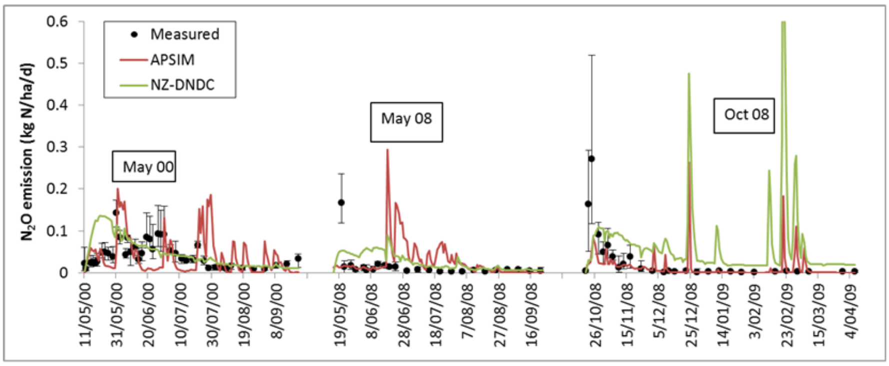

Figure 1. Measured and simulated, based on default parameters, N_2O emissions following urine applications of 500 to 600 kg N/ha at three different times to the Horotiu soil.

Keywords: *APSIM, DNDC, nitrous oxide emissions, soil nitrate and ammonium*

1. INTRODUCTION

Agricultural greenhouse gas (GHG) emissions are a major contributor to New Zealand's total GHG emissions, and nitrous oxide (N_2O) emissions from animal excreta deposited onto pastures are a main source of these emissions. To reduce N_2O emissions better understanding of the factors governing nitrogen (N) cycling and driving N_2O emissions, as well as evaluation of mitigation strategies is required. Various simulation approaches, such as NGAS (Mosier et al., 1983), DAYCENT (Parton et al., 1996), DNDC (Li et al., 1992), and WNMM (Li et al., 2007) have been developed to better understand how environmental conditions combined with management strategies interact to control N cycling and losses (Schmid et al., 2001). These models have, however, often been found to poorly simulate both annual totals and daily rates and patterns of N_2O emissions (Dalal et al., 2003; Wang et al., 1997). Comparing various models (CENTURY, DNDC, CASA, ExpertN) Frolking et al. (1998) concluded that further model inter-comparisons, as well as comparisons to measured data sets, are required to better evaluate the models strengths and advice on future development.

For this study two process-based models, the Agricultural Production Systems sIMulator (APSIM: Keating et al., 2003) and NZ-DNDC, a modified version of DNDC adapted to New Zealand grazed pasture conditions, were chosen for a sensitivity analysis and comparison with data from field experiments. These two models are conceptually different but both simulate the main N processes in the soil leading to N_2O emissions. A more detailed appraisal of the concepts and functions in the two models, including the effect of environmental conditions on N cycling, is given by Vogeler et al. (2012). Here, the models were used to simulate nitrogen cycling, including N_2O emissions, from soils following a urine deposition on to a pasture soil. The two models, APSIM and DNDC, have previously been compared by Giltrap et al (2013) with data from a series of field measurements of N_2O emissions from applications of known amounts of urinary N applied at different times of the year (February, May, August, October) to four different soil types (Horotiu, Te Kowhai, Wingatui, and Otokia), in two regions of New Zealand (Waikato and Otago). The models predicted total N_2O emissions rather poorly over the complete datasets. However, for the emissions the APSIM model performed well in winter while NZ-DNDC performed well on the Otago soils. This suggests that the model functions and/or parameters need to be improved. In that work the model parameters were not altered; that is, only default values were used. The objective of this study was to test the sensitivity of predicted N_2O emissions from both APSIM and DNDC to variations in parameters that affect N_2O emissions from urine patches.

2. METHODS

2.1. Model Setup

APSIM and DNDC runs were setup to simulate N transformations in the soil and N_2O emissions following urine application in three different seasons and years (May 2000, May 2008, October 2008) to the Horotiu soil in the Waikato region of New Zealand. This corresponded with previously conducted experiments designed to evaluate GHG emission factors. The methodology used followed the standard IPCC protocol, the experimental details and associated N_2O emissions have been reported previously (de Klein et al., 2003, 2004; Sherlock et al., 2003a,b; van der Weerden et al., 2011). The sensitivity of the models to the various parameters was examined by varying the parameters' values and comparing the model results to experimental data. Model parameters that were varied, one at a time, included for APSIM: the two parameters of the nitrification rate function (K_{max} and K_{NH4}), the optimum soil temperature for nitrification, the fraction of nitrified N emitted as N_2O ($K_{N2O\text{nit}}$), the denitrification rate (K_{denit}), the curvature of the function for water content effect on denitrification, and the rainfall intensity; and for NZ-DNDC: microbial activity index, nitrification rate, denitrification rate, the fraction of nitrified N emitted as N_2O, rainfall intensity, ammonia volatilization and plant growth (Table1). The simulations were run for one year and the simulation outputs analysed included daily values of soil nitrate and ammonium, as well as N_2O emissions.

