(comments of the referees are printed in blue, responses of authors are held in black)

We would like to thank the reviewer #1 for his highly constructive comments on the manuscript bg-2017-96 "Constraining a complex biogeochemical model for multi-site greenhouse gas emission simulations by model-data fusion"

Response letter to Reviewer #1

General comments

In this study the authors compare the DNDC model simulations of N2O and CO2 emissions against measurements across three different landuse types (arable cropping, grassland, forest). This comparison against different land-use types, as well as the multi-objective Bayesian model calibration method should be of interest to other researchers in this area.

One weakness of this study is that there is no attempt to verify the model calibrations with a independent data. Given that there were three years' data it would have been possible to use two years for the parameterisation and then test the model using the third year's data. (Although this might not work so well for the arable land where the crop types change between years).

We agree with the reviewer in this point . Conducting a split time series calibration and validation test would have been ideal. However, our simulations ran from Jan 2010 to Jan 2016 while measurements for model testing are only available for two years (from Nov 2013 to Dec 2015, see Figure 5, we added this information in section 2.1). We therefore decided not to split up the available 24 months data set, as this would have resulted in a very short period for model testing. In general, it would be very nice to investigate how many data points are needed to test such a complex model set up as we used and how much uncertainty is introduced by reducing the calibration period. For the moment, we cannot answer this question.

Another problem is that the CO2-equivalent values of N2O emissions are incorrectly calculated. It should be noted that the GWP values convert from kg N2O to kg CO2, not kg N2O-N to kg CO2-c.

We acknowledge this important comment. We corrected the GWP values throughout the manuscript.

This MS would benefit from editing by a native English speaker as there a numerous grammatical errors.

We sent the MS to the Nature Research Editing Service. Native English-speaking editors revised it for English language usage, grammar, spelling and punctuation.

Also, results should be consistently presented with their corresponding errors.

We included the communication of the corresponding errors consistently throughout the text.

Specific comments

2.2 Trace gas measurements

- Were any measurements other than CO2 and N2O made?

Yes, there are other measurements like soil moisture, wet deposition, and meteorological data as outlined in chapter 2.1. We decided to combine both chapters to have a stringent structure.

2.3 Modelling approach

- This section contains very little information about how the LandscapeDNDC model works. What processes does it consider, what timestep does it work at, what drivers does it consider? Is it 1, 2, or 3-dimensional? Later in the MS it is mentioned that the model does not consider lateral flows of water and nutrients. This should be mentioned here as many readers might expect that a "Landscape" model would consider horizontal flows.

We agree with the reviewer. We added the following information into this chapter:

"The biogeochemical model MeTr^x simulates the turnover of soil organic matter and plant debris depending on their chemical structures (e.g., lignin and cellulose content, C/N ratio), soil properties (e.g., pH value) and meteorological drivers. Following the 'anaerobic balloon' concept of Li et al. (2000), major metabolites (e.g., NO_3) are distinguished between aerobic and anaerobic counterparts in order to simulate the share of nitrification and denitrification and the related production of GHG emissions. Simulated model outputs are, among others, emissions of CO_2 and N_2O. The watercycleDNDC model simulates soil water dynamics, i.e., potential evapotranspiration based on Thornthwaite and Mather (1957), transpiration depending on gross primary productivity, the water use efficiency of the modelled plant types and soil water flow based on a cascading bucket model approach (Kiese et al., 2011). The latter determines the advective transport of nutrients into deeper soil layers. All models refer to a one-dimensional soil column, i.e., assuming homogeneous conditions in lateral directions, and were run with a daily time step resolution."

- pg 5, line 3: If only G1 can be modelled then G2 should not be included in Tables 2 and 3. If G2 is sufficiently different from G1 then it does not make sense to average the results for these two systems

We see the problem with Table 2 and 3. However, we think it makes sense to report the measured fluxes of G2. Instead of deleting this data, we decided to split the rows/columns in Table 2 and 3 for G1 and G2 and explicitly state again, that G2 is not part of the modelling part to prevent confusion.

Table 1

- A column with management practices applied (e.g. manure and fertiliser applications) would also be informative

We like the reviewer's idea and added information about management practices in Table 1.

- Why are the ranges for organic C and N expressed as high-low when all the other ranges are low-high?

We added the missing explanation in the table header: "In case spans are given, they reflect observed ranges for measurements used throughout the set up of the soil profile, given from the top layer setting to the bottom layer of the model."

3.1 Measured N2O fluxes

- pg 6, line 27: Need to clarify what you mean by "no statistical difference over time". Do you mean no differences in the annual cumulative emissions?

We added the following details: "There were no significant differences over time between the three weekly measured transects on arable land (Table 2)". The header of Table 2 explains the underlying statistical test.

- pg 6, line 27: "Highest emissions occur after management events". This is not always true. For example, between May and Sept 2014 there's a measured peak several months after the last management practice

Changed to: "The highest emissions occur mostly after management events."

- pg 6, line 30: CO2e incorrectly calculated. 4.5 kg N2O-N = 7.07 kg N2O (4.5 * 44/28) = 2107 kg CO2e (7.07 * 298) = 575 kg CO2e-C (2107*12/44)

We thank the reviewer for detecting this mistake. We corrected the calculation accordingly throughout the manuscript.

- Grassland N2O: Given that the grazed site and the wetland have different management, soil and vegetation properties it seems strange to combine them both as a single "grassland" type.

We are in line with the reviewer and separated the description of G1 and G2 into the subchapters "Grassland N2O fluxes" and "Wetland N2O fluxes". To be consistent, we did the same in chapter 3.2.

- pg 7, lines 21-22: Conversion of emissions to CO2-Ce is incorrect (see comment for pg 6, line 30)

Changed accordingly.

- pg 7, line 22: How was the emission factor of 5.4% calculated? According to Table 4 the manure N input was 7.57 kg N/ha/a. Assuming no background emissions this gives an emission factor of 0.29/7.57 *100% = 3.8%

Our emission factor value was based on older results, the reviewer is right: the correct emission factor is 3.8%. We changed it accordingly.

- pg 7, line 7: The percentage differences between the forest transects are incorrectly stated. For example, W1 has 3x the emissions of W2, but this is a difference of +200% not +300%. Similarly for the difference between W3 and W2
Changed accordingly.
- pg 7, line 30: The measured negative fluxes are all small compared to the measurement error. Therefore, how do you know that the negative fluxes are real and not just the result of measurement error?
We thank the reviewer for this comment and added it into the manuscript: "However, our measured negative emissions are low compared to the variance between transects (W1-3), i.e., they could also originate from measurement errors."

- pg 7, line 33: Figure A3 shows the WFPS, but it doesn't the correlation between negative emissions and WFPS
We changed the text to: "Negative emissions occur during times with high WFPS (Fig. A3)."

- pg 7, line 34: Conversion of emissions to CO2-Ce is incorrect (see comment for pg 6, line 30)
Changed accordingly.

- pg 8, line 1: 0.08 is almost two orders of magnitude smaller than 5.1
Changed accordingly.

Table 2
- The A3:A3 and G1:G1 squares should be blocked out
Changed accordingly.
- G1 and G2 should be separated into two separate categories (grassland and wetland)
Changed accordingly.

3.2 Measured CO2 fluxes
- I disagree with the decision to use different definitions of 'CO2 emission' depending on land use. I think it would be clearer to use distinct terms such as TER and belowground respiration to avoid the potential for reader confusion
We accept the reviewer suggestion. We explicitly differentiate TER and belowground respiration values now throughout the manuscript, instead of defining them all as CO2 emissions.

- In general measured values should be quoted with uncertainties in this section
Added accordingly.

- pg 8, line 21-22: It is confusing to talk about a weekly measured value and then give the units in day^-1
We removed the word weekly.

- pg 8, line 21-22: What are these results "not significantly different" from?
We added the missing information: "are not significantly different between the transects A1-3 (compare Table 3)."

- pg 9, line 5: What were the measured CO2 fluxes negatively correlated with?
We added the missing information: "with WFPS".

Table 3
- The measurements from G1 and G2 should not be averaged as these systems were sufficiently different that only G1 was able to be modelled. Also, Table 2 explicitly states that G2 was not modelled. This should also be stated in Table 3
Changed accordingly.

Figures 3 and 6
- For the arable and grassland sites the total DNDC results contain values higher than any that occur in the individual seasons. How is this possible?

The “Total” column was showing all simulations of DNDC, while the season columns were showing simulation results only where measurements were available. We changed the “Total” column to only show simulations for days where measurements are available. Accordingly, the revised column does not show any higher values as for the individual seasons.
- It is confusing to include G2 in the grassland results as the model was only run for the G1 system

We removed G2 from Figures 2 and 6.

3.3 Modeled N fluxes
- pg 10, line 17: The uncertainty in NO3- leaching is actually the largest in Table 4
The reviewer is right. We corrected the text at this point.

- pg 11, line 1: Need to be more specific about what you mean when you say emissions were highest in spring. Are you talking about the total, mean, median, variance, upper quartile, or maximum of the emissions?
We added the missing information by stating that we mean the total emissions.

- pg 11, line 16: It is not clear what is the simulated N loss large in comparison to? It could be the grassland N inputs or the losses from the arable system.
We are now more specific at this point. The text reads now: “The simulated N loss is substantially larger than the N input …”
- pg 11, line 19: Do you have any evidence of what is happening to organic N stock in the real system?
We do not have any evidence of the N stocks in the soil so far. We added this information into the manuscript: “The model suggests decreasing soil organic N stocks. So far, we have only initial measurements of soil organic N content. However, we assume that the source of additional N in the form of nitrate in shallow groundwater…”

- pg 11, 19-20: It does not make sense to say that the model is mimicking an additional N source that is not included in the model. The model can only simulate what has been included in the model.
We deleted this statement.

- pg 11, line 26-29: What stocking rate was used for the grazing? Note that for grazed systems the emissions will be spatially as well as temporally peaky. In the grazed system the animal urine patches will create emissions hot spots. With only 5 chambers it is possible that the measurements could miss these hot spots. Meanwhile, the DNDC model will assume that the manure is uniformly spread over the field, producing emissions that are likely to be higher than those from non-urine patches, but lower than those from urine patches.
We thank the reviewer for this point. We added this discussion and the stocking rate (n=70 sheep per hectare) into the manuscript.

- pg 11, line 34: Total output is 1.82, total leaching is 0.04, therefore leaching is 0.04/1.82 *100% = 2% of output.
Changed accordingly.

- pg 12, line 7-9: Measured range 0.18-0.48 kg N2O-N/ha/a does not overlap the measured range of 0.03-0.09 kg N2O-N/ha/a.
The reviewer is right, we changed the text accordingly: “The mean modelled annual emissions (0.33 ± 0.15 kg N ha^{-1} a^{-1}) overestimate the observed emissions on all transects.”

Table 4
- Should the forest NH3 emission be "<0.01" rather than ">0.01"?
Yes, changed accordingly.

3.4 Modeled C flux
- pg 14, line 12-13: Not sure what the relevance of Figure 7 is here. The statement "mean modeled fluxes are substantially lower than measured ones" contradicts the results in Table 3
We added the missing information with regard to Figure 7: “…mean modelled fluxes are substantially lower than those measured before and after the harvest (Fig. 7).”

- Arable C cycle: There will be some confounding effects in the before/after tillage and before/after harvest emissions in Figure 7. Unless there is a >2 week gap between harvest and tillage the "pre-tillage" results will include some post-harvest effects and the "post-harvest" results will also include some post-tillage effects. Some discussion of how the model handles tillage and harvest events might be informative here.

We agree with the reviewer that e.g., harvest and tillage effects on soil respiration are not distinguishable by sharp points of time. We added the reviewers concern about confounding effects and added a discussion about the model behavior: “However, unless there is a gap of two weeks or more between harvest and tillage, the "pre-tillage" results will include some post-harvest effects, and the "post-harvest" results will also include some post-tillage effects. Our intention to present the data grouped by these events are the discrepancies between modeled and observed CO_2 dynamics. There is a sharp drop of modeled CO_2 emissions after harvest due to the prompt absence of autotrophic respiration. In reality, there will likely be some ongoing metabolic respiration of plant tissue remaining in the field, which is not represented by the 'assumed' dead plant material in the model. After incorporation of harvest residues (by tilling) modeled CO_2 emissions increase again sharply. The sharp increase is due to the incorporation and hence availability of fresh litter (stubble) and a temporary stimulation of decomposition by the model due to the disruption/aeration of the soil structure. Both, overestimation of fresh litter and/or stimulation of decomposition by the model may contribute to the discrepancies between observed and modelled CO_2 emissions.”

- pg 15, line 6: it is a little odd to describe increasing soil C as an "output" as the C is remaining within the system

Changed to “The rest is related to grazing…”

- pg 15, line 6: Include uncertainties here. In particular it is important to note that the model cannot determine whether the system is net gaining or losing carbon.

We included the uncertainties and the statement of the C balance accordingly.

Table 5

- Should DOC leaching be "<0.01" rather than ">0.01"?

Yes, changed accordingly.

Conclusion

- Table 6: New results shouldn’t be presented in the conclusions. This Table should be in the Results and discussion. There also needs to be an explanation of how the model performance was classified as good, medium, or poor.

We see the reviewers point. However, we do not think that Table 6 presents any new results. It is just summarizing the results of chapter 3.3 and 3.4, which is why we would like to keep this table in the conclusion chapter. We included an explanation how the model performance was classified in the text and in the table header.

- Include uncertainties with results

Changed accordingly.

- It is uncertain whether the grassland was acting as a sink or source of C as the balance 1.35 +/- 4.74 t C/ha/a. Therefore both positive and negative values are within the uncertainty range.

We added this statement in the manuscript. The text reads now: “Whether the extensive grazed grassland is also acting as a sink for C with 1.4 ± 4.7 t C ha^{-1} per year remains uncertain …”

Technical corrections

pg 2, line 14-15: Models are not "driven by" uncertainties. Might be better to use "with"?

Changed as proposed.

pg 2, line 15-16: Revise to "During model application further uncertainties arise due to the uncertainties in the applied forcing data"

Changed as proposed.

pg 6, line 24-25: reference to (Fig. 3), (Fig. 4), and (Fig. 5) should be (Fig. 2), (Fig. 3), and (Fig. 4) respectively
Changed accordingly.

pg 6, line 25: Table 4 is referred to before Table 3
We deleted the reference to Table 4 at this point.

pg 7, line 28: "contribute" should be "attribute"
Changed as proposed.

pg 8, line 20: "N" should be "C"
We deleted the reference to Table 5 at this point.

pg 14, line 10: Delete "perfect"
Changed as proposed.

pg 14, line 17: There is no section 3.1.2
Changed to “chapter 2.1”.

