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Modelling nitrous oxide emission from water-logged soils of a spruce forest ecosystem using the biogeochemical model Wetland-DNDC

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Abstract During the last decades, decision makers and policy have increasingly demanded for regional and national inventories of greenhouse gas emission, such as nitrous oxide (N_2O), to develop appropriate strategies and mitigation options. A potential way to derive large-scale estimates of N_2O emission is the use of process-based models, such as PnET-N-DNDC or Wetland-DNDC. While PnET-N-DNDC has been effectively applied for various upland forest ecosystems, the Wetland-DNDC model has not yet been validated with regard to N_2O emission. We calibrated and validated the Wetland-DNDC model on the basis of a 4-year field data set of two water-logged soils (*Humic Gleysol* and *Histic Gleysol*) of a spruce forest ecosystem. Model calibration by means of the Levenberg–Marquardt algorithm considerably improved the model performance for the period of calibration (2001–2002). The error variance was reduced by up to a factor of two and the modelling efficiency was increased from –1.24 to –0.15 (*Humic Gleysol*) and from –0.42 to 0.1 (*Histic Gleysol*). However, the model performance for the period of validation (2003–2004) and particularly for the extreme dry period in summer 2003 was not fully satisfying, notably with regard to the temporal pattern of the N_2O emission.

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Introduction

During the last decades, decision makers and policy have increasingly demanded for regional and national inventories of greenhouse gas emission to develop and verify appropriate strategies and mitigation options. Besides water (H_2O), carbon dioxide (CO_2), ozone (O_3) and methane (CH_4), nitrous oxide (N_2O) is regarded as one of the most important natural greenhouse gases because (1) it has a huge radiative forcing of about 300 times that of CO_2 (IPCC 2001), (2) a long atmospheric lifetime of about 120 years, (3) its atmospheric concentration is continuously rising by 0.27 ± 0.01% year^{-1} (Khalil and Rasmussen 1992) and (4) N_2O contributes to the stratospheric ozone depletion (Cliff and Thiemens 1997).

N_2O is naturally produced in soil mainly as a by-product of the microbial processes nitrification and denitrification (Bremner 1997). In forest ecosystems soil moisture, soil temperature and the availability of nitrogen were identified to be the key factors controlling N_2O fluxes (Schindlbacher et al. 2004; Smith et al. 2003).

Total N_2O emissions from temperate forest soils are estimated to be in the range of 0.1–2.0 Tg N year^{-1} (Kroeze et al. 1999). However, due to the high temporal, spatial and inter-annual variability of N_2O fluxes, estimates of N_2O emission are still highly uncertain (Ambus and Christensen 1995; Schulte-Bisping et al. 2003). Since field measurements are costly and time consuming, only few long-term measurements are available, which cannot cover the wide variety of ecological and environmental conditions in forest ecosystems (Schmidt et al. 1988; Ambus and Christensen 1995; Hahn et al. 2000; Butterbach-Bahl et al. 2002; Zechmeister-Boltenstern et al. 2002; Jungkunst et al. 2004; von Arnold et al. 2005a, b; Lamers et al. 2007a). Moreover, the measurement area is typically <1 m^2. A potential way to overcome these shortcomings is the use of process-based models such as PnET-N-DNDC (Li et al. 2000) or Wetland-DNDC (Zhang et al. 2002), among others. These models were developed to simulate carbon (C) and nitrogen (N) dynamics as well as trace gas emissions from upland and wetland forest ecosystems.

Highest N_2O emission rates with up to 7.0 kg N ha^{-1} $year^{-1}$ were mainly reported for forest soils affected by stagnant water (Brumme et al. 1999; Zechmeister-Boltenstern et al. 2002; Jungkunst et al. 2004; Lamers et al. 2007a). Fluctuating water table promote constantly alternating aeration conditions and thus incomplete denitrification, which was identified to be the major N_2O forming process in soil (Vor et al. 2003). The final step of the denitrification pathway, the reduction from N_2O to N_2, occurs only under anaerobic conditions when efficient electron acceptors are absent. Hence, soils affected by alternating aeration conditions tend to emit more N_2O than constantly aerobic or anaerobic soils (Jungkunst et al. 2004). However, no efforts have been made so far to simulate N_2O emissions from water-logged soils. As a consequence, model-based regional estimates of N_2O emission from temperate forest ecosystems are limited to upland soils (Butterbach-Bahl et al. 2004; Kesik et al. 2005).

While PnET-N-DNDC has been successfully applied to various upland forest ecosystems (Stange et al. 2000; Lamers et al. 2007b), the Wetland-DNDC model has not yet been validated with regard to N_2O emission. Most studies in which the Wetland-DNDC model was used focused on soil organic carbon (SOC) dynamics or methane fluxes from wetland sites (e.g. Zhang et al. 2002; Cui et al. 2005a). Li et al. (2004) modified the model to simulate the impact of management on carbon sequestration and emissions of trace gases including N_2O in forested wetland ecosystems over a period of 150 years but without any pre-validation.

In this paper, we present the first study that aims at calibrating and validating the Wetland-DNDC model with regard to N_2O emission from two water-logged soils (*Humic Gleysol* and *Histic Gleysol*) of a spruce forest ecosystem in the Central Black Forest (South-west Germany).