2.2. Data Analysis

The models were evaluated with the Nash-Sutcliff efficiency (NSE), also called model efficiency, and several error indices. The NSE compares the model mean square error with the variance of the observations, and its value can vary from -∞ to +1. A positive ME indicates that the model has more predictive power than simply applying the mean observed value. NSE is given by:

$$NSE = 1 - \frac{\sum_{i=1}^{n}(p_i - o_i)^2}{\sum_{i=1}^{n}(o_i - \bar{o})^2}$$

Where o_i is the *i*th observation of the constituent being evaluated, $\bar{o}$ is the mean of the observed data, and p_i is the *i*th simulated value. The error indexes included the percent bias (PBIAS), which is a measure of the average tendency of the simulated data being either larger than their observed counterparts (negative values) or smaller (positive values), with an optimum value of zero. PBIAS is calculated by:

$$PBIAS = \frac{\frac{1}{n}\sum_{i=1}^{n}(o_i - p_i)}{\bar{o}} \times 100$$

The other measure was the standard deviation ratio (RSR), which is a measure that scales the RMSE (root mean square error) to the observed standard deviation (Moriasi et al., 2007), and varies from zero, for perfect model simulation, to large positive values. The RSR is given by:

$$RSR = \frac{RMSE}{STDEV_o} = \frac{\sqrt{\sum_{i=1}^{n}(o_i - p_i)^2}}{\sqrt{\sum_{i=1}^{n}(o_i - \bar{o})^2}}$$

In addition to assessing the model performance using daily values, we also assessed the model performance for estimating N_2O emissions cumulative over 7 days. For the measured data the weekly cumulative value were found by linear interpolation of measured values (Li et al., 2011).

Table 1. Decreased, default and increased values of APSIM and DNDC parameters in sensitivity analysis

				Parameter values		
	Parameter name	Abbrev.	Unit	Decrease	Default	Increase
APSIM	Maximum nitrification rate	K_{max}	mg/kg/d	30	40	50
	NH_4 concentration for half the maximum response to [NH_4]	K_{NH4}	K_{NH4}	40	90	140
	Optimum temperature for nitrification	T_{opt}	°C	20	32	40
	Denitrification rate	K_{denit}		0.0001	0.0006	0.001
	Denitrification water function shape	WFS_{denit}	-	concave	linear	Convex
	Rainfall intensity	RFI	mm/h	3	unifor m	5
	Fraction of N_2O produced during nitrification	$K_{N2O\mathrm{nit}}$	-	0.001	0.002	0.005
DNDC	Microbial activity	MA	-	0.1 & 0.5	1	
	Nitrification rate	*Nitr.*		0.1	1	10
	Denitrification rate	*Denit.*		0.1	1	10
	Fraction of N_2O produced during nitrification	N_2O_{nit}	-	0.001	0.02	0.05
	Rainfall intensity	RFI	mm/h	1&2	5	10
	Ammonia volatilization	NH_3		0.005	0.025	0.1
	Plant growth	PG	-		1	2 & 5

3. RESULTS

3.1. Model Data comparison – default model parameters

Measured values of NH_4^+ (0-75mm) and NO_3^- (0-75 mm) concentrations in the soil compared reasonably well with APSIM and NZ-DNDC simulated values for two of the three datasets (Figure 2). Soil NH_4 and NO_3 concentrations were, in general, well predicted by APSIM, apart from the NO_3 in the October 2008 dataset. The NSE values for were all positive (data not shown) and the RSR below 1, there was no clear trend with regard to over or underestimation, with PBIAS values oscillating from positive and negative between different days. For the DNDC model the agreement with experimental data was also good for the two May datasets (Figure 2). The NSE was positive for the both mineral N forms, and for the NO_3 for the May 08 dataset close to 1, indicating very good model performance. Similarly the RSR values for NH_4 and NO_3 were below 1 for the two May datasets but higher for the October dataset. In general, both NH_4 and NO_3 concentrations in the soil were overestimated by DNDC, suggesting either too little movement of these solutes in the soil, too little plant uptake, or too little N loss via volatilization after urine application.