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We would like to thank the reviewer #2 for his highly constructive comments on the manuscript bg-2017-96 "Constraining a complex biogeochemical model for multi-site greenhouse gas emission simulations by model-data fusion"

Response letter to Reviewer #2

The authors used a model-data fusion method to constrain the LandscapeDNDC model with multiple-year greenhouse gas fluxes from arable, forest and grassland sites. I appreciate the authors' effort to parameterize biogeochemistry models using long-term field data. I would like the authors to further clarify some of my concerns:

(1) Is LandscapeDNDC a multi-layer (i.e., vertically-resolved) model? If yes, how many soil layers are included and how do you model the fluxes between layers?

The reviewer's assumption is correct, LandscapeDNDC is vertically-resolved. We included the missing information about the number of layers (arable=85, grassland=40 and forest=45) into the description of the model set up (chapter 2.3.1) and added more details on how the fluxes are modeled: "The watercycleDNDC model simulates soil water dynamics, i.e., potential evapotranspiration based on Thornthwaite and Mather (1957), transpiration depending on gross primary productivity, the water use efficiency of the modelled plant types and soil water flow based on a cascading bucket model approach (Kiese et al., 2011). The latter determines the advective transport of nutrients into deeper soil layers.

All models refer to a one-dimensional soil column, i.e., assuming homogeneous conditions in lateral directions, and were run with a daily time step resolution."

(2) In Tier I and TierII, do you include the same parameters, e.g., all parameters in Table A1? To my understanding, hydrological parameters (e.g., in wcDNDC module) controlling soil water (represented by WFPS) in Teir I will also influence N2O and CO2 in Teir II; however, some key parameters governing the biogeochemistry processes (e.g., in METRX module) do not necessarily affect soil water.

We investigated this potential effect and found no major differences between the WFPS simulation between tierI and tierII. We included this statement into the manuscript and added also some information, which parameters of Table A1 were used in tier I and II.

(3) page 6: please further explain "within best 5% of all simulated RMSEs". Do you mean the best 5% of total number of simulations or the best 5% of unduplicated RMSEs? If it's the former, the number of accepted model runs depends on the total number of model runs. Since multiple objectives (e.g., WFPS in different depths) are considered, do you integrate them (RMSEs) into one single objective? If not, how do you determine the acceptance of a model run?

We added the missing information in the manuscript. The text reads now: "This time, we considered the best 5% of all RMSEs in terms of the respective N_2O and CO_2 emissions for each land use (A1-3, G1 and W1-3).".

(4) Table 6: what are the criteria used to classify model performance?

The criteria result from a subjective classification of the model performances compared with each other. We added this information in the table header and where it is referenced in the manuscript.

Other minor comments:

(5) Table 1: Since the model DNDC include inorganic N, what's the inorganic N amount used in the model?

The model considers various inorganic N species (NH3, NH4, NO3, NO, N2O, NO2). Respective amounts are dynamically calculated during the simulation and depend strongly on field management such as fertilizer (i.e. inorganic nitrogen) application, which we added in Table 1. Regarding model initialization Tab. 1 presents initial values of total soil nitrogen (inorganic and organic). We changed the term accordingly. However, organic soil nitrogen represents by far the dominating initial N pool (>99%).

How do you initialize the model? Using measured values (e.g., Table 1) or implementing model spin-up?

We added the missing information in the manuscript. The text reads now: “We run simulations for all land uses at a daily time resolution for 6 years, starting on 1st January 2010, using the data from Table 1 as initialization and using a model spin-up time of two years.”

(6) please use month names (e.g., January, February,...) to indicate the month in a date (e.g., 01.11.2013)

Changed as proposed.

Constraining a complex biogeochemical model for multi-site greenhouse gas emission simulations by model-data fusion

Tobias Houska[1], David Kraus[2], Ralf Kiese[2], and Lutz Breuer[1,3]

[1] Institute for Landscape Ecology and Resources Management (ILR), Research Centre for BioSystems, Land Use and Nutrition (iFZ), Justus Liebig University Giessen, Giessen, 35392, Germany
[2] Institute of Meteorology and Climate Research - Atmospheric Environmental Research (IMK-IFU), Garmisch-Partenkirchen, 82467, Germany
[3] Centre for International Development and Environmental Research (ZEU), Justus Liebig University Giessen, Giessen, 35392, Germany

Correspondence to: Tobias Houska (tobias.houska@umwelt.uni-giessen.de)

Abstract~~.~~: This ~~paper~~study presents the results of a combined measurement and modelling strategy to analyse N_2O and CO_2 emissions from adjacent arable land, forest and grassland sites in Germany. ~~Measured~~The measured emissions reveal seasonal patterns and management effects ~~like~~, including fertilizer application, tillage, harvest and grazing. ~~Measured~~The measured annual N_2O fluxes are 4.5, 0.4 and 0.1 kg N ha^{-1} a^{-1}, ~~while~~and the CO_2 fluxes are 20.0, 12.2 and 3.0 t C ha^{-1} a^{-1} for the arable land, grassland and forest sites, respectively. An innovative model-data fusion concept based on a multi-criteria evaluation (soil moisture ~~in~~at different depths, yield, CO_2 and N_2O emissions) is used to rigorously test the LandscapeDNDC biogeochemical ~~LandscapeDNDC~~ model. The model is run in a Latin Hypercube based uncertainty ~~analyses~~analysis framework to constrain model parameter uncertainty and derive ~~behavioral~~behavioural model runs. ~~Results~~The results indicate that the model is ~~in general~~generally capable ~~to predict the~~of predicting trace gas emissions, as evaluated ~~by~~with RMSE as ~~an~~the objective function. The model shows a reasonable performance in simulating the ~~ecosystems~~ecosystem C and N balances. The model-data fusion concept helps to detect remaining model errors ~~like~~, such as missing (e.g.~~.~~., freeze-thaw cycling) or incomplete model processes (e.g.~~.~~., respiration ~~amount~~rates after harvest). ~~It~~This concept further elucidates ~~identifying~~the identification of missing model input sources (e.g.~~.~~., the uptake of N through shallow groundwater on grassland during the vegetation period) and uncertainty in the measured validation data (e.g.~~.~~., forest N_2O emissions in winter months). Guidance is provided to improve the model structure and field measurements to further advance landscape~~ ~~-scale model predictions.

1 Introduction

Carbon dioxide (CO_2) and nitrous oxide (N_2O) are two prominent greenhouse gases (GHG) contributing to global warming, the latter having a ~~300 times higher~~ global warming potential (GWP) 300 times higher than that of CO_2 considering a 100~~ ~~-year time horizon (Myhre et al., 2013). Terrestrial ecosystems play an important role in the global atmospheric budgets of both GHGs (Cole et al., 1997). ~~Global~~The global CO_2 emissions from soils are five times higher than anthropogenic (mainly fossil fuel) CO_2 emissions (Raich and Schlesinger, 1992; updated with recent fossil fuel data by Boden, et al., 2010), while agricultural land use ~~release~~released over 60% of the global anthropogenic N_2O emissions in 2005 (IPCC, 2007). ~~Besides~~In addition to the radiative forcing of both GHGs, N_2O is currently the main driver of stratospheric ozone depletion (Ravishankara et al., 2009), causing increased ultraviolet radiation, which could result in skin cancer and other health problems (Graedel and Crutzen, 1989). While CO_2 is exchanged with the soil (heterotrophic respiration) and ~~the~~ vegetation (photosynthesis and autotrophic respiration), N_2O fluxes refer mainly to the nitrification and denitrification processes occurring only in the soil (Butterbach-Bahl et al., 2013).

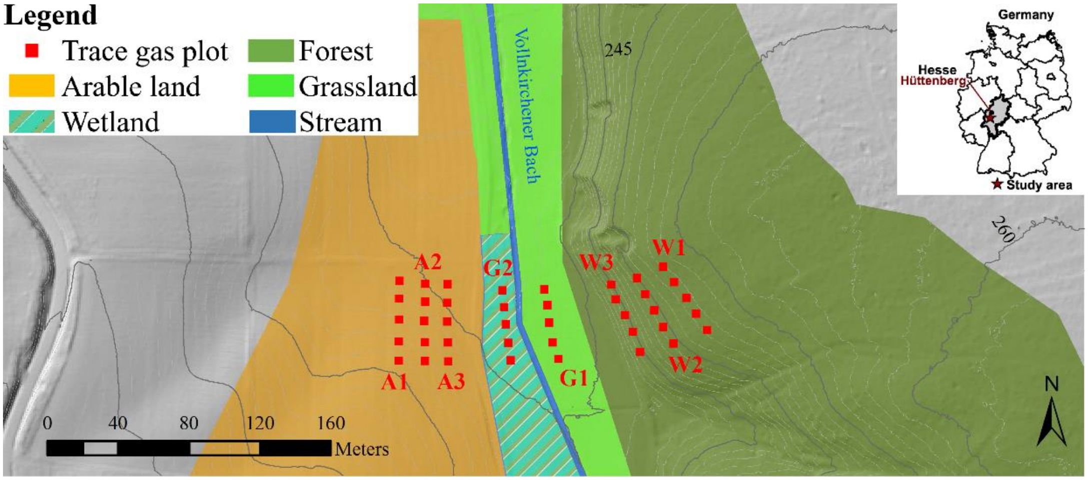
Emissions of both GHGs are highly variable in space~~,~~ and time and depend on a multitude of different interacting environmental factors, e.g., land use/management, nitrogen/carbon inputs, meteorological conditions and physical and chemical soil properties (Davidson, 1992; Smith et al., 2003). They are largely regulated by plant physiological (Rochette et al., 1999) and microbial processes (Burton et al., 2008). Field measurements of GHG emissions and environmental drivers have ~~allowed~~paved the way for a basic understanding of observed emissions patterns. Nevertheless, the large number and complexity of the processes involved in the production and consumption of CO_2 and N_2O are still ~~challenge~~challenges in the reliable quantification of related GHG ~~emission~~emissions (Butterbach-Bahl et al., 2013). ~~Therefore, various~~Various biogeochemical models have been developed in recent years. These models are used for temporal as well as spatial up-scaling of GHG emissions, hypothesis testing of our ~~process~~ understanding of processes, and~~, moreover~~, for scenario analyses and the evaluation of efficient mitigation options (Kim et al., 2015; Molina-Herrera et al., 2016). These include, e.g~~.~~., BASFOR (Oijen et al., 2005), CERES-EGC (Gabrielle et al., 2006), COUP (Jansson, 2012), DAYCENT (Parton et al., 1998) ~~or~~and DNDC and its descendant LandscapeDNDC (Haas et al., 2013). However, models ~~remain as~~are still simplifications of the real world~~, driven by uncertainties due to intrinsic~~ and are prone to multiple sources of uncertainty, i.e., defective model structure~~,~~ and/or parameterization and the current model state (Vrugt, 2016). During model application, ~~further uncertainties are added by applied~~poor-quality model forcing data results in further uncertainties about the predicted model outcome (Kavetski et al., 2006). However, ~~currently~~ there is still no method available ~~dealing~~to properly ~~with all those~~address these sources of uncertainty at the same time (Vrugt, 2016). One promising way to reduce the magnitude of ~~model output~~ uncertainties in model output is to use model-data fusion techniques, i.e~~.~~., matching model prediction with multiple observations by varying model parameters or states using statistical uncertainty estimation (Keenan et al., 2011). There are several statistical uncertainty estimation methods available, e.g., formal Bayesian approaches ~~like~~such as DREAM (Vrugt, 2016) ~~or~~and informal Bayesian approaches ~~like~~such as GLUE (Beven and Binley, 1992). However, ~~they~~these approaches are mostly used to fit models to single types of ~~observation~~observations (Giltrap et al., 2010). Innovative multiple observation data ~~evaluation~~evaluations with model-data fusion ~~is getting~~are becoming common in ecosystem carbon modelling ~~(Wang et al., 2009) and is getting~~(Wang et al., 2009) and are more and more important in the nitrogen modelling community~~, too~~ (Wang and Chen, 2012). ~~Gained~~The knowledge gained can and should be used to guide further model improvements (Vrugt, 2016).

This work focuses on establishing model-data fusion in the biogeochemical community – i.e~~.~~., showing ~~their~~the capability of this technique to ~~gain knowledge with~~improve process understanding through the application of process-based ~~model application.~~models. We present weekly measurements of CO_2 and N_2O emissions from a developed landscape ~~including~~with different land uses, i.e., arable land, grassland and forest ecosystems, covering a two~~ years~~-year period of observations. In addition to field measurements, we set up the biogeochemical LandscapeDNDC model for each of the three land uses. During model-data fusion with GLUE, we rigorously accept only model runs~~, which~~ that return concurrent, acceptable outputs for N_2O, CO_2, and soil moisture ~~in~~at different depths and yields. Posterior model runs are not only evaluated ~~fulfilling~~as to whether they fulfil appropriate objective functions~~,~~ but also regarding realistic simulations of GHG emissions for separate seasons, annual sums as well as before and after land management. The model is finally used to estimate the magnitude and uncertainty of C and N fluxes, ~~like~~such as N_2 emissions or autotrophic and heterotrophic CO_2 emissions, which are not yet experimentally ~~not yet~~ quantifiable *in situ*. ~~Remaining~~The remaining model and data errors are traced back to their potential sources to improve ongoing measurements and future model applications.

2 ~~Material~~Materials and methods

2.1 Study area

The study area is located in the catchment of a low-mountainous creek (Vollnkirchener Bach) in the municipality of Hüttenberg, Hesse, Germany (50°29′56″ N, 8°33′2″ E). One ~~kilometer~~kilometre north of the village of Vollnkirchen, next to the creek, we established eight transects (oriented mostly ~~vertical~~vertically to slope) along a valley cross-section covering different types of land uses (Fig. 1) for GHG emission measurements. See Table 1 for detailed information on soils characteristics. Three transects (A1-A3) are located on arable land ~~westwards~~to the west of the creek and were cultivated with the same field management and crop rotations (Table 1). Three transects are located in a light beech (*Fagus sylvatica*) forest (W1-W3) with young and old trees on a steep hillside (slope: 10%) ~~eastwards~~east of the creek. A shallow 0.05 m litter layer characterizes the forest soils. Furthermore, there are two transects (G1, G2) located ~~on grassland~~ in the riparian zone at a 4 m distance ~~on~~to each side to the Vollnkirchener Bach. One of the two transects is managed and grazed grassland (G1~~) and is~~), mainly covered with brown knapweed (*Centaurea jacea*), meadow foxtail (*Alopecurus pratensis*), red clover (*Trifolium ~~pretense~~pratense*) and ribwort plantain (*Plantago ~~lanceolate~~lanceolata*). The second~~ grassland~~ transect (G2) represents a wetland and is mainly covered by meadowsweet (*Filipendula ulmaria*), common nettle (*Urtica dioica*), hoary ragwort (*Senecio erucifolius*) and field bindweed (*Convolvulus arvensis*). The groundwater table is close to the surface on both grassland sites. ~~Mean~~The mean annual wet ~~deposition~~depositions of nitrate and ammonium were measured from 2013–2015 with 1.66 kg N ha^{-1} and 3.45 kg N ha^{-1}, respectively. In the catchment, the mean annual precipitation is 588 mm, and the mean annual temperature is 10.5 °C for the hydrological year ~~01.11.~~1st Nov. 2013~~ 31.10.~~ - 31st Oct. 2014 ~~(Seifert et al., 2016). Soil~~(Seifert et al., 2016). The soil moisture is measured at A3 [0.2, 0.4 and 0.6 m], at G2 [0.1 and 0.25 m] and at W1 [0.15 and 0.25 m] and has been recorded ~~in~~at an hourly resolution since 2013.