Materials and methods

Study area

The study area "Wildmooswald" (7 ha) is located in the Central Black Forest, South-west Germany (47°57′N, 8°07′E; 1,085–1,150 m above sea level). The study site is a convex–concave shaped southward falling slope with an average inclination of 4.2%. The annual averages of precipitation and temperature are 1,700 mm and 7°C, respectively (Deutscher Wetterdienst 1999). The vegetation is dominated by an about 86-year old stand of Norway spruce (*Picea abies*). The hydrology of the investigation area is strongly affected by an impermeable layer, which temporarily causes water-logging and extensive lateral water flow. Due to this hydrological situation *Histic* and *Humic Gleysols* [Food and Agricultural Organisation (FAO) 1998] have formed which together cover ~24% of the study site. These soil types are typical for the Central Black Forest. A more detailed description of the study site can be found in Fiedler et al. (2002).

The Wetland-DNDC model

The general structure of the Wetland-DNDC model is identical to that of the PnET-N-DNDC model. Both models have been combined to yield the Forest-DNDC model, which can either be run in the upland (PnET-N-DNDC) or in the wetland mode (Wetland-DNDC). To adopt the Wetland-DNDC model for the specific features of wetland ecosystems the model includes enhanced functions and algorithms for simulating soil moisture and water table dynamics, C fixation by mosses and herbaceous plants, and considers the effect of anaerobic conditions on decomposition and on other biogeochemical processes (Zhang et al. 2002).

In Wetland-DNDC the soil profile is subdivided into forest floor and mineral or organic layer. The thickness of the forest floor and mineral/organic layer is preset by the model to 12 and 2 cm, respectively (C. Li personal communication, March 2005). These values are hard-coded and cannot be changed by the user. For the present study, we used a version downloaded from the DNDC-homepage (http://www.dndc.sr.unh.edu) on 8 December 2006. PnET-N-DNDC and Wetland-DNDC are not open source models, that is, the user has no access to the source code. Parameter changes or calibration are hence restricted to those parameters which are accessible via the graphical user interface (GUI).

Model input data

Model calibration and validation was carried out using N_2O emission data of the years 2001–2002 (Jungkunst et al. 2004) and 2003–2004 (Lamers et al. 2007a), respectively. Both authors extensively investigated the influence of environmental parameters on N_2O emission and comprehensively discussed the relevance of N_2O emission from forest wetland ecosystems in the context of climate change. N_2O flux measurements were conducted weekly or biweekly using the "closed chamber" technique. Measurements were taken in replicates. The area covered by the stainless-steel chambers was 1 m^2, while the volume of the chambers ranged from 0.196 to 0.275 m^3. N_2O flux rates were determined by measuring N_2O concentration changes in the chamber headspace using linear regression (Livingston and Hutchinson 1995). On sampling days, gas samples were taken 0, 30, 60 and 90 min after closing the chambers by connecting the chamber atmosphere with a vacutainer (22.5 ml) through a constantly mounted septum using a multi-sample needle (Venoject double-cannula, 0.7×40 mm^2, Terumo Inc., Germany). N_2O concentrations were analysed in the laboratory using a gas chromatograph (GC) equipped with a ^{63}Ni electron capture detector (ECD). The GC was coupled with an HS 40 autosampler (Perkin-Elmer, Foster City, CA, USA). Cumulative annual emission rates were calculated by linear interpolation. For details see Lamers et al. (2007a). Daily precipitation and air temperature were obtained from a weather station (Campbell Scientific, Logan, UT, USA) located at an open site about 400 m west of the study area. The water table was measured weekly using polyvinyl chloride (PVC) tubes (diameter 6 cm) slotted at two sites (Eijkelkamp, The Netherlands). Daily water table data, which were needed as model input, were computed by linear interpolation between weekly records. Since the pipes had only been installed to a depth of 100 cm, values for simulation were set to 100 cm if the pipes were waterless. Data for N-concentration in precipitation (nitrate and ammonium) were taken from the monitoring station "Schauinsland" (German Federal Environmental Agency, 47°55′N, 7°55′E, 1,205 m above sea level) and was found to be 0.9 mg N l^{-1} on average. For the *Humic Gleysol* and the *Histic Gleysol* the type of the forest floor was set to "moder", the mineral/organic soil was set to "silty loam" and "organic or peat", respectively. All other soil related model input is listed in Table 1.

Model optimization and sensitivity analysis

For automatic calibration, we linked Wetland-DNDC to UCODE (Version 3.02) (Poeter and Hill 1999). UCODE estimates an optimum set of parameters minimizing a weighted least-square objective function using the Levenberg–Marquardt method. It further calculates important statistics, e.g. linear confidence intervals and parameter correlations. Additional information is given in (Hill et al. 1998) and (Poeter and Hill 1999). Because the structure of the ASCII input files compiled by Wetland-DNDC is not documented the change of the input variables during the optimization cannot directly be performed in the input files but must be done through the GUI. To overcome this shortcoming, we used the freeware scripting language AutoIt (Version 3) (Benett 2005). AutoIt is able to automatically enter the inputs through the GUI. A more detailed description of the automatic calibration routine can be found in Lamers et al. (2007b).