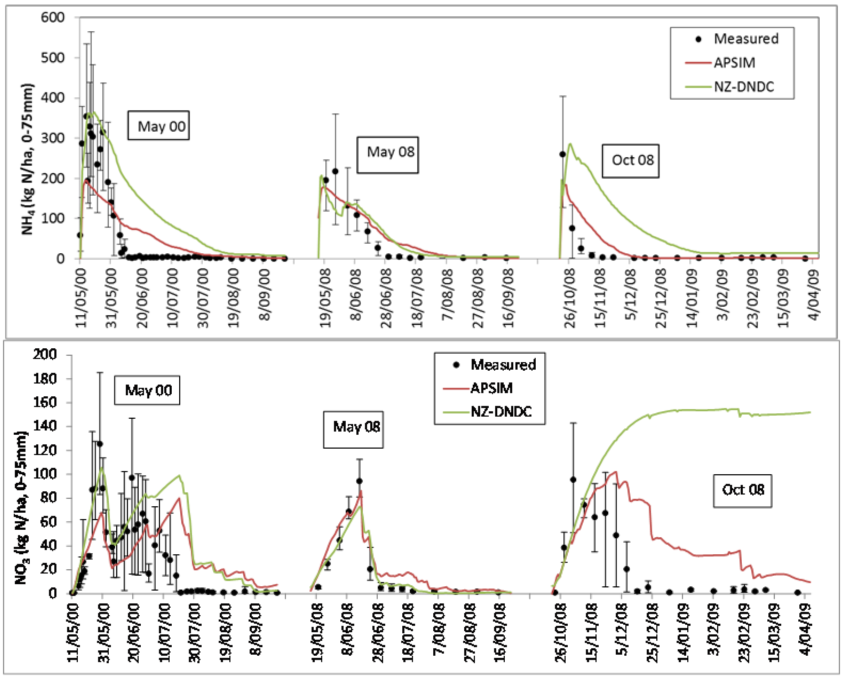

Figure 2. Measured and simulated (using default parameter values) soil NH_4 (top) and NO_3 (bottom) concentrations in the top 75 mm following urine applications of 500 to 600 kg N/ha at different times to the Horotiu soil.

Measured N_2O emissions presented high variability, with large differences between replicates (see Figure 1). These differences demonstrate the large sensitivity of N_2O emissions to differences in soil properties over comparatively short distances. This is also an indication of the difficulties in simulating N_2O emissions. In our case both models frequently produced results outside the measured range (both over- and under-estimates). For APSIM, the comparisons based on cumulative N_2O emissions over 7 days, showed NSE positive only for the October dataset, the RSR was below 1, but the model underestimated the emissions. For the other two datasets the APSIM model could not predict the emissions well. The DNDC model showed negative NSE values for all three datasets, RSR values between 1.5 and 3.4, and an overestimation of emissions.

Table 2. Statistics from APSIM and NZ-DNDC model output comparison with measured cumulative N_2O emissions over 7 days from three different datasets following urine application to the Horotiu soil, with NSE being the Nash-Sutcliffe efficiency, RSR the RMSE-observation standard deviation ratio, and PBIAS the percent bias (%).

				K_{max}		K_{NH4}		K_{denit}		K_{N2Onit}		WFS_{denit}		RFI		T_{opt}	
			Default	30	50	10	140	0.0001	0.001	0.001	0.005	concave	convex	3	5	20	40
APSIM - N_2O	N	May-00	-1.18	-0.93	-1.43	-1.69	-0.94	-0.63	-5.05	-1.18	-1.67	-4.19	-0.35	-1.63	-1.63	-3.68	-0.80
	S	May-08	-3.25	-2.15	-4.21	-5.73	-2.42	0.03	-9.04	-2.99	-4.47	-7.13	-0.88	-1.44	-1.43	-7.10	-1.66
	E	Oct-08	0.15	0.02	0.26	0.34	0.08	0.18	-0.10	-0.01	0.42	-0.01	0.19	0.24	0.24	0.56	-0.02
	R	May-00	1.44	1.36	1.52	1.60	1.36	1.24	2.40	1.44	1.59	2.22	1.13	1.58	1.58	2.11	1.31
	S	May-08	2.01	1.73	2.22	2.52	1.80	0.96	3.08	1.94	2.28	2.77	1.34	1.52	1.52	2.77	1.59
	R	Oct-08	0.89	0.95	0.82	0.78	0.92	0.87	1.01	0.97	0.73	0.97	0.86	0.84	0.84	0.64	0.97
	P	May-00	-12	0	-18	-22	-3	64	-69	-2	-41	-66	35	91	91	-33	8
	BIAS	May-08	-135	-105	-152	-172	-112	20	-251	-110	-207	-221	-51	-76	-76	-185	-87
		Oct-08	21	26	18	15	24	61	-10	39	-29	-7	45	56	57	-1	30