~~**Figure 1: Map of the study area. Red squares represent GHG chamber positions at the different transects. Dark grey contour lines represent 5 m differences in elevation, light grey areas are outside of the catchment area.**~~

~~2.2 Trace gas measurement~~

The weekly trace gas measurements ~~started~~began in November 2013~~.~~ and range so far until December 2015. GHG exchange fluxes were measured manually ~~measured~~ with non-steady state opaque chambers, each covering a basal area of 0.12 m^2. Chambers were placed on frames (both polypropylene~~)~~), which were inserted approx. 8 cm into the soil in order to facilitate gas~~-~~-tight sampling as well as to avoid soil ~~structure~~structural damage and lateral trace gas leakage. Each chamber is equipped with an extraction septum, a counterbalance valve (in-box pressure balance) and a small fan/ventilator for homogenous mixing of the headspace air. During a 40~~ minutes~~-minute closure period, five air samples are taken from the chamber headspace at regular time intervals t0-t4 of ten minutes (0, 10, 20, 30 and 40 min.). Samples are ~~analyzed~~analysed by gas chromatography (GC 8610C, SRI Instruments, Torrance, US) with an ECD for N_2O and a methanizer and FID for CO_2. Sampling was performed on a weekly basis, with five replicated chambers per transect sampled by the gas sample pooling technique (Arias-Navarro et al., 2013). According to this approach, at any time interval (t0-t4~~)~~), 10~~ ~~-ml headspace ~~sample~~samples are collected subsequently from any of the five replicated chambers and are pooled into one gas~~-~~-tight glass vial (SRI Instruments). ~~Trace~~The trace gas fluxes are calculated from the rate of change in the headspace gas concentration over time by linear regression and were corrected ~~by~~for the chamber temperature, atmospheric pressure and chamber volume according to Barton et al. (2008). All measurements with a regression quality of $r^2 < 0.7$ for CO_2 (using at least four individual samples) were rejected.

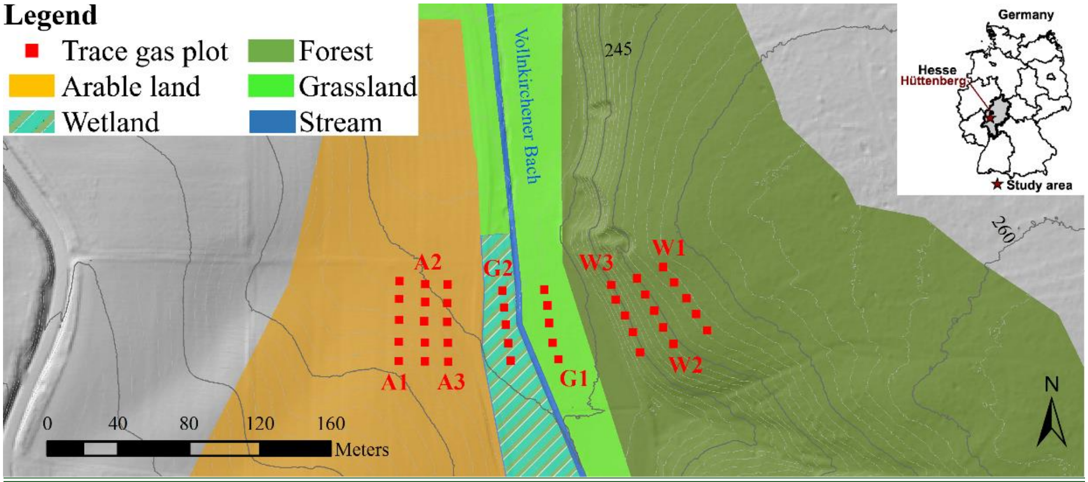


Figure 1: Map of the study area. Red squares represent GHG chamber positions at the different transects. Dark grey contour lines represent 5 m differences in elevation. Light grey areas are outside of the catchment area.

Soil emissions of CO_2 and N_2O can be subject to significant diurnal patterns, with peak values observed in the early afternoon (Savage et al., 2014), ~~making an~~impeding the up-~~scale process~~scaling of hourly measured emissions (usually obtained at midday) to daily values~~ difficult~~. We performed multiple linear regression (ordinary least ~~square~~squares regression including air temperature, relative humidity and water filled pores space~~),~~) to account for the difference between, e.g., daytime (Wohlfahrt et al., 2005a) and ~~nighttime~~night-time respiration (Wohlfahrt et al., 2005b). In our dataset, only CO_2 emissions showed significant correlations with the mentioned environmental drivers on arable land ($r^2 = 0.53$), grassland ($r^2 = 0.59$) and forest ($r^2 = 0.51$). Following Subke et al. (2003), we derived an hourly integration formula in order to obtain daily representative mean values of CO_2 emissions from our field measurements conducted mostly between ~~9am–5pm.~~9 am and 5 pm. N_2O emissions are up-scaled to daily mean values with the common approach, i.e., by multiplying hourly emissions ~~with~~by 24. Annual CO_2 and N_2O emissions are calculated by linear interpolation between the measurements. All the underlying data ~~of chapter~~in sections 2.1 and 2.2 ~~is~~are available ~~on~~upon request from a database (http://fb09-pasig.umwelt.uni-giessen.de:8081/).

2.3 Modelling approach

2.3.1 Model set up

We tested the biogeochemical model framework LandscapeDNDC (Haas et al., 2013) with the observed data ~~of~~from our study area. Individual models were set up for arable land, grassland and forest ecosystems. The ~~modules~~models describe different processes in ecosystem compartments, i.e~~.~~., mathematical descriptions of microclimate, water cycle, plant physiology and soil biogeochemical processes. We applied the biogeochemical ~~module~~model MeTr^x (Kraus et al., 2015) and the ~~watercycle module~~water cycle model watercycleDNDC (Kiese et al., 2011) for all land uses~~, but selected individual physiology modules, i.e. arableDNDC for arable, PSIM/TREEDYN for forest and grasslandDNDC for grassland simulations. As LandscapeDNDC~~

is not yet capable for wetland simulation, we included only G1 within the modelling activities. The three different model setups were driven by the same meteorological data and initialized by land use specific soil and vegetation characteristics (Table 1). . The biogeochemical model MeTr^x simulates the turnover of soil organic matter and plant debris depending on their chemical structures (e.g., lignin and cellulose content, C/N ratio), soil properties (e.g., pH value) and meteorological drivers. Following the 'anaerobic balloon' concept of Li et al. (2000), major metabolites (e.g., NO_3) are distinguished between aerobic and anaerobic counterparts in order to simulate the share of nitrification and denitrification and the related production of GHG emissions. Simulated model outputs are, among others, emissions of CO_2 and N_2O. The watercycleDNDC model simulates soil water dynamics, i.e., potential evapotranspiration based on Thornthwaite and Mather (1957), transpiration depending on gross primary productivity, the water use efficiency of the modelled plant types and soil water flow based on a cascading bucket model approach (Kiese et al., 2011). The latter determines the advective transport of nutrients into deeper soil layers.

All models refer to a one-dimensional soil column, i.e., assuming homogeneous conditions in lateral directions, and were run with a daily time step resolution. Tab. 1 provides an overview of the major model driving data, i.e., meteorological data and land use-specific soil and vegetation characteristics. To simulate plant growth on the three different land use types, we selected the individual physiology modules arableDNDC, grasslandDNDC (Kim et al., 2015; Molina-Herrera et al., 2016) and PSIM (Grote et al., 2009).

Arable soils are stagnic luvisols with a thick loess layer, modelled down to 2.0 m with 80 layers, while the actual soil depth is unknown. Gleysols in the meadow grassland site were modelled down to 0.5 m (set up with 40 layers), corresponding to the mean annual groundwater table depth. The thin and stony soil at the forest site is a cambisol and modelled down to bedrock (0.55 m, set up with 45 layers) with a litter height of 0.05 m. The bulk density increases with depth for every land use, while soil organic carbon and nitrogen decrease with depth. We run simulations for all land uses at a daily time resolution for 6 years, starting on 1st January 2010, using the data from Table 1 as initialization and using a model spin-up time of two years.

Table 1: Input settings of the LandscapeDNDC model for the three different land uses in the Vollnkirchener study region, based on measurements and farmers management documentation. In case spans are given, they reflect observed ranges for measurements used throughout the set up of the soil profile~~.~~, given from the top layer setting to the bottom layer. The soil depth was estimated for model set up. F = fertilizer application, M = manure application.

Input	Arable (A1-3)	Grassland (G1)	Forest (W1-3)	Unit
Vegetation type	~~09/10–07/11 Winter Barley~~ ~~08/11–08/12 Rape~~ ~~10/12–08/13 Winter Wheat~~ ~~10/13–08/14 Triticale~~ ~~09/14–08/15 Triticale~~ ~~10/15–07/16 Rape~~ Sep 10 - Jul 11 Winter Barley Aug 11 - Aug 12 Rape Oct 12 - Aug 13 Winter Wheat Oct 13 - Aug 14 Triticale Sep 14 - Aug 15 Triticale Oct 15 - Jul 16 Rape	Perennial grass	Light beech forest	-
Management	2 Mar12 166.5 kg N ha^{-1} (F) 2 Apr 12 49.9 kg N ha^{-1} (F) 8 Nov 12 56.2 kg N ha^{-1} (F) 11 Mar 13 54.0 kg N ha^{-1} (F) 23 Apr 13 53.8 kg N ha^{-1} (F) 3 May 13 29.3 kg N ha^{-1} (M) 3 May 13 538.0 kg C ha^{-1} (M) 12 Nov 13 29.0 kg N ha^{-1} (M) 12 Nov 13 533.0 kg C ha^{-1} (M) 11 Mar 14 54.0 kg N ha^{-1} (F) 1 Apr 14 53.8 kg N ha^{-1} (F) 8 May 14 40.5 kg N ha^{-1} (F) 22 Sep 14 149.0 kg C ha^{-1} (M) 22 Sep 14 8.1 kg N ha^{-1} (M) 8 Nov 14 1032.0 kg C ha^{-1} (M) 8 Nov 14 56.2 kg N ha^{-1} (M) 11 Mar 15 1564.0 kg C ha^{-1} (M) 11 Mar 15 85.1 kg N ha^{-1} (M) 10 Apr 15 59.4 kg N ha^{-1} (F) 30 Aug 15 59.4 kg N ha^{-1} (F) 12 Nov 15 29.0 kg N ha^{-1} (M) 12 Nov 15 532.0 kg C ha^{-1} (M)	01 Feb 13 Grazing 01 May13 Harvest 01 Sep 13 Grazing 02 Mar 14 Grazing 01 May 14 Harvest 01 Sep 14 Grazing 20 Jan 15 Grazing 29 Jun 15 Harvest 26 Sep 15 Grazing		-
Soil texture	Sandy clay loam	Sandy clay loam	Sandy clay loam	-
Soil type	Stagnic Luvisol	Gleysol	Cambisol	
Bulk density	1.55–1.60	1.20–1.44	1.36–1.49	g cm^{-3}

Organic carbon	1.57–0.91	2.55–0.71	3.61–1.73	%
~~Organic~~Total soil nitrogen	0.16–0.09	0.29–0.08	0.21–0.11	%
Clay content	23–26	24–25	24–26	%
pH	6.45	4.42	3.5–5.5	-
Soil depth	2.00	0.50	0.55	m

~~Arable soils are Stagnic Luvisols with a thick loess layer, modeled down to 2.0 m, while actual soil depth is unknown. Gleysols at the meadow grassland site was modeled down to 0.5 m, which is approximately the mean annual groundwater table depth. The thin and stony soil at the forest site is a Cambisol and modeled until bedrock (0.55 m) with a litter height of 0.05 m. Bulk density is increasing for every land use in depth, while soil organic carbon and nitrogen are decreasing with depth. We run simulations for any land use in daily time resolution for 6 years, starting on 1st January 2010 with a model spin-up time of two years.~~

2.3.2 Model-data fusion

For the multi-objective Bayesian model calibration, we used a two-tiered Generalized Likelihood Uncertainty Estimation (GLUE) approach (Beven and Binley, 1992). The model was ~~started~~iterated in both ~~tier for~~tiers 100,000 times by changing the parameter sets ~~by~~using Latin ~~Hypercube~~hypercube sampling ~~using~~with the Python software SPOTPY ~~(Houska et al., 2015). Parameters for the physiology and the water-cycle modules where treated land use-specifically, while the parameters of the biogeochemical module were calibrated using data of all land uses (Table A1). We assume no prior knowledge than the given parameter ranges, i.e. consider~~(Houska et al., 2015). The parameters for the physiology and the water-cycle modules were treated as land use-specific, while the parameters of the biogeochemical model were calibrated using the data from all land uses (Table A1). We presuppose no prior knowledge besides the given parameter ranges, i.e., we assume a uniform (non-informative) prior probability distribution for all parameters. We statistically judged the performance of every parameter set to reproduce measurements with a root mean squared error (RMSE). Similar to Bloom and Williams (2015), we do not explicitly consider measurement uncertainty during the model data fusion. As shown in Houska et al. (2017), one-tier GLUE based multi-objective model calibration can result in very low acceptance rates, down to 0.01%. We ~~therefor~~therefore considered a two-~~tiered~~tier GLUE approach~~,~~ in order to increase the identifiability and accuracy of the accepted model runs:

Tier I: In ~~a~~the first step, we constrained the parameter space of the hydrology and plant physiology modules of LandscapeDNDC by investigating the respective parameters of both models (Table A1). We accepted only model runs~~, which are~~ that were within the best 5% of all simulated RMSEs in terms of the respective variable (WFPS ~~in~~at different depths [arable ~~in~~land at 0.2, 0.4 and 0.6 m, grassland ~~in~~at 0.1 and 0.25 m and forest ~~in~~at 0.15 and 0.25 m], as well as yield on arable land). Parameter sets were accepted~~,~~ if they ~~belong~~belonged to the 5% best model runs for each land use. ~~Results~~ That is, we took the best 5% of the RMSEs for each respective output variable and took only the intersecting parameter set, which are all from the selected variables for one land use. The results of tier~~-~~ I are summarized in ~~supplement~~supplementary Fig. A1-A4 and are not further discussed in this ~~paper~~study, as they belong to the initialization of the model.