Simulation results were assessed using the following statistical criteria based on Loague and Green (1991):

Table 1 Results of the sensitivity analysis performed with UCODE for input parameters of Wetland-DNDC for the Humic Gleysol and the Histic Gleysol of the investigation area "Wildmooswald" and the default and optimized parameter values used for simulating N_2O emission

Parameter	Initial conditions	Humic Gleysol			Histic Gleysol		
		Sensitivity		Optimized values	Sensitivity		Optimized values
		1%	10%		1%	10%	
General data							
N in prec	0.9[a]	2.36	0.93		0.08	0.04	
Latitude	47[a]	627	61.3		21.5	24.5	
Tree age	86[a]	333	11.8		6.02	2.7	
Soil fertility	2.3[b]	0	0		0	0	
	SGn/Sgo			*Forest floor data*			
pH ($CaCl_2$)	3.2[a]/3.0[a]	104	103		18.7	13.9	
SOC 5 cm	0.3[a]/0.4[a]	0	0		0	0	
Clay	0.0[a]/0.0[a]	0	0		0	0	
BD	0.2[a]/0.1[a]	0	0		0	0	
Ks	1[b]/1[b]	0	0		0	0	
Porosity	0.9[a]/0.84[a]	15.1	4.3		0.28	0.96	
FC	0.35[b]/0.35[b]	475	25.7	0.56 (0.43–0.74)	0.05	0.06	
WP	0.2[b]/0.2[b]	0	0		0	0	
Humads	0.9[b]/0.9[b]	0	0		0	0	
Litter	0.01[b]/0.01[b]	0	0		0	0	
			Mineral/organic soil data				
pH ($CaCl_2$)	3.2[a]/3.4[a]	182	180		35.8	27	
SOC	0.05[a]/0.3[a]	110	115		6.23	5.98	
Clay	0.2[a]/0.0[a]	31.1	4.13		0.18	0.2	
BD	0.8[a]/0.25[a]	8.98	9.13		7.12	10.8	
Ks	0.2[b]/1[b]	50.8	5.27	0.22 (0.14–0.35)	0.15	0.9	6.6 (4.7–9.9)
Porosity	0.7[a]/0.65[a]	161	294		1.92	1.67	
FC	0.17[b]/0.625[b]	802	568	0.2 (0.16–0.27)	0.76	2.16	0.64 (0.45–0.82)
WP	0.05[b]/0.5[b]	522	8.82	0.05 (0.033–0.083)	3.44	6.04	0.49 (0.26–0.94)
Humads	0.2[b]/0.2[b]	58.6	52.9	0.07 (0.05–0.087)	15.5	14.8	0.058 (0.034–0.099)
Litter	0.1[b]/0.1[b]	58.1	4.05	0.12 (0.039–0.4)	0.11	0.12	

For the optimized parameters 95% confidence intervals are listed in brackets

N in prec nitrogen in precipitation [mg l^{-1}], *SOC* soil organic carbon [kg C (kg soil)$^{-1}$], *clay* clay content [%], *BD* bulk density [g cm^{-3}], *Ks* hydrological conductivity [cm min^{-1}], *FC* water filled pore space (*wfps*) at field capacity, *WP* wfps at permanent wilting point, *Humads* fraction of humads [%], *Litter* fraction of litter [%]

[a] Measured data

[b] Default values by Wetland-DNDC

Modelling efficiency

$$\mathrm{MEF} = \frac{\left[\sum_{i=1}^{n} (y_i - \bar{y})^2 - \sum_{i=1}^{n} (x_i - y_i)^2\right]}{\sum_{i=1}^{n} (y_i - \bar{y})^2}. \tag{1}$$

Coefficient of determination

$$\mathrm{CD} = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2}{\sum_{i=1}^{n} (x_i - \bar{y})^2}. \tag{2}$$

Error variance

$$\mathrm{EV} = \frac{1}{n}\sum_{i=1}^{n} (x_i - y_i)^2. \tag{3}$$

Root mean square error

$$\mathrm{RMSE} = \left[\frac{1}{n}\sum_{i=1}^{n} (x_i - y_\mathrm{i})^2\right]^{0.5}. \tag{4}$$

Mean error

$$\mathrm{ME} = \frac{1}{n}\sum_{i=1}^{n} (x_i - y_i), \tag{5}$$

where x_i and y_i denote simulated and observed values, respectively, $\bar{y}$ represents the mean of the measured data, and n is the number of observations.

To evaluate the performance of the calibration, calibrated simulation results were compared to those based on the default values provided by Wetland-DNDC. In the following the latter type of simulation will be denoted "cold simulation".

Based on the soil input data given in Table 1, a sensitivity analysis was performed. Input variables were changed from the initial values by 1 and 10%. Since Wetland-DNDC calculates the initial SOC content as a function of tree age and latitude and the *soil fertility factor* as a function of the wet N-deposition, these general data were additionally included in the sensitivity analyses.

For forward differences, UCODE calculates scaled sensitivities, ss_{ij}, by (Hill et al. 1998)

$$\mathrm{ss}_{ij} = \left(\frac{\partial y_i}{\partial b_j}\right) b_j \varpi_i^{0.5}, \tag{6}$$

where y_i denotes the simulated value associated with the xth observation, b_j the jth parameter and ω_i the weight of the ith observation. Observations were weighted by the reciprocal of the observed variance. The composite scaled sensitivity for the ith parameter, css_i, is then calculated by

$$\mathrm{css}_i = \left[\frac{1}{N}\sum_{i=1}^{N} \left(\mathrm{ss}_{ij}\right)^2\right]^{0.5}, \tag{7}$$

where N denotes the number of observations being used in the regression.