				Denitri_factor		Nitri_factor		NH_3		K_{N2Onit}		PG		RFI			MA	
			default	0.1	10	0.1	10	0.005	0.1	0.2	0.5	2	5	1	2	10	0.1	0.5
NZ-DNDC - N_2O	N	May-00	-1.33	-1.26	-12.1	-0.86	-46.4	-2.51	-0.49	-1.57	-24.5	-1.54	-1.88	-1.47	-1.28	-1.76	-1.17	0.34
	S	May-08	-1.29	-1.02	-11.0	-0.12	-25.3	-5.91	0.48	-0.26	-16.4	-1.54	-0.49	-1.13	-1.29	-1.73	-0.04	0.12
	E	Oct-08	-10.9	-0.26	-352	-4.52	-19.7	-27.3	-15.6	-7.59	-18.7	-29.0	-0.54	-1.96	-1.00	-1.06	-19.4	-13.3
	R	May-00	1.49	1.47	3.52	1.33	6.71	1.83	1.19	1.56	4.93	1.55	1.65	1.53	1.47	1.62	1.44	0.79
	S	May-08	1.57	1.38	3.37	1.03	4.99	2.56	0.70	1.09	4.06	1.55	1.19	1.42	1.47	1.61	1.93	0.98
	R	Oct-08	3.39	1.10	18.4	2.30	4.45	5.19	3.98	2.87	4.35	5.37	1.22	1.69	1.39	1.41	4.43	3.70
	P	May-00	-30	-26	-121	70	-141	-57	9	88	-216	-27	-7	37	5	-66	80	17
	BIAS	May-08	-142	-107	-326	42	-460	-253	-39	48	-443	-146	-103	-47	-83	-170	75	-31
		Oct-08	-389	-130	2116	-154	-596	-472	-270	-178	-722	-571	-113	-97	-162	-200	68	-114

3.2. Sensitivity Analysis

The sensitivity analysis based on the selected model parameters for APSIM and DNDC (Table 1) shows that changing some of the default model parameters can improve the agreement between simulated and measured soil nitrogen concentrations and N_2O emissions. APSIM prediction of temporal soil NH_4 and NO_3 concentrations improved generally with increased K_{max}, decreased K_{NH4}, and decreased T_{opt}. The improvement results in a higher positive value for NSE and a lower RSR. There was no clear trend for either over- or under-prediction of the APSIM model, with PBIAS being both positive and negative. Predictions of soil NH_4 and NO_3 concentrations by NZ-DNDC improved in general with increased volatilization rate, plant growth, and when setting the rainfall intensity to either 1 or 2 mm. Changing the various model parameters in APSIM improved the predictions of weekly sums of N_2O emissions in some cases (Table 2), especially for the October 2008 dataset when N_2O_{nit} was increased to 0.005, or T_{opt} decreased to 20^oC. But neither of the parameters improved the prediction for the other two datasets. Contrasting to findings from Thorburn et al. (2010) increasing the default value of K_{denit} in APSIM did not improve predictions of N2O emissions in the three datasets. Similarly, for DNDC, while some of the model parameters improved the prediction of N_2O, especially increasing the volatilization rate and the microbial activity, none of the parameters changed could improve the predictions for all three datasets satisfactory (Table 2).

4. DISCUSSION

The results from this work demonstrate the sensitivity of two distinct models to their parameters when predicting soil nitrogen concentrations and N_2O emissions following urine application to the soil. The measured data are highly variable and none of the models performed consistently in describing the N_2O emission pattern, although the mineral N in the soil was reasonably well predicted by both models. Changing some of the default model parameters improved the agreement in some cases, e.g. for APSIM when the fraction of nitrified N emitted as N_2O was increased or the optimum temperature for nitrification was decreased to 20^oC, and for DNDC when microbial activity was decreased or volatilization rate increased. However, so far none of the model parameters investigated could be pin pointed separately to improve the predictions that agreed reasonably with values measured. This indicates that either the underlying functions need to be advanced or that parameters need to be changed in combination. A sensitivity analysis with further parameters and model functions, as well as changing various parameters simultaneously is needed. Testing the models against more comprehensive datasets, e.g. that had more detailed measurements of soil conditions and higher frequency N_2O measurements, would also be valuable in better developing the models.

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