Tier II: ~~In order to~~To achieve realistic GHG simulations from the $MeTr^x$ biogeochemical module ~~$MeTr^x$~~ of LandscapeDNDC, we took the posterior parameter boundaries of tier I and ran GLUE with all parameters of Table A1 again. This time, we considered the best 5% of all RMSEs in terms of the respective N_2O and CO_2 emissions for each land use (A1-3, G1 and W1-3). Again, only the 5% best intersecting parameter sets were accepted per land use. These results are shown in the following chapters. There was no major effect of the biogeochemical model parameters on the WFPS simulation.

Posterior model runs of tier II were further investigated in three different ways:

(1) Seasonal comparisons of measured and ~~modeled~~modelled emissions for spring (~~21.03-20.06.),~~21st March - 20th June), summer (~~21.06.-20.09.),~~21st June - 20th September), autumn (~~21.09.-20.12.),~~21st September - 20th December), and winter (~~21.12.-20.03.).~~21st December - 20th March).

(2) Management comparison of measured and ~~modeled~~modelled emissions, i.e~~.~~., investigation of model performance within two weeks before and two weeks after management events to check model performance in generating hot moments, e.g~~.~~., after fertilizer application.

(3) Model performance in simulating magnitude and uncertainty of C and N fluxes not measured *in situ*, ~~like~~such as N_2 or autotrophic and heterotrophic components of CO_2 emissions.

3 Results and discussion

3.1 Measured N_2O fluxes

To determine the representativeness of each transect for a given land use, the respective differences ~~of~~in measured N_2O emissions were compared (Table 2). ~~Temporal~~The temporal dynamics of N_2O emissions are presented (Fig. ~~3), separated into~~2), distinguishing between different seasons (Fig. ~~4~~3) and before/after management~~-~~ events ~~occur~~ (Fig. ~~5). The mean annual N cycle is given in Table 4.~~4).

Arable land N_2O fluxes: Emissions on arable land vary between 0 and 0.3 kg N_2O-N ha^{-1} day^{-1}. There were no ~~statistical~~significant differences over time between the three ~~arable~~ weekly measured transects~~. Highest~~ on arable land (Table 2). The highest emissions occur mostly after management events. ~~Especially mineral~~Mineral fertilizer application in particular stimulates N_2O emissions, causing hot moments from~~ e.g.,~~, for example, March to May 2014. ~~Input~~The input of N through manure application has a minor influence on the magnitude of N_2O emissions. ~~Mean~~The mean annual measured N_2O emissions from arable land are comparably high with 4.5 kg N_2O-N ha^{-1} a^{-1} ~~(Jungkunst et al., 2006)~~(Jungkunst et al., 2006), ~~equaling~~equalling a GWP of ~~1,338~~ 575 kg~~-~~ CO_2-C equiv. ha^{-1} a^{-1}. With a yearly fertilizer application of 248.2 kg N a^{-1} a mean annual emission factor (EF) of 1.4% (varying between 1.2% for A2 and 1.8% for A3) can be calculated, where 1 kg N ha^{-1} a^{-1} is attributed to the background emissions of unfertilized soil (IPCC, 1997). This EF is inside the IPCC~~-~~-assumed range of 1.25

±1% and close to the average EF (1.56%) of several (n=56) agricultural sites in Germany (Jungkunst et al., 2006). A robust finding throughout the literature is that reduced nitrogen input would lead to lower emissions and therefore more climate-friendly agriculture (Bouwman et al., 2002).

Grassland N_2O fluxes: N_2O emissions ~~vary~~ significantly vary between the grazed site G1 and the wetland site G2, which can be ~~attribute~~attributed to differences in management, hydrological, soil and vegetation characteristics. Most likely, the nitrate supply through groundwater and uptake by the rooting system of the plants is important (Liebermann et al., 2017). Even though the groundwater table (0.2 - 0.4 m ~~below ground~~belowground) is rather shallow in the winter/spring, the uptake rates in summer/autumn (groundwater table 0.3 - 1.0 m ~~below ground~~belowground) are supposedly larger due to the vegetation period. Here, capillary rise ~~might~~may play a relevant role ~~(Orlowski et al., 2016). While G1, with a mix of *Centaurea jacea, Alopercurus pratensis*, *Plantago lancelotata* and *Trifolium prantense*, is grazed by sheep twice a year and cut once a year, the non-managed transect G2 is dominated by other species like *Urtica dioca*, *Filipendula ulmaria* and *Senecio erucifolius*. Typically, a deeper rooting system is found compared to G1 and accordingly, additional nitrate uptake from the groundwater is more prevalent. Mean measured emissions are higher on non-managed G2 than on grazed G1 throughout the year, especially during summer and autumn (Fig. 3). Emissions from~~(Orlowski et al., 2016). G1 is characterized by a mix of *Centaurea jacea, Alopecurus pratensis*, *Plantago lanceolata* and *Trifolium pratense*, is grazed by sheep twice a year and is cut once a year. Emissions from the grazed grassland vary between -0.0019 and 0.014 kg N ha^{-1} day^{-1}. High emissions were measured after grazing, e.g~~.~~., in March 2014 when sheep dung was stimulating N_2O emissions. Negative values depict N_2O uptake~~,~~ and are frequently found under prevailing wet conditions in spring, a finding that was also reported by ~~Glatzel and Stahr (2001).~~Glatzel and Stahr (2001). The grassland annual N_2O emissions are much lower than those observed for the arable system (A1-3). However, with 0.29 ~~(G1) and 0.52~~ kg N_2O-N ha^{-1} a^{-1} ~~(G2)~~are they ~~are~~ in ~~line~~accordance with a study site 12 km northeast of our site, where annual emissions ~~amount to~~range from 0.18 to 0.79 kg N_2O-N ha^{-1} a^{-1} on an unfertilized grassland with shallow groundwater table (Kammann et al., 1998). ~~They~~Their study also ~~report~~reports a similar seasonal pattern ~~we found~~to our measurements, with emissions close to zero in the dry and colder autumn months. ~~Measured~~The measured annual emissions

Table 2: Mean measured annual fluxes (Nov 2013 - Dec 2015) on the different land use transects of the Vollnkirchener Bach study area. Differences between the investigated transects and land uses for measured and modelled N_2O emissions in kg N-N_2O ha^{-1} a^{-1}. * = significant difference ($p < 0.05$, Kruskal-Wallis test). Arable (A1-3), Grassland (G1), Wetland (G2), Forest (W1-3), RMSE in kg N-N_2O ha^{-1} day^{-1}.

	A1	A2	A3	G1	G2	W1	W2	Measured	Mean measured	Mean simulated	Posterior RMSE
A1								4.08			0.0326 - 0.0353
A2								3.87	4.49	7.33	0.0238 - 0.0278
A3								5.53			0.0285 - 0.0329
G1	*	*	*					0.29	0.29	0.69	0.0029 - 0.0038
G2	*	*	*	*				0.52	0.52	-	not simulated
W1	*	*	*		*			0.09			0.0022 - 0.0025
W2	*	*	*	*	*			0.03	0.08	0.33	0.0014 - 0.0021
W3	*	*	*		*		*	0.13			0.0018 - 0.0021

are below the assumed background level of N_2O-N emissions of 1 kg N_2O-N ha^{-1} a^{-1} from agricultural soils (IPCC, 1997). ~~Our~~The annual N_2O emissions are equal to a GWP of ~~87 (G1) and 156~~37 kg CO_2-C equiv.~~-~~ ha^{-1}~~-~~ a^{-1} ~~(G2).~~. The EF through grazing is ~~5.4~~3.8%, which is in ~~line~~accordance with ~~usually found~~typical emissions factors from extensive grazed grasslands, ranging globally from 0.2 - 9.9% (Oenema et al., 1997).

Wetland N_2O fluxes: The non-managed transect G2 is dominated by species such as *Urtica dioica*, *Filipendula ulmaria* and *Senecio erucifolius*. Typically, a deeper rooting system is found compared to that in the grazed grassland transect G1, and accordingly, additional nitrate uptake from the groundwater is more prevalent. The mean measured emissions are higher on the non-managed G2 than on the grazed G1 throughout the year, especially during summer and autumn (Fig. 3). The annual emissions are accordingly nearly two times higher at 0.52 kg N_2O-N ha^{-1} a^{-1}, which is equal to a GWP of 66 kg CO_2-C equiv. ha^{-1} a^{-1}.

Forest N_2O fluxes: Significant differences were found for the forest transects W2 and W3, which can be explained by natural variations along the steep hillslope: On the hillside (W2) the soil is potentially washed out through lateral transport, leading to decreased ~~nutrition~~nutrient availability, compared to the ~~dryer~~drier top (W1, +~~300~~200% N_2O emissions) and the wetter hillfoot (W3, +~~430~~330% N_2O emissions). The N_2O emissions from the forest transects are ~~most of the time~~mostly low, ranging between -0.003 and 0.004 kg N ha^{-1} day^{-1}. Higher emissions were measured only for several weeks in January 2014, with the highest values observed at W1. We ~~contribute~~attribute this to freeze~~-~~-thaw effects, typically found when year-around measurements are considered (Papen and Butterbach-Bahl, 1999). Negative fluxes were measured~~ e.g.~~, for example in March and May 2014. The underlying process of N_2O uptake has been reported before (e.g., Flechard et al., 2005; Neftel et al., 2007) and is assumed to be a microbial process, in which ~~denitrifier~~denitrifiers use N_2O as an electron acceptor for respiration under wet/anaerobic conditions (Bremner, 1997). Negative emissions ~~are positively correlated~~occur during times with high WFPS (Fig. A3~~) being~~), which is in ~~line~~accordance with Bremner~~-~~ (1997)~~.~~. However, our measured negative emissions are low compared to the variance between transects (W1-3), i.e., they could also originate from measurement errors. Our annual measured emissions in ~~forest~~forests are ~~with~~ 0.08 kg N_2O-N ha^{-1} a^{-1} (GWP of ~~25~~10 kg CO_2-C equiv.~~-~~ ha^{-1} a^{-1} CO_2 emissions~~)~~), which is much lower than that at adjacent grassland and arable sites. ~~Even more they are a~~Moreover, this value is almost two orders of magnitude lower than the N_2O emissions (5.1 kg N_2O-N ha^{-1} a^{-1}) measured from a beech forest in~~ the~~ Högelwald, Germany (Papen and Butterbach-Bahl, 1999). A likely reason is the substantially higher annual deposition rate of 25 kg N ha^{-1} a^{-1}, ~~a~~an N input five times higher ~~N input as compared to~~than that in our system. However, our measurements of N deposition only ~~includes~~include wet deposition. Additional dry depositions ~~is~~are often assumed to add another 30-60% to total atmospheric N deposition (Flechard et al., 2011).

~~**Table 2: Mean measured annual fluxes (11/2013-12/2015) on the different land use transects of the Vollnkirchener Bach study area. Differences between the investigated transects and land uses for measured and modeled N_2O emissions in kg N-N_2O ha^{-1} a^{-1}. * = significant difference ($p < 0.05$, Kruskal-Wallis test). Arable (A1-3), Grassland (G1), Wetland (G2), Forest (W1-3), RMSE in kg N-N_2O ha^{-1} day^{-1}.**~~

	A1	A2	A3	G1	G2	W1	W2	Measured	Mean measured	Mean simulated	Posterior RMSE
A1								4.08	4.49	7.33	0.0326 - 0.0353
A2								3.87			0.0238 - 0.0278
A3								5.53			0.0285 - 0.0329
G1	*	*	*					0.29	0.29	0.69	0.0029 - 0.0038
G2	*	*	*	*				0.52			not simulated
W1	*	*	*		*			0.09	0.08	0.33	0.0022 - 0.0025
W2	*	*	*	*	*			0.03			0.0014 - 0.0021
W3	*	*	*		*		*	0.13			0.0018 - 0.0021

3.2 Measured CO_2 fluxes

Emissions measured using our closed chamber on arable land and grassland include those from soil and vegetation, as the entire plants are covered by the chamber. Therefore, we interpret these emissions as total ecosystem respiration (TER). In contrast, chambers in the forest were placed on the forest floor without any vegetation inside,; thus, these measurements include soil (heterotrophheterotrophic) and root (autotrophautotrophic) respiration, only. For the sake of a better read-flow, we decide to define emissions from the different land use as 'CO_2 emissions', even though we considered the different flux components on different land use.i.e., below ground respiration only. To determine the representativeness of each transect for a given land use, the respective differences ofin measured CO_2 emissions were compared to each other (Table 3). MeasuredThe measured CO_2 emissions are given inover time (Fig. 65), separated into different seasons (Fig. 76) and before/after management-events occur (Fig. 8). The mean annual N cycle is given in Table 5.7).

Arable CO_2 fluxes: Weekly measuredTER: Measured values from our arable transects range between 0 andto 175.2, 199.6 and 143.1 kg C-CO_2 ha^{-1} day^{-1} for A1, A2 and A3 respectively and are not significantly different. between the transects (compare Table 3). Emissions occur mainly during the growing season, starting in March and ending in November. For a comparable study site in southern Finland, reported daily TER values under barley during May and September were between 23.6 to 235.6 kg C-CO_2 ha^{-1} day^{-1} during May and September (Lohila et al., 2003), which is in the same range as our observations.(Lohila et al., 2003), which is in the same range as our observations. The annual sum of our TER emissions is 19.96 ± 2.36 t C-CO_2 ha^{-1} a^{-1}. This is slightly lower than yearly TER measured on a winter wheat study site in Belgium with 23.18 t C-CO_2 ha^{-1} a^{-1} (Suleau et al., 2011). Demyan et al. (2016) reported lower values, with an average sumtotal of 11.43 t C-CO_2 ha^{-1} a^{-1}, derived from observations spanning six growing seasons in southwestsouthwestern Germany. However, all studies are possibly prone to overestimations of the emissions from September to November, as daily emissions are generated with a multiple linear regression, model, and in our case, are based on our hourly measurements of air temperature and soil moisture. Such methods do not fully account for management effects like harvest, such as harvests (Subke et al., 2003)(Subke et al., 2003).