UCODE calculates the standard deviation of predicted values (s_z) by (Hill 1998)

$$s_z = \left[\sum_{i=1}^{\mathrm{NP}}\sum_{j=1}^{\mathrm{NP}} \frac{\partial z_l}{\partial b_j} V(b') \frac{\partial z_l}{\partial b_i}\right]^{0.5}, \tag{8}$$

where NP is the number of estimated parameters, z_l denotes the simulated prediction, b_j and b_i stands for the jth and ith estimated parameter, respectively, and $V(b')$ is the covariance matrix for the final estimated parameters.

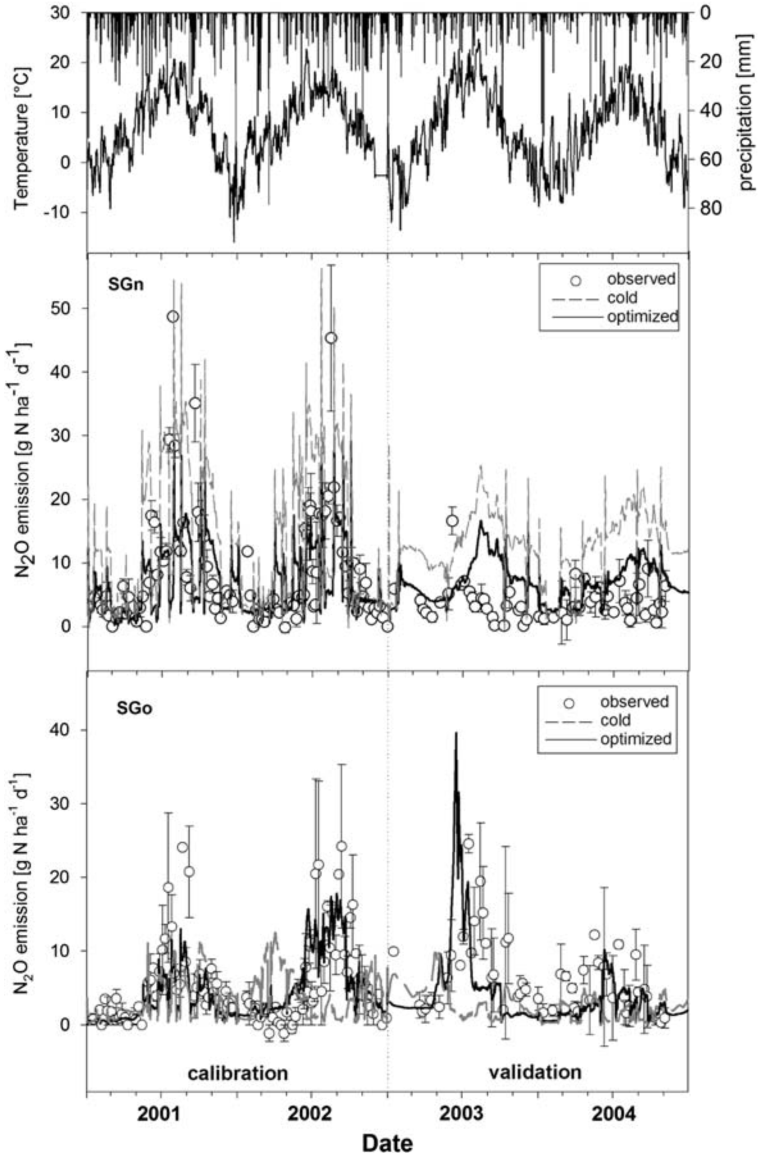
Results and discussion

Sensitivity analysis

The simulation of N_2O emissions was sensitive to all general parameters as well as all mineral/organic soil parameters except the *soil fertility factor* (Table 1). Since Wetland-DNDC computes the *soil fertility factor* on the basis of the atmospheric N-deposition it was not possible to independently modify *N-deposition* and *soil fertility factor*. High leverage inputs were *latitude*, *tree age*, *field capacity*, *SOC*, *pH value, porosity* and *water content at the permanent wilting point*. The strong impact of *tree age* and *latitude* on model prediction results from the algorithm that calculates the initial soil organic matter content (SOC) as a function of tree age, latitude and soil fertility (Stange 2001).

With regard to the forest floor depth, however, simulated N_2O emissions for the *Humic Gleysol* (SGn) and *Histic Gleysol* (SGo) were only sensitive to three input variables (*pH*, *field capacity* and *porosity)*. Sensitivities of the remaining model input were zero. This finding was unexpected because among the zero-sensitive input there were several variables that should affect the emission of N_2O

Fig. 1 Precipitation, air temperature, and measured and simulated N_2O emission rates for the Histic Gleysol (*SGo*) and the Humic Gleysol (*SGn*) for the years 2001–2004. Field data of N_2O fluxes represent mean and standard deviation of emission rates. Measured data for 2001–2002 and for 2003–2004 were taken from Jungkunst et al. (2004) and Lamers et al. (2007a), respectively



(e.g. *SOM* and *saturated hydraulic conductivity*). Although these parameters are asked for in the soil input dialogue box, so that a user has the impression that it is possible to change these parameters, the values of the zero-sensitive parameters are hard-coded and cannot be changed by the user via the GUI (C. Li personal communication, February 2005).

Therefore, we restricted the calibration to those input variables that were sensitive with regard to the simulation of N_2O emission and were not available from measurements (Table 1).