Grassland CO_2 fluxesTER: Emissions from grassland vary from 5.0 to 68.3 (G1) and from 0 to 92 kg t C-CO_2 ha^{-1} day a^{-1} (G2),, with no significant difference between the two transects G1 and G2. Emissions are close to zero in the winter months

(December to February) and highest during the growing season. A distinct negative correlation between the measured TER with WFPS was found during wet conditions from end of June to July in 2014. In this time, emissions decrease to 41.0 kg C-CO_2 ha^{-1} day^{-1}. The total yearly emissions are 11.79 t C-CO_2 ha^{-1} a^{-1}, which agrees well with the mean yearly emissions reported for 19 different grassland sites across Europe, with mean annual emissions of 12.83 t C-CO_2 ha^{-1} a^{-1} (Gilmanov et al., 2007). However, due to the many different grassland sites considered in their study, Gilmanov et al. report a much wider range of observed annual TER valuesof measured CO_2 fluxes was found during wet conditions from end of June to July in 2014. In this time emissions drop to values of 41.0 kg C-CO_2 ha^{-1} day^{-1}. The TER of a grassland CO_2 is mainly driven by the growing season (Soussana et al., 2007). Emissions typically end with, from 4.9 to 16.4 t C-CO_2 ha^{-1} a^{-1}. They also found that management is a main influencer of TER, where intensively managed grasslands produce higher emissions than extensively managed grasslands. With regard to grazing, we found only a minor direct impact on the measured flux rates (Fig. 7).

Wetland TER: Emissions from the study site G2 vary from 0 to 92 kg C-CO_2 ha^{-1} day^{-1} and are higher than those from G1, especially in the growing season. This is due to the higher above ground biomass of the different species present and represents a common pattern in unmanaged grasslands (Soussana et al., 2007). Emissions typically end with the cessation of pasture growth during temperatures under 5°C (Parsons, 1988). Total yearly emissions are 11.79 t C-CO_2 ha^{-1} a^{-1}, which agrees well with mean yearly emissions reported for 19 different grassland sites across Europe with mean annual emissions of 12.83 t C-CO_2 ha^{-1} a^{-1} (Gilmanov et al., 2007)The annual emissions are 12.54 t C-CO_2 ha^{-1} a^{-1}, driven by the growing season.. However, due to the many different grassland sites considered in their study, Gilmanov et al. report a much wider range of observed annual TER values from 4.9 to 16.4 t C-CO_2 ha^{-1} a^{-1}. They also found that management as a main influence on TER, where intensively managed grassland produce higher emissions than extensively managed grasslands. With regard to grazing, we found only a minor direct impact on measured flux rates (Fig. 7).

Forest CO_2 fluxes: Mean measured soilbelow ground respiration span from: The mean measured belowground respiration spans between minimum values of 2.1 to 4.5 and maximum values of 9.3 to 19.9 kg C-CO_2 ha^{-1} day^{-1}. between the different transects (W1-3). While we found higher emissions in the summer months, seasonal differences have a lower magnitude asof TER on arable and grassland. This was expected, as we do not measure above ground biomass respiration on our forest study site. Overall, rewetting has the strongest influence on changes of soilin belowground respiration in our forest study sites. HighestThe highest emissions occuroccurred in July 2014 after several rewetting events of the uppermost soil layer (Fig. A1). Xiang et al. (2008) reported that multiple rewetting led leads to respiration rates of up to eight-times higher respiration rates. Total. The total yearly soil emissions are with 2.98 ± 0.89 t C-CO_2 ha^{-1} a^{-1}, which is at the lower end of other European forest ecosystems, e.g.., 6.6 ± 2.9 t C-CO_2 ha^{-1} a^{-1}, as reported by Janssens et al., (2001). The uphill transect W1 has the highest emission rates throughout the year and shows significant differences when compared to W2 and W3. This transect is less shaded throughby trees, resulting in a 1.3°C higher annual mean soil temperature compared to W2 and W3, likely causing higher CO_2-emissions (Table 3).

Table 3: Mean measured annual fluxes (~~11/~~Nov 2013~~-12/~~ - Dec 2015) ~~on~~from the different land use transects of the Vollnkirchener Bach study area. Differences between the investigated transects and land uses for measured and ~~modeled~~modelled CO_2 emissions in t C-CO_2 ha^{-1} a^{-1}. * = significant difference ($p < 0.05$, Kruskal-Wallis test). Arable (A1-3), Grassland (G1), Wetland (G2), Forest (W1-3~~),~~), RMSE in kg C-CO_2 ha^{-1} day^{-1}.

	A1	A2	A3	G1	G2	W1	W2	Measured	Mean measured	Mean simulated	Posterior RMSE
A1								20.10	19.96	20.53	30.73 - 36.38
A2								22.25			35.66 - 42.26
A3								17.54			22.90 - 28.46
G1								11.79	~~12.17~~11.79	13.24	7.01 - 9.08
G2								12.54	12.54	-	not simulated
W1	*	*	*	*	*			4.00	2.98	3.28	3.53 - 3.89
W2	*	*	*	*	*	*		2.38			3.37 - 4.07
W3	*	*	*	*	*	*		2.56			3.15 - 3.96

3.3 ~~Modeled~~Modelled N fluxes

After selecting the posterior model runs ~~according to chapter~~as described in section 2.3.2, we found the model to be generally capable ~~in~~of reproducing the measured data and consequently ~~investigate~~investigated the ~~modeled~~modelled C and N ~~cycle~~cycles in more detail. ~~Modeled~~The modelled N_2O emissions are shown for the different land ~~use~~uses over time (Fig. 2), separated into different seasons (Fig. 3) and before/after management-events occur (Fig. 4). The complete ~~modeled~~modelled N cycle is given in Table 4.

Arable land N cycle: ~~Arable~~ The arable land simulations consider an annual N input of 198 kg N ha^{-1} a^{-1}. This input is balanced by ~~109~~108.6 ± 50.1 kg N ha^{-1} a^{-1} gaseous (primarily N_2), 30.0 ± 29.9 kg N ha^{-1} a^{-1} nitrate leaching and 99.7 ± 7.8 kg N ha^{-1} a^{-1} harvest losses (Table 4), meaning that ~~modeled~~the modelled outputs are higher ~~as~~than the given inputs. This gap in the annual N cycle is fed by ~~storages of the~~ soil storage in the model, indicating N depletion over time. Even though N losses ~~of~~through NO_3^- and particularly N_2O ~~emission~~emissions (7.3 ± 2.3 kg N ha^{-1} a^{-1}) ~~have~~are only a minor ~~percentage in~~proportion of the total N balance, both rates are high regarding their environmental ~~impact~~impacts as a GHG contributing to global warming and as a water pollutant regarding eutrophication and drinking water supply, respectively. However, the uncertainty related to our estimated NO_3^- leaching rate is overall the ~~second~~ largest source of uncertainty ~~source~~ in our N balance. These estimates cannot be sufficiently ~~constraint~~constrained with the given observation data, but they are in ~~line~~accordance with other reported N leaching rates on arable land in Germany (Siemens and Kaupenjohann, 2002).

The simulated N_2O ~~emission~~emissions contribute 3.1% to the total simulated N losses. The underlying model runs follow the trend of the observation data. Hot moments can be observed after fertilizer applications, ~~which~~and they are predicted by the model in time~~,~~ but sometimes not in magnitude (e.g.~~.~~., March to May 2014). During these events, soil moisture is often not ~~modeled~~modelled accurately: The model predicts rewetting processes that have not been measured ~~in~~at the same magnitude (Fig. A1), which might explain the overestimated fluxes. ~~A~~One possible reason ~~can~~may also be uncertain rainfall model input data. Kavetski et al. (2006) found the measurements of precipitation within a catchment to be uncertain, as the trajectory of storm cells through a catchment may be different for each storm and may not have ~~its center~~their centres at the rain gauge, where ~~traditionally~~ rainfall inputs are traditionally measured. Our rainfall data ~~is~~are measured 4 km northeast of the trace gas study area and is likely ~~effected~~affected by such uncertainties.

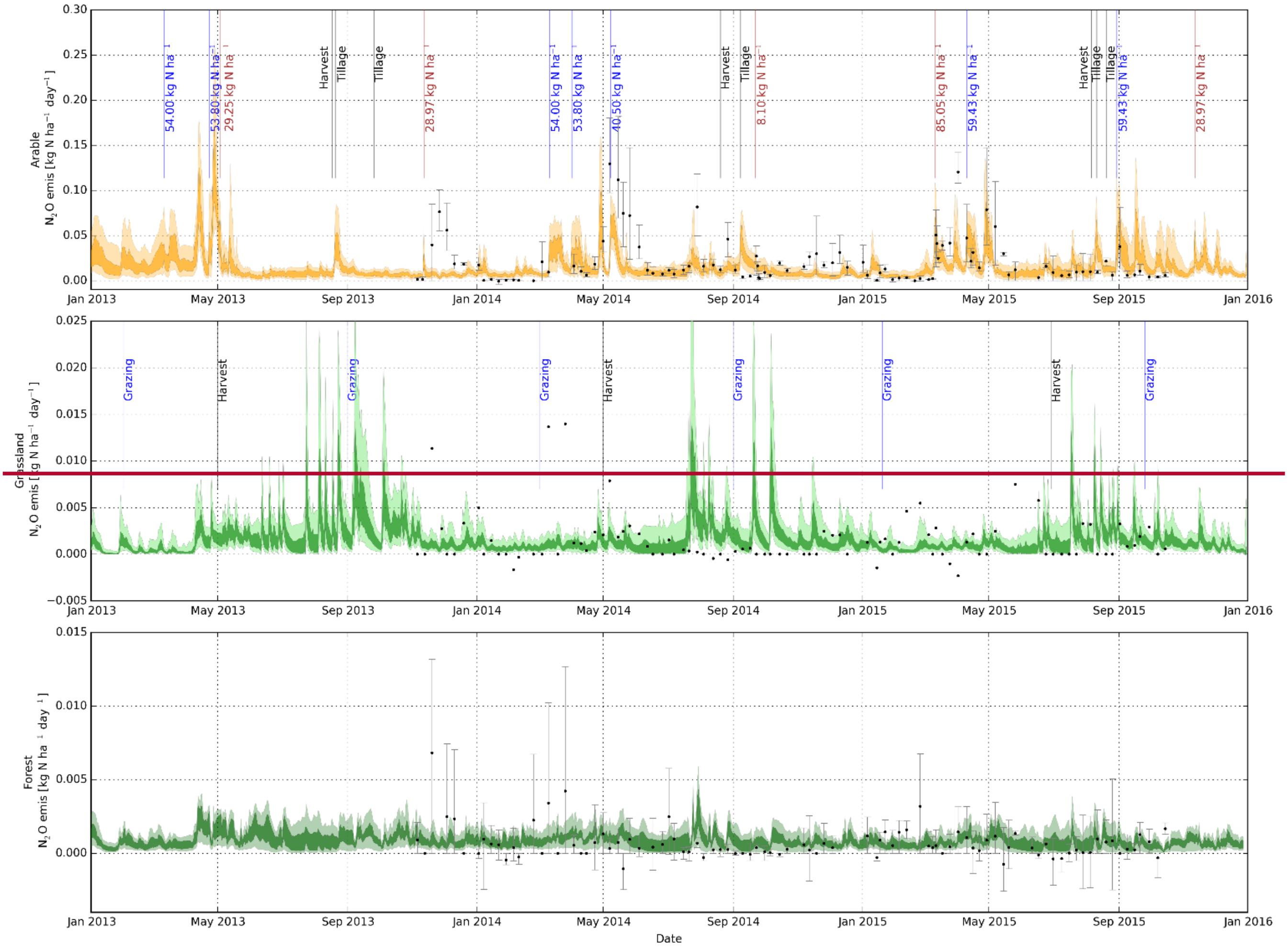
~~For both,~~The total simulated and measured emissions on the arable site are highest in the spring (Fig. 3). While the transects A1 and A2 vary, with 95% of the values between 0 and 0.05 kg N_2O-N ha^{-1} day^{-1}, A3 shows ~~a higher~~more variation, up to 0.15 kg N_2O-N ha^{-1} day^{-1}. As A3 is located at the hill toe, we attribute this effect to the lateral transport of nitrate from uphill. However, our one-dimensional model ~~set up~~setup does not cover lateral water and ~~nutrition~~nutrient transport~~,~~; accordingly, the model is not able to predict the higher emissions at A3 in the spring. While such a process is part of complex integrated hydro-biogeochemical catchment models (Haas et al., 2013; Klatt et al., 2017; Wlotzka et al., 2013), it has not yet been confirmed experimentally. The distributions of the measured emissions in the summer, autumn and winter seasons ~~measured emissions~~ are well in ~~line~~accordance with the ~~modeled~~modelled emissions. Furthermore, the ~~modeled~~modelled emissions are also in agreement with ~~measured~~ emissions measured before and after manure applications (Fig.~~-~~ 4). This result ~~corresponds~~agrees with a study by Molina-Herrera et al., (2016) who found LandscapeDNDC to be capable of simulating agricultural N_2O emissions. However, in our case, the model overestimates peak emissions before fertilizer applications, which leads to higher mean annual ~~modeled~~modelled emissions (7.33 kg N_2O-N ha^{-1} a^{-1}). This is 2.8 kg N_2O-N ha^{-1} a^{-1} higher than our observed emissions and is even outside the large model uncertainty of 2.3 kg N_2O-N ha^{-1} a^{-1}. Hence, future research should ~~particularly~~specifically investigate the reason for this overestimation of peaks, either by revising the model structure or ~~identification of~~by identifying other sources of model uncertainty.

Grassland N cycle: Grassland simulations consider an annual N input of 12.7 kg, with 7.6 kg coming from ~~modeled~~modelled biomass that is transferred into ~~applied~~ dung and urine ~~through~~applied by grazing sheep. ~~Simulated~~The simulated N loss is substantially larger than the N input, with 22.3 ± 13.3 kg N ha^{-1} a^{-1} gaseous losses (primarily N_2), 1.5 ± 3.19 kg N ha^{-1} a^{-1} occurring as nitrate leaching and 29.8~~-~~ ± 9.4 kg~~-~~ N~~-~~ ha^{-1} a^{-1} ~~by~~as biomass removal through grazing sheep and harvest (hay making). Comparing inputs and outputs, we simulated a mean nitrogen gap of ~~41~~40.9 ± 25.9 kg N ha^{-1} a^{-1}. ~~Decreasing~~The model suggests decreasing soil organic N stocks ~~in model simulations indicate~~. So far, we have only initial measurements of soil organic N content. However, we assume that the ~~model is currently mimicking an additional N~~ source~~, which is not included in the current modelling approach. We assume uptake~~ of additional N in the form of nitrate ~~by the~~in shallow groundwater ~~as~~is a potential dominating process that is not included in the current LandscapeDNDC version we used. Liebermann et al. (2017) used a revised LandscapeDNDC ~~set up~~setup for hypothesis testing to identify potential additional N sources in groundwater-dominated grasslands and showed~~,~~ that groundwater N uptake is a likely contributor.

Taking a closer look at the ~~modeled~~modelled N_2O emissions, one can see that the model did not reproduce high ~~as well as~~or negative (N_2O uptake) emissions. Currently, LandscapeDNDC does not consider any N_2O uptake, and accordingly, negative fluxes cannot be simulated by the model. The peaky dynamics of the simulated N_2O emissions, especially from August 2014 to January 2015, are not confirmed by the measurements, indicating possible measurement errors ~~in~~during this period of time. In a grazed system with, in our case, approximately 70 sheep per hectare, the animal urine patches create emissions hot spots. With only five chambers, it is possible that the measurements could miss these hot spots. Additionally, the LandscapeDNDC model will assume that the manure is uniformly spread over the field, producing emissions that are likely to be higher than those from non-urine patches, but lower than those from urine patches. One has also to consider the temporal mismatch of our weekly N_2O measurements and the hourly simulations, making a full match of the observations versuswith the simulations difficult.

ThereSo far, there is no clear effect of grazing on the N_2O emissions on the grassland site in both the measurements and modeledmodelled results (Fig. 4). Mean modeledThe mean modelled annual emissions overestimate the observations by 0.4 kg N_2O-N ha^{-1} a^{-1}, and even the simulated uncertainty bounds of 0.27 kg N_2O-N ha^{-1} a^{-1} do not capture the measured dynamics.

Forest N cylce:cycle: The N input is given for the forest model only byconsidering atmospheric deposition with an annual amount of 5.1 kg N ha^{-1} a^{-1}. Gaseous losses amount to 1.8 ± 2.0 kg N ha^{-1} a^{-1}. Leaching contributes to 2.0.6% of the N output. The rest (3.3 ± 2.0 kg N ha^{-1} a^{-1}) is allocated into biomass and soil. By taking a closer look onat the N_2O emissions (Fig. 2), we see that the model failingfails to reproduce the observed emission dynamics. ObservedThe observed N_2O emissions have high error bars, and not all transects are driven by frost-thaw cycles or N_2O uptake at the same time (Table 2). Parameterizing and simulating the forest transects independentindependently from each other, would improve the simulations. One limiting factor is that both N_2O uptake and frost-thaw cycles are not included in the current version of LandscapeDNDC version. We therefore recommend to particularly include the inclusion of frost-thaw cycles into (e.g., based on De Bruijn et al., 2009) in the model (De Bruijn et al., 2009), as this process can have a major influence on N_2O inventories, e.g.., up to 73% of the total annual N_2O loss ofat a forest site in Högelwald, Germany (Papen and Butterbach-Bahl, 1999) was occurring during such cycles.(Papen and Butterbach-Bahl, 1999). The mean modeledmodelled annual emissions (0.33 ± 0.15 kg N ha^{-1} a^{-1}) overestimate the observed emissions, but capture the mean observed annual emissions with their uncertainty bands of 0.15 kg N_2O-N ha^{-1} a^{-1}. on all transects.


Arable
N2O emis [kg N ha−1 day−1]
0.30
0.25
0.20
0.15
0.10
0.05
0.00
54.00 kg N ha−1
53.80 kg N ha−1
29.25 kg N ha−1
Harvest
Tillage
Tillage
28.97 kg N ha−1
54.00 kg N ha−1
53.80 kg N ha−1
40.50 kg N ha−1
Harvest
Tillage
8.10 kg N ha−1
85.05 kg N ha−1
59.43 kg N ha−1
Harvest
Tillage
Tillage
59.43 kg N ha−1
28.97 kg N ha−1
Jan 2013
May 2013
Sep 2013
Jan 2014
May 2014
Sep 2014
Jan 2015
May 2015
Sep 2015
Jan 2016
Grassland
N2O emis [kg N ha−1 day−1]
0.025
0.020
0.015
0.010
0.005
0.000
−0.005
Grazing
Harvest
Grazing
Grazing
Harvest
Grazing
Grazing
Harvest
Grazing
Forest
N2O emis [kg N ha−1 day−1]
0.015
0.010
0.005
0.000
Date

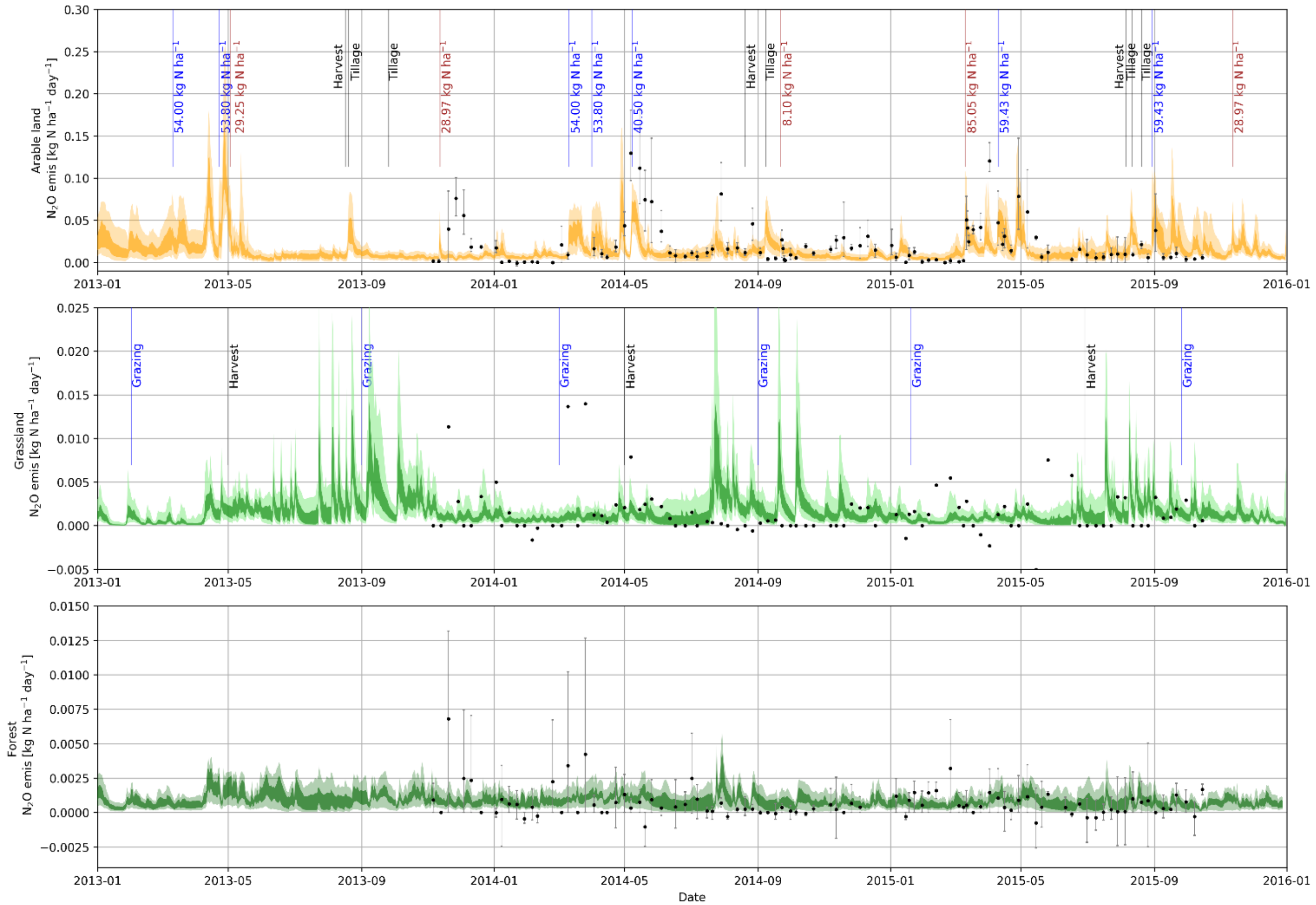
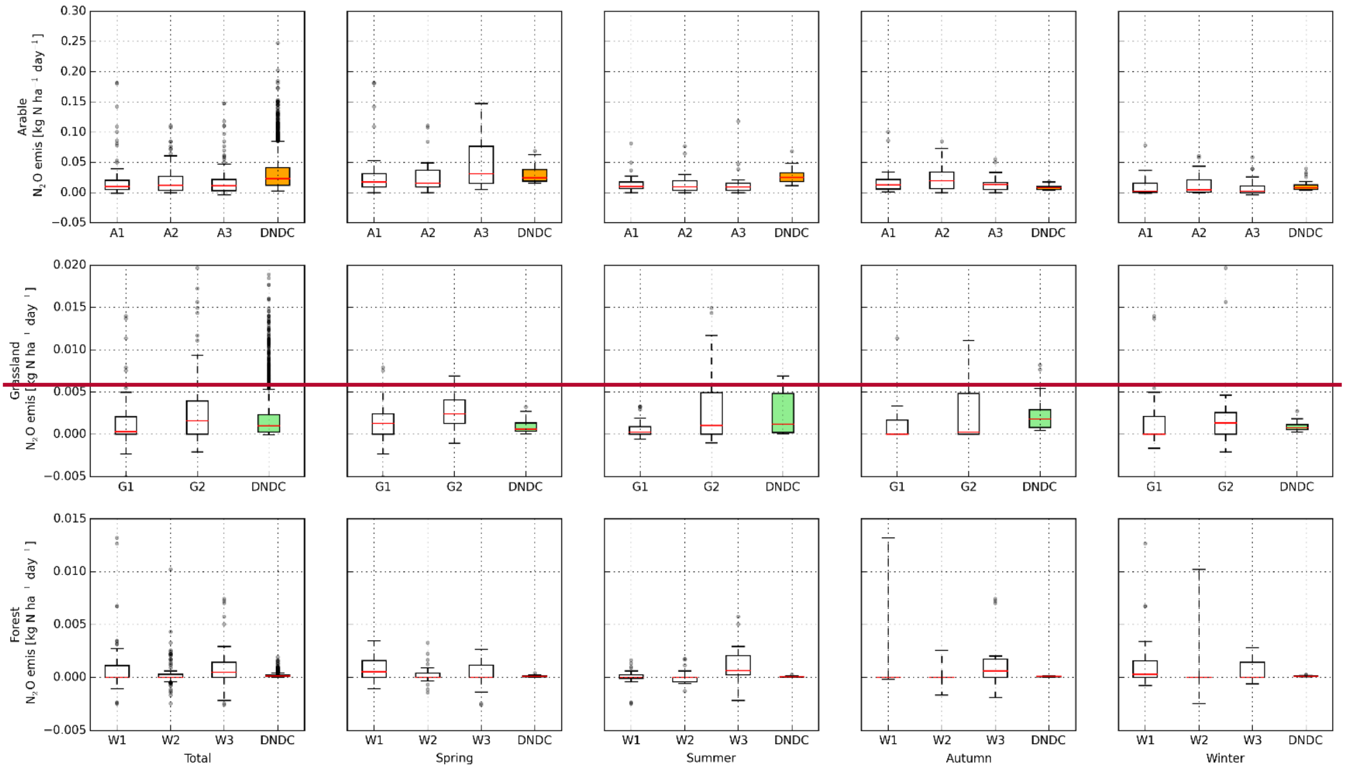


Figure 2: Measured and ~~modeled~~modelled N_2O emissions from different land use. Measurements are given as grey error bars showing the variance between the replicated transects and the mean value as a black dot. Posterior model uncertainty is given in light ~~color~~colour for the 5 and 95 ~~percentile~~percentiles and dark ~~color~~colour for the 25 and 75 ~~percentile~~percentiles. Vertical lines indicate management events. In the uppermost panel, blue ~~colored~~coloured vertical bars indicate fertilizer application, while brown ~~color~~colours indicate manure application.


Arable
N2O emis [kg N ha-1 day-1]
A1
A2
A3
DNDC
Grassland
G1
G2
Forest
W1
W2
W3
Total
Spring
Summer
Autumn
Winter

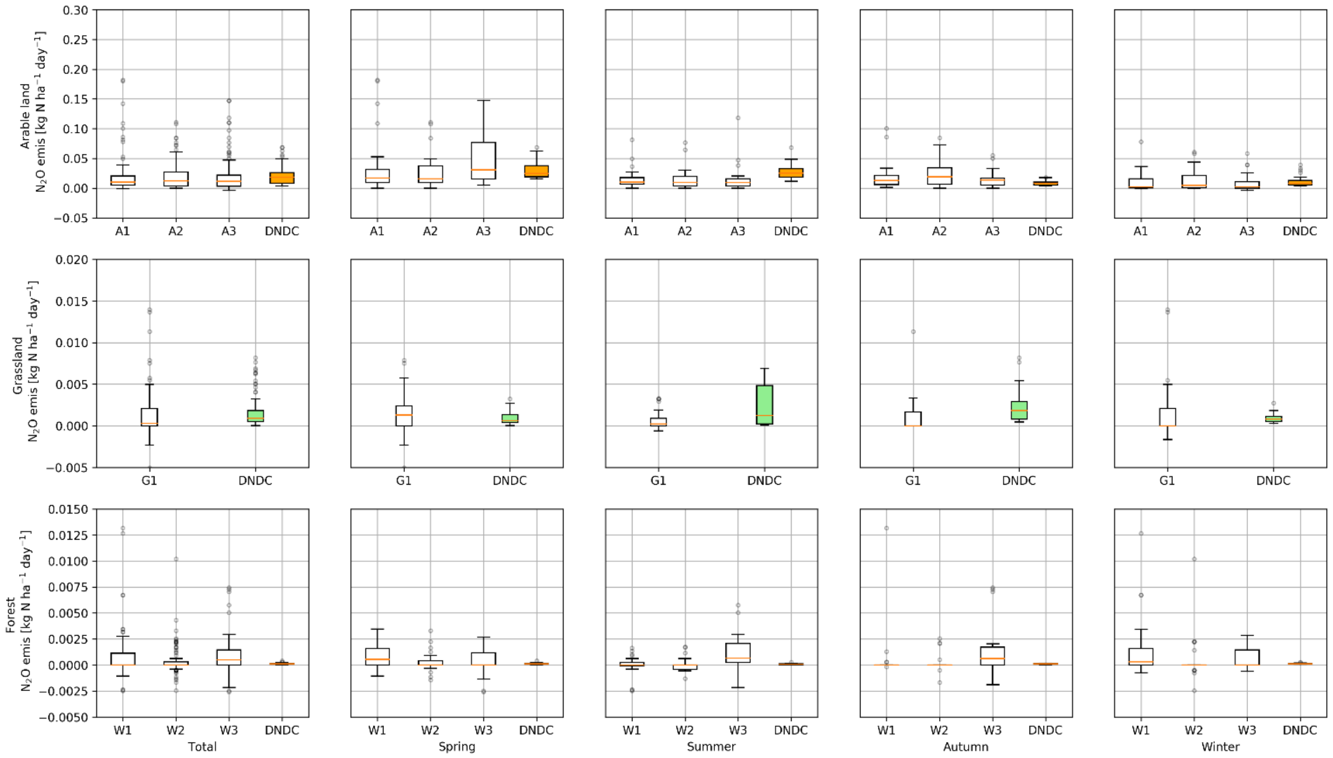
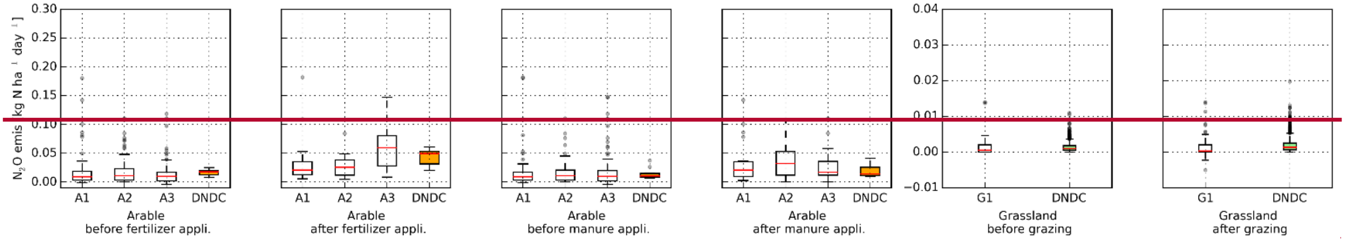