Modelling results

Cold simulations

Simulation results for the period from 2001 to 2004 using default modelling input are shown in Fig. 1. The results clearly indicate that the cold simulations did not reproduce observed values well (Table 2). For *SGn* the model systematically overestimated measured values over the entire simulation period. Especially for the period of validation (2003–2004)

Table 2 Model performance for simulating N_2O emission with Wetland-DNDC for the Histic Gleysol (*SGn*) and Humic Gleysol (*SGo*) using default (cold) and optimized (opt) input variables

Criteria	Calibration period (2001–2002)				Validation period (2003–2004)			
	SGn		SGo		SGn		SGo	
	Cold	Optimized	Cold	Optimized	Cold	Optimized	Cold	Optimized
MEF	–1.24	–0.15	–4.2	0.1	–15.1	–6.6	–0.69	–1.0
CD	0.54	2.52	2.23	2.54	0.07	0.14	1.43	0.42
EV	183	94.1	116.5	74.9	129.1	60.7	13.5	16.1
RMSE	13.6	9.7	10.7	8.65	11.4	7.8	3.7	4.01
ME	4.92	–2.05	–5.41	–3.69	+9.5	+6.0	–1.34	0.35
Mean daily emission rate[a]	+56.9	–25.1	–42.3	–11.6	+243	+153	–55.2	–27
Annual emission rate[a]	+61.9	–23.2	–33.8	–17.6	+199	+117	–53.3	–29.6

MEF modelling efficiency, *CD* coefficient of determination, *EV* error variance, *RMSE* root mean square error, *ME* mean error, for details see Eqs. 1–5

[a] Per cent error calculated by: (simulated/observed–1) × 100

the model did not roughly reproduce measured N_2O fluxes with regard to magnitude and seasonal pattern (Fig. 1). Taking the mean daily and annual emission rate the model overestimated observed values for the period of calibration and the period of validation by 57 and 243% and by 62 and 199%, respectively (Table 2). Only during summer 2001 the model satisfactorily captured single peak events in terms of magnitude and time of occurrence (Fig. 1).

For *SGo* cold simulation results did not adequately capture observed values. For the period of calibration, for example, differences between measured and predicted N_2O fluxes are largely due to an overestimation and underestimation of N_2O fluxes during the winter period and the summer period in 2002, respectively. The predicted mean daily and annual emission rate was 42 and 34% lower than the N_2O emission rate calculated from the measured data. For the period of validation the model systematically underestimated observed values, e.g. up to a factor of 8 in summer 2003 (Table 3). Taking the mean daily and annual emission rate the model underestimated observed values for the period of calibration and the period of validation by 42 and 34% and by 55 and 53%, respectively (Table 2).

Calibrated simulation

For both soils model performance could markedly be improved by parameter calibration (Fig. 1). At the *SGo* site the modelling efficiency, for example, could be improved from –4.2 to 0.1. For *SGn* the error variance was reduced from 183 to 94 (Table 2). In all cases parameter correlations were below 0.5. Their 95% confidence intervals were reasonable. The statistical results indicated that simultaneous fitting of parameters make sense, and that input values could reliably be estimated from the available data (Table 1). For *SGn* the highest parameter correlation (–0.39) was found between *field capacity* and *hydraulic conductivity* of the mineral soil. For *SGo* the highest parameter correlation (0.44) was found between *humads fraction* and *the water content at the permanent wilting point* of the organic layer.

For the period of calibration (2001–2002) measured and modelled N_2O emission were in fairly good agreement with regard to the seasonal pattern (Fig. 1). For *SGn*, periods of lower emissions (<10 g N ha^{-1} day^{-1}) were well reproduced by the model. Observed emission peaks in 2001 and 2002, however, were systematically underestimated by the model (Fig. 2). Taking the mean daily and the mean annual N_2O emission rates the simulation underestimated the measured N_2O emission by 25 and 23%.

For the *SGo* similar as for the *SGn* differences between observed and predicted N_2O emission were largely due to underestimated N_2O fluxes during the summer and spring period in 2001 and 2002, respectively (Table 3). Mean daily and mean annual N_2O emissions were fairly well reproduced by the model with only a slight underestimation of 12 and

Table 3 Seasonal perspective of measured and modelled N_2O emission for the *Humic Gleysol* and *Histic Gleysol*

Year	Spring (20.04–20.06)			Summer (21.06–22.08)			Fall (23.08–31.12)			Winter (01.01–19.04)		
	Observed	Simulation		Observed	Simulation		Observed	Simulation		Observed	Simulation	
		Cold	Optimized		Cold	Optimized		Cold	Optimized		Cold	Optimized
Humic Gleysol												
2001	5.7 ± 5.3	11.6 ± 9.6	4.6 ± 3.9	19 ± 12.6	25 ± 11.2	10.2 ± 4.4	7.7 ± 5.3	16 ± 9.7	7.7 ± 4.4	2.5 ± 1.5	5.9 ± 4.8	2.9 ± 2.7
2002	6.0 ± 5.6	16.9 ± 6.8	7.9 ± 4.7	16 ± 9.5	21 ± 11.9	10.2 ± 5.4	4.4 ± 3.2	11 ± 10.6	5.9 ± 5.3	3.1 ± 3.4	6.6 ± 5.6	3.6 ± 3.3
2003	6.3 ± 5.2	10.0 ± 1.2	11 ± 2.4	4.0 ± 2.1	18.1 ± 3.8	16 ± 2.5	2.3 ± 1.8	14 ± 4.1	10 ± 3.3	5.0 ± 0.9	10 ± 3.9	6.3 ± 3.5
2004	4.9 ± 1.9	12.7 ± 3.2	8.4 ± 2.7	4.3 ± 2.6	17.3 ± 2.0	12.7 ± 1.8	3.1 ± 1.9	15 ± 3.7	9.5 ± 2.5	1.5 ± 0.4	5.5 ± 3.8	4.0 ± 2.9
Histic Gleysol												
2001	2.9 ± 2.7	2.1 ± 1.8	2.4 ± 1.6	11.1 ± 6.5	4.7 ± 2.9	5.7 ± 2.7	4.2 ± 1.7	4.4 ± 3.0	3.6 ± 2.6	1.8 ± 1.2	1.1 ± 0.6	0.72 ± 0.2
2002	2.4 ± 2.6	5.4 ± 2.1	5.2 ± 2.7	12 ± 6.7	1.7 ± 1.0	12.2 ± 2.2	5.8 ± 4.7	3.2 ± 2.5	6.5 ± 4.8	1.3 ± 1.2	5.4 ± 3.9	1.9 ± 0.63
2003	4.3 ± 2.8	5.3 ± 2.8	12 ± 9.8	12.7 ± 5.5	1.6 ± 0.7	11 ± 7.4	6.2 ± 3.5	2.3 ± 1.3	2.5 ± 1.7	6.3 ± 3.6	5.2 ± 1	2.5 ± 0.3
2004	6.1 ± 3.1	2.6 ± 1.5	3.7 ± 2.5	5.0 ± 2.9	1.3 ± 0.8	4.6 ± 1.9	1.0 ± 0.4	2.2 ± 1.2	2.1 ± 1.0	4.1 ± 2.2	1.2 ± 1.1	1.1 ± 0.5

Values represent mean daily N_2O emission [g N ha^{-1} day^{-1}] (±standard deviation) (2001–2002 period of calibration, 2003–2004 period of validation)

18%, respectively. The results show that the model yields acceptable estimates for daily and annual emission but to some extent unsatisfying results with regard to the seasonal dynamics of the N_2O fluxes.

For the period of calibration, the modelling uncertainty of the predictions using optimized parameter values was quantified by calculating their standard deviation (Eq. 8). For 2001 and 2002 the standard deviation of predicted mean daily N_2O emission [g N ha^{-1} day^{-1}] was 2.7 and 2.2 for the *SGn*, and 1.8 and 3.1 for the *SGo*, respectively (Table 4).

For the validation period (2003–2004) the model performance strongly decreased for both soils (Table 2). For *SGn* modelling efficiency dropped to –6.6 indicating that simulated values were less accurate than the observed mean (Loague and Green 1991). The model systematically overestimated N_2O emission almost over the entire simulation period. Especially during the summer period 2003 the simulation overestimated measured values by up to a factor of 4. The summer 2003 was extremely dry with only half of the average annual precipitation. This resulted in significantly deeper water tables throughout the year and thus a completely different soil water regime compared to the calibration period. However, this was not sufficiently reproduced by the model on the basis of the calibrated parameter values. This was probably the reason for the particularly bad model performance in 2003 (Fig. 3).

Since the pipes for measuring water table had only been installed to a depth of 100 cm, values for simulation were set to 100 cm if pipes were waterless. The influence of the lowest water table depth on simulation results was assessed by rerunning the model assuming a lowest water table of 120 and 140 cm. However, for both soils the simulation results did not differ between the individual runs indicating that the lowest water table depth had no influence on presented simulation results.

For *SGo* the modelling efficiency and the error variance slightly increased from –0.69 to –1.0 and from 13.5 to 16.1, respectively. Taking the mean daily and annual N_2O emission rate the model underestimated observed values by 27 and 30% (Table 2). Both the magnitude and the seasonal trend of measured N_2O emission was not sufficiently reproduced by the model. In 2003 the period of elevated N_2O emission, for example, was captured by

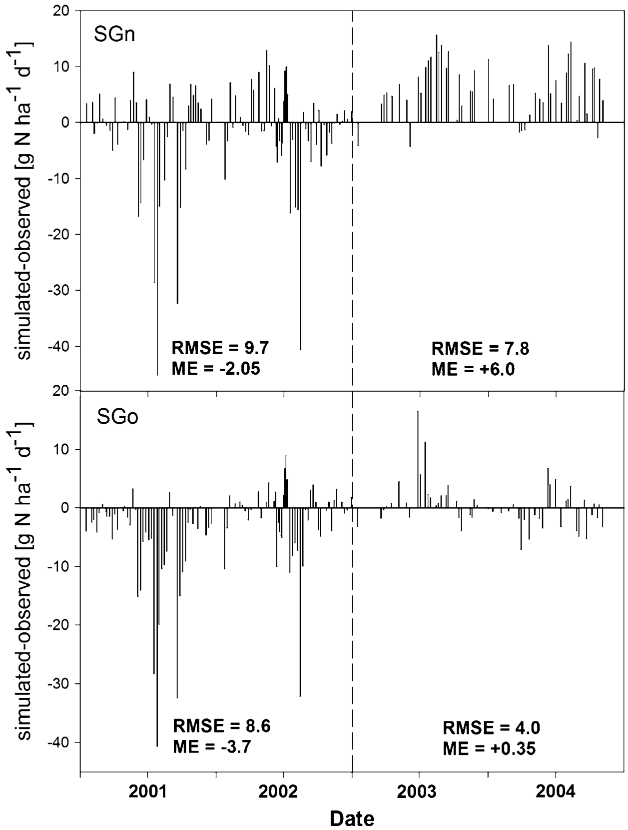


Fig. 2 Residuals of measured and simulated N_2O emission for the Humic Gleysol (*SGn*) and the Histic Gleysol (*SGo*) for the years 2001–2004 (*RMSE* root mean square error, *ME* mean error)