Figure 3: Observed and ~~modeled~~modelled N_2O emissions for spring (~~21.03-20.06~~21st Mar. - 20th Jun.), summer (~~21.06. 20.09~~21st Jun. - 20th Sep.), autumn (~~21.09. 20.12~~21st Sep. - 20th Dec.), and winter (~~21.12. 20.03~~21st Dec. - 20th Mar.).



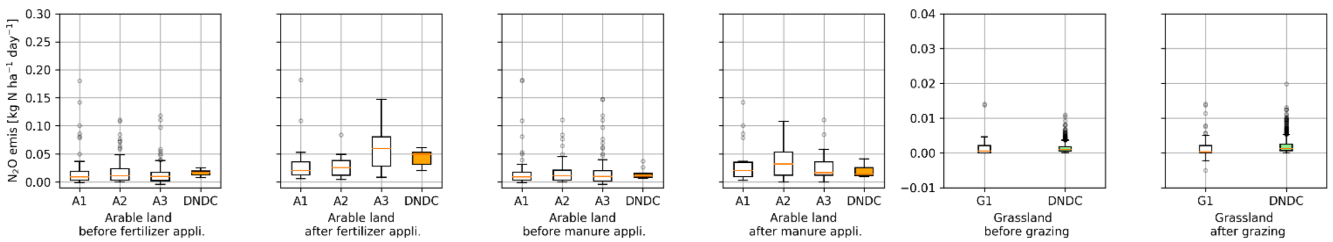


Figure 4: Management effects on N_2O emissions. Measured and ~~modeled~~modelled emissions ~~where selected in~~within a time window of 2 weeks before and 2 weeks after a management.

Table 4: Simulated nitrogen fluxes given by posterior model runs and their uncertainty on different land use in [kg N ha^{-1} a^{-1}]. N manure on grassland includes urine and dung input by sheep. Biomass output on grasslands combines harvest export and biomass leaving the system through sheep. Arable land model assumes 20% return of stubble to field.

Modeled N flux	Arable land		Grassland		Forest	
N deposition	5.11		5.11		5.11	
N manure	57.55		7.57		0	
N fertilizer	135.37		0		0	
Total input	**198.03**		**12.68**		**5.11**	
NO emis.	0.57	±0.16	0.46	±0.21	0.45	±0.33
N_2 emis.	62.55	±26.83	18.69	±10.91	1	±1.5
N_2O emis.	7.33	±2.3	0.69	±0.27	0.33	±0.15
NH_3 emis.	38.15	±20.8	2.45	±1.89	~~>~~<0.01	~~±>~~±<0.01
Total gaseous output	**108.6**	**±50.09**	**22.29**	**±13.28**	**1.78**	**±1.98**
DON leaching	0.01	~~±>~~±<0.01	0.01	~~±>~~±<0.01	0.01	~~±>~~±<0.01
NO_3 leaching	30.01	±29.9	1.46	±3.19	0.03	±0.04
Total leaching output	**30.02**	**±29.9**	**1.47**	**±3.19**	**0.04**	**±0.04**
N grain export	63.92	±5.17	0		0	
N straw export	35.75	±2.67	29.77	±9.44	0	
Total biomass output	**99.67**	**±7.84**	**29.77**	**±9.44**	**0**	
Balance	**-40.26**	**±87.83**	**-40.85**	**±25.91**	**3.29**	**±2.02**

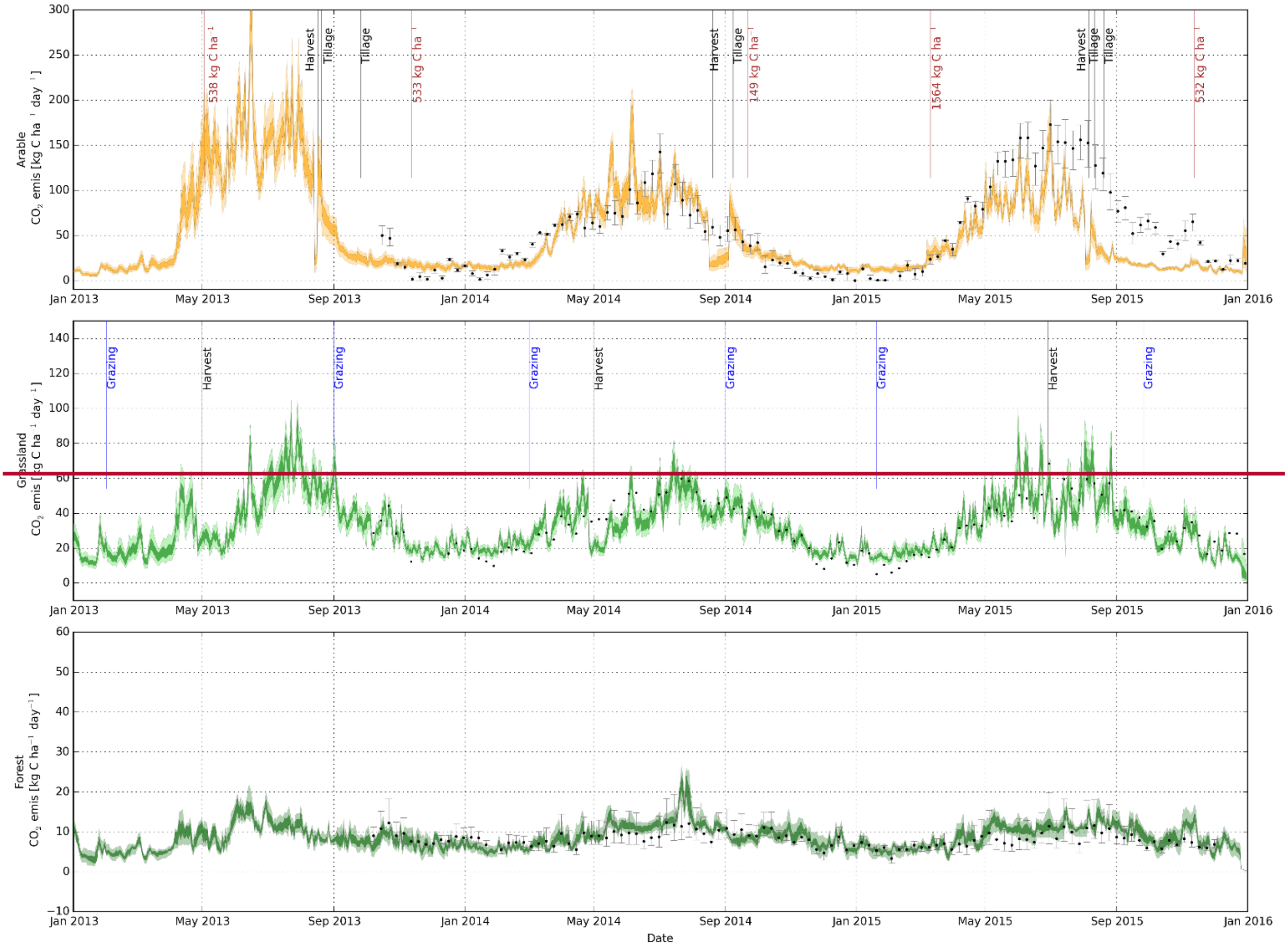
3.4 ~~Modeled~~Modelled C fluxes

~~Modeled~~The modelled CO_2 emissions are shown for the different land uses over time (Fig. 5), separated into different seasons (Fig. 6) and before/after management~~-~~ events ~~occur~~ (Fig. 7). The complete ~~modeled~~modelled C cycle is given in Table 5. Arable land C cycle: The LandscapeDNDC simulations for the arable system predict a mean annual gross carbon uptake of 25.7 ± 1.3 t C-CO_2 ha^{-1} a^{-1}. 20.5 ± 1.8 t C-CO_2 ha^{-1} a^{-1} ~~leave~~leaves the system through respiration, ~~from~~to which maintenance respiration contributes the largest proportion (65%). This is ~~perfect~~ in ~~line~~accordance with annual measured losses (Table 3). ~~Harvest~~The harvest output is with 4.7 ± 0.4 t C ha^{-1} a^{-1} and is in good agreement with the observed yields (Fig. A4). However, the temporal ~~dynamic~~dynamics of the ~~modeled~~modelled TER on the arable land study site ~~underestimates~~underestimate the emissions in the summer season (Fig. 6~~)~~), and the mean ~~modeled~~modelled fluxes are substantially lower than those measured ~~ones~~ before and after the harvest (Fig. 7).

Tillage and harvest events ~~fall into~~occur in the summer season. While the observed emissions drop after harvest by 25%, the ~~modeled~~modelled emissions drop by ~~even~~ 50%. The reason for this is either an underestimation of the emissions through LandscapeDNDC (after harvest events until tillage occurs~~),~~) or ~~the uncertainty in the upscaling method of~~ uncertainties in the measured CO_2 emissions upscaling method (discussed in chapter ~~3.1.~~2.1). As microbial processes can oxidize more soil carbon after ~~harvest~~harvests (resulting in higher heterotrophic respiration), we assume that the discrepancy ~~is rather stemming~~stems from the model simulations. There are ~~also~~ studies, e.g~~.~~., Buyanovsky et al. (1986), ~~who~~which report the highest soil respiration rates after ~~harvest. Modelled~~harvests. The modelled and measured soil CO_2 emissions agree well after tillage. However, unless there is a gap of two weeks or more between harvest and tillage, the "pre-tillage" results will include some post-harvest effects, and the "post-harvest" results will also include some post-tillage effects. Our intention to present the data grouped by these events are the discrepancies between modeled and observed CO_2 dynamics. There is a sharp drop of modeled CO_2 emissions after harvest due to the prompt absence of autotrophic respiration. In reality, there will likely be some ongoing metabolic respiration of plant tissue remaining in the field, which is not represented by the 'assumed' dead plant material in the model. After incorporation of harvest residues (at tilling) modeled CO_2 emissions increase again sharply. The sharp increase is due to the incorporation and hence availability of fresh litter (stubble) and a temporary stimulation of decomposition by the model due to the disruption/aeration of the soil structure. Both, overestimation of fresh litter and/or stimulation of decomposition by the model may contribute to the discrepancies between observed and modelled CO_2 emissions.

Grassland C cycle: The LandscapeDNDC simulations for the grassland system (G1) predict a mean annual gross carbon uptake of 16.9 ± 1.7 t C-CO_2 ha^{-1} a^{-1} and an annual loss of 13.2 ± 2.3 t C-CO_2 ha^{-1} a^{-1} through respiration. ~~Further minor outputs are~~The rest is related to grazing (0.2 ±< 0.01 t C-CO_2 ha^{-1} a^{-1}), ~~harvest~~harvesting (2.1 ± 0.7 t C-CO_2 ha^{-1} a^{-1}) and allocation in the soil (1.4 ± 4.7 t C-CO_2 ha^{-1} a^{-1}). ~~Mean~~The model cannot determine whether the system is net gaining or losing carbon. The annual ~~as well as~~mean and temporal dynamics of ~~modeled~~the modelled emissions are well in ~~line~~accordance with the measured emissions. ~~Effect~~The effect of grazing has a minor influence on the total ecosystem respiration (Fig. 7), resulting in a wider range of both measured and ~~modeled~~modelled emissions. Grazing, i.e~~.~~., the reduction of root biomass, results in two contrary processes: a reduction ~~of~~in maintenance respiration and ~~increasing~~an increase in autotrophic respiration (Raich and Tufekciogul, 2000).

Forest C cycle: The forest model predicts an annual C input of 8.9 ± 0.6 t C-CO_2 ha^{-1} a^{-1}, which is quite low compared to the estimations for old-growth beech forests in Europe, with reported rates from 14.4 to 18.3 t C-CO_2 ha^{-1} a^{-1} (Molina-Herrera et al., 2015). However, C uptake rates vary in magnitude, with values ~~presented~~ranging from 3 to 34 t C-CO_2 ha^{-1} a^{-1} for different forests in different growing stages (Waring et al., 1998). As our study site is a mixture of young and old beech trees, we assume that it has 40~~-~~ - 50% less biomass compared to an old beech forest. Of the ~~modeled~~modelled C input, 6.6 ± 0.5 t C-CO_2 ha^{-1} a^{-1} ~~leave~~leaves the system as gaseous CO_2. The rest is accumulated in the biomass and soil. ~~Mean~~The annual ~~sum~~mean and ~~dynamic~~dynamics of ~~modeled~~the modelled emissions are in ~~line~~accordance with the measured emissions. We expected to see rising emissions with litter fall in autumn (Raich and Tufekciogul, 2000), but cannot report this effect, ~~neither~~either with measurements~~, nor~~ or with model results (Fig. 6).