Table 4 Comparison of measured and modelled mean daily and annual N_2O emission rates

Year	Mean daily N_2O emission rate [g N ha^{-1} day^{-1}]						Cummulative annual N_2O emission rate [kg N ha^{-1} year^{-1}]					
	SGn			SGo			SGn			SGo		
	Observed	Simulated		Observed	Simulated		Observed	Simulated		Observed	Simulated	
		Cold	Optimized		Cold	Optimized		Cold	Optimized		Cold	Optimized
2001	9.4	13.5	6.2 (±2.7)[a]	5.3	3.3	3.0 (±1.8)[a]	3.2	5.0	2.0	1.8	1.1	1.05
2002	8.1	13.6	6.9 (±2.2)[a]	5.9	3.1	6.6 (±3.1)[a]	2.7	4.6	2.5	2.1	1.5	2.16
2003	3.9	13.2	10.4	8.3	3.2	5.5	1.7	4.8	2.6	2.7	1.3	2.06
2004	3.8	12.9	9.1	4.5	1.8	2.9	1.4	4.4	2.3	1.5	0.7	0.91

For the period of calibration (2001–2002) values in brackets indicate the standard deviation of the prediction with optimized parameter values

[a] Standard deviation was calculated according to Eq. 8

the model only with a pre-lag of up to 3 weeks. In 2004 the simulation systematically underestimated observed values by nearly 100%.

For both soils pattern of N_2O fluxes switched from highest to lowest emission rates and vice versa within one time step throughout the entire simulation period. Figure 4 clearly indicates that these abrupt changes of simulated N_2O emission were strongly related to water table dynamics. As soon as the mineral/organic layer are completely water saturated, that is the water table reaches the lower boundary of the forest floor layer of 24 cm (*SGn*) and 12 cm (*SGo*), N_2O fluxes are sharply decreased to low emission rates <5 and 3 g N ha^{-1} day^{-1}, respectively (Fig. 4). Soil water

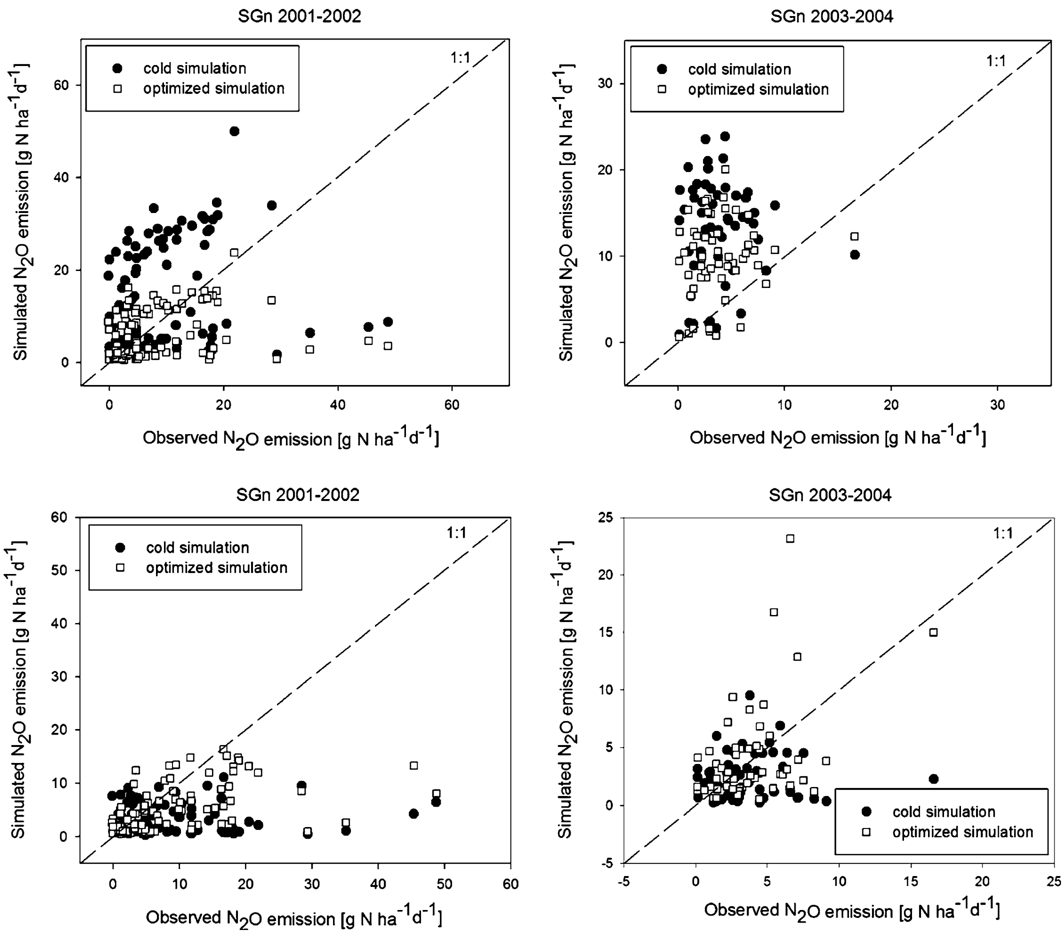


Fig. 3 Scatter plot of observed and simulated N_2O emission for the Humic Gleysol (SGn) and the Histic Gleysol (SGo2) for the period of calibration (2001–2002) and the period of validation (2003–2004)

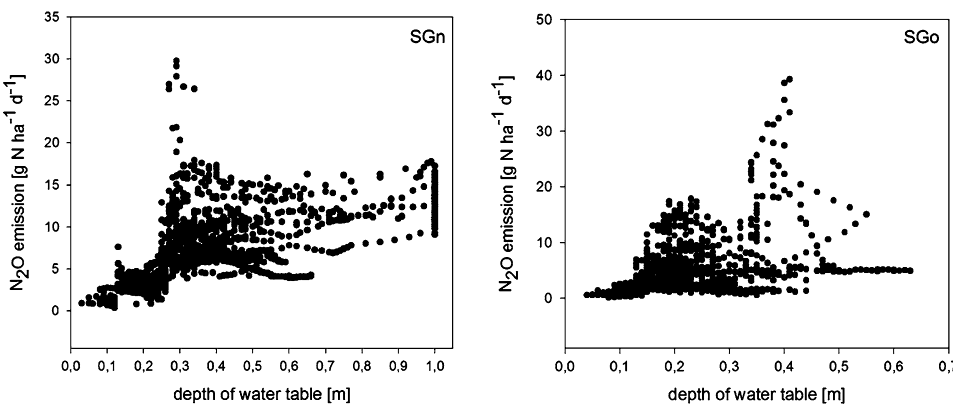


Fig. 4 Scatter plot of simulated N_2O emission and depth of water table for the *Humic Gleysol* (SGn) and the *Histic Gleysol* (SGo) for the entire simulation period (2001–2004)

content nearby saturation yields predominantly anaerobic conditions, which are favourable to promote the final step of denitrification, the reduction from N_2O to dinitrogen (N_2). Since elevated N_2O emissions were restricted to periods of non-saturated conditions within the mineral/organic layer, the forest floor layer appeared to contribute only marginally to the total N_2O fluxes. However, since the Wetland-DNDC output was limited and provided, for example, no further information about the denitrification rate, the reason for this model behaviour cannot definitely be analysed.

In a previous study (Lamers et al. 2007b) we calibrated the Forest-DNDC (in PnET-N-DNDC mode) model for an upland soil. Also for this soil calibration markedly improved model performance, which demonstrates that automatic parameter optimization should be an essential of any modelling application. Although especially the Forest-DNDC model has been applied in a huge number of studies (Stange et al. 2000; Zhang et al. 2002; Butterbach-Bahl et al. 2004; Li et al. 2004; Cui et al. 2005a, b; Kesik et al. 2005), only little effort has been made in parameter optimization. Most studies do not disclose the method used for model calibration and do not discuss the effectiveness of calibration efforts. Stange et al. (2000) applied the PnET-N-DNDC model to seven different forest ecosystems. For each forest type the authors presented a specific parameter set but it remains unclear how the model was calibrated. Zhang et al. (2002) used the Wetland-DNDC model to simulate water table dynamics and methane emissions, among others, from wetland ecosystems. They calibrated empirical hydrological and plant respiration parameters to match field observations, but no further information is given. Kesik et al. (2005) applied the Forest-DNDC model to 19 forest sites across Europe. Again, details of model calibration were not documented.

The lack of studies dealing with the state-of-the-art calibration of the Wetland-DNDC model is remarkable in view of the fact that in related disciplines huge efforts have been made during the last decades to develop appropriate strategies for the calibration of complex models and to analyse the limitations of optimization procedures. In soil physics and groundwater engineering, for example, automatic optimization procedures, mainly by inverse simulation, have been used for a long time, mainly to parameterize hydraulic models (e.g. Zurmuhl and Durner 1998; Bitterlich et al. 2005; Kohne et al. 2006; Spohrer et al. 2006).

It is well known, that calibration of complex models is difficult even if detailed measurements are available. Franks et al. (1997), Franks and Beven (1997) and Schulz et al. (1999) have pointed out that model calibration can lead to the problem of equifinality. Schulz and Beven (2003) use the term equifinality in the sense that a satisfying model performance can be achieved by using different, physically reasonable parameter sets or different model structures. Moreover, even with advanced procedures it cannot completely be ruled out that the minimum found is only a local, but not the global one. Up to now, the questions of equifinality and uncertainty in parameter value specification have not yet been discussed with N_2O emission models.

Summary and conclusion

Applying the Wetland-DNDC model with the default input variables did not produce satisfying simulations of the N_2O emissions from the water-logged soils at the study site “Wildmosswald”. Model calibration using inverse techniques considerably improved model performance during the calibration period. For the validation period and notably the extremely dry summer in 2003, however, model performance was still partly unsatisfying, in particular with regard to the temporal emission pattern. Our data show that the predictive power of the Wetland-DNDC model can be limited when weather conditions become exceptional. This is distressing in view of the fact that models become more and more popular among policy and decision makers as tools for forecasting the effect of climate change on the emission of greenhouse gases.

During the last decades inverse simulation techniques have been utilized in many areas of environmental research. In biogeochemical modelling, this important technique should no longer be disregarded. Further, we strongly recommend to routinely disclose the source code for Wetland-DNDC and other biogeochemical models. An open source code philosophy would not only help in identifying errors in the source codes but also enable model users to better understand contents and hence limitations of popular models.

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