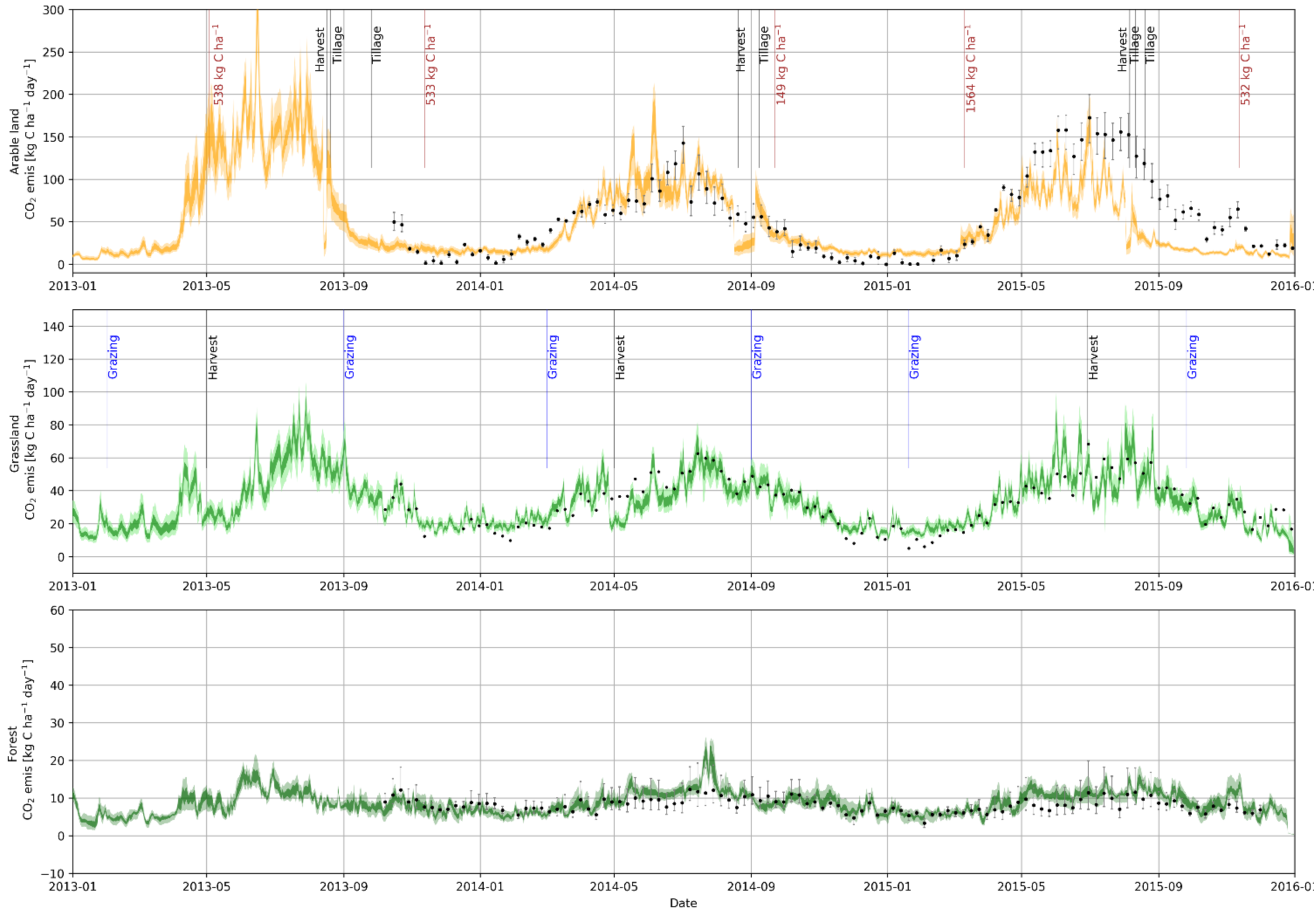
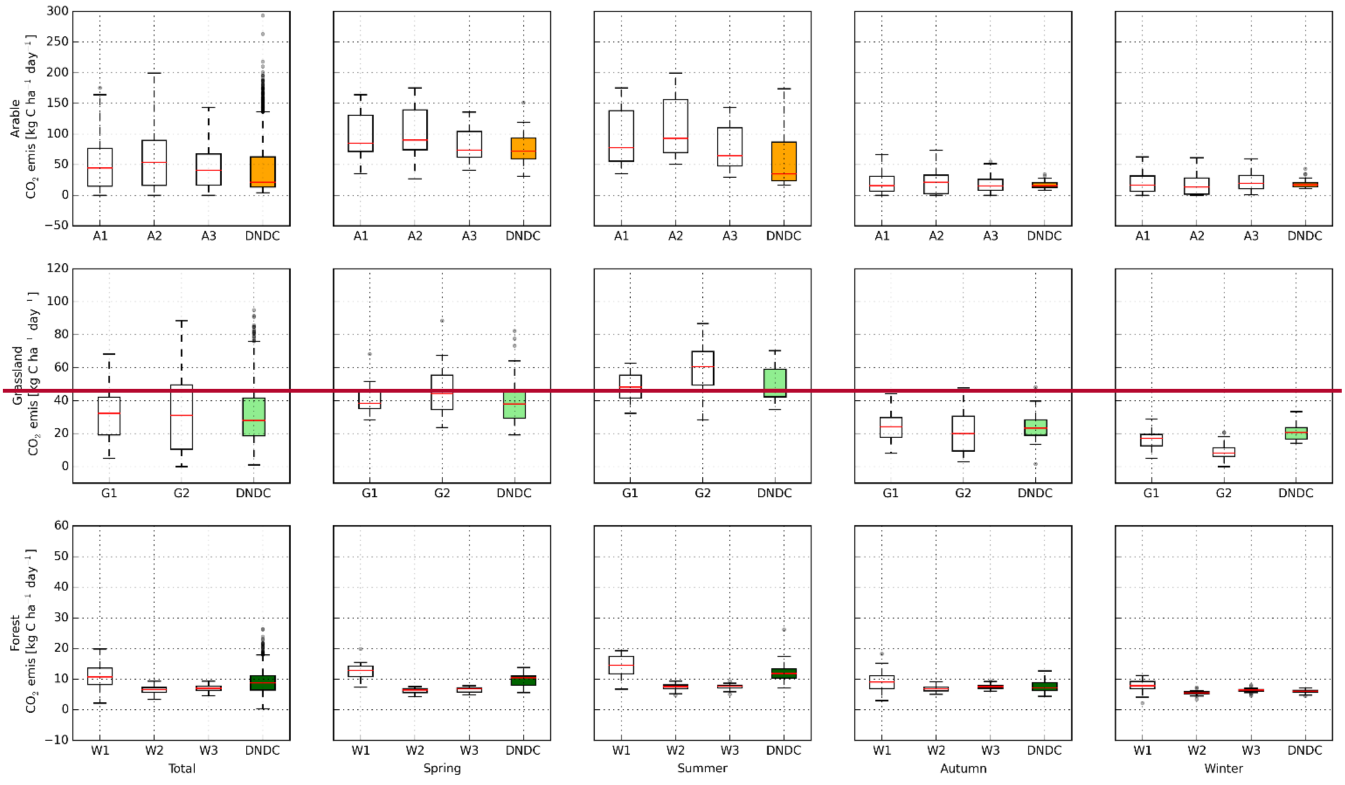


Figure 5: ~~Modeled~~Modelled CO_2 emissions and management. Measurements are given as grey error bars showing the variance between the replicated transects and the mean value as a black dot. Posterior model uncertainty is given in light ~~color~~colour for the 5 and 95 ~~percentile~~percentiles and dark ~~color~~colour for the 25 and 75 ~~percentile~~percentiles. Vertical lines indicate management events. Brown ~~colored~~coloured bars in the uppermost panel indicate manure application.



Arable
CO2 emis [kg C ha⁻¹ day⁻¹]
Grassland
CO2 emis [kg C ha⁻¹ day⁻¹]
Forest
CO2 emis [kg C ha⁻¹ day⁻¹]
A1
A2
A3
DNDC
G1
G2
DNDC
W1
W2
W3
DNDC
Total
Spring
Summer
Autumn
Winter

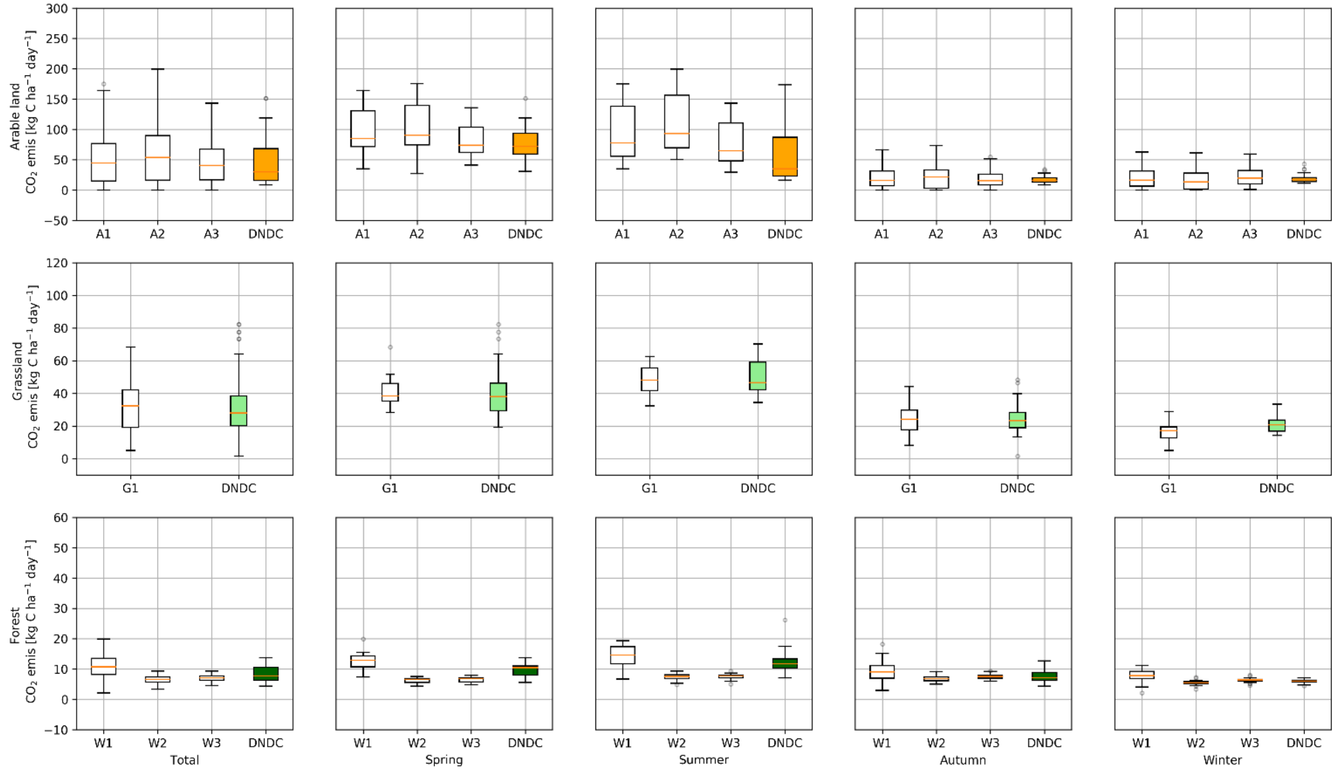
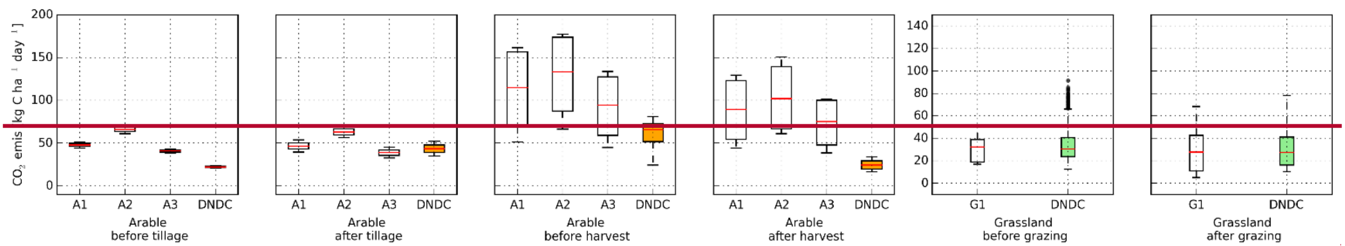


Figure 6: Observed and ~~modeled~~modelled CO_2 emissions for spring (~~21.03-20.06~~21st Mar. - 20th Jun.), summer (~~21.06.-20.09~~21st Jun. - 20th Sep.), autumn (~~21.09.-20.12~~21st Sep. - 20th Dec.), and winter (~~21.12.-20.03~~21st Dec. - 20th Mar.).



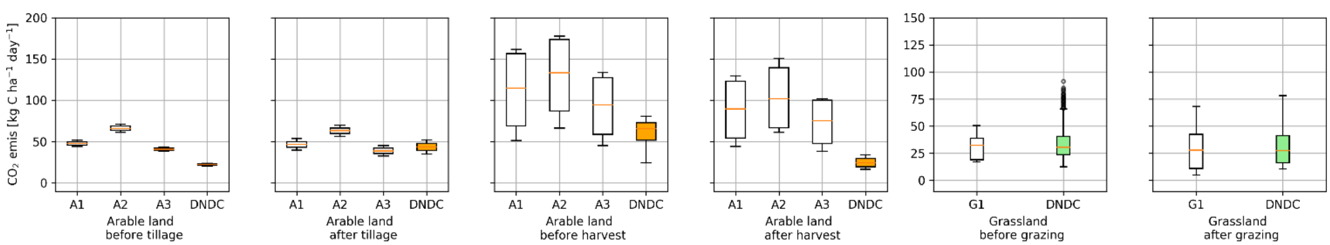


Figure 7: Management effects on CO_2 emissions. Measured and ~~modeled~~modelled emissions ~~where selected~~ in a time window of 2 weeks before and 2 weeks after a management.

Table 5: Simulated carbon fluxes given by posterior model runs and their uncertainty on different land use in [t C ha^{-1} a^{-1}]. C manure on grassland includes input by sheep's dung. Arable land model assumes 20% return of stubble to field.

Modeled C flux	Arable land		Grassland		Forest	
CO_2 uptake	24.65	±1.32	16.8	±1.72	8.94	±0.56
C manure	1.06		0.07		0	
Total input	**25.71**	**±1.32**	**16.87**	**±1.72**	**8.94**	**±0.56**
Growth respiration	2.53	±0.2	0.81	±0.27	1.44	±0.05
Heterotrophic respiration	4.69	±0.53	2.27	±0.9	2.04	±0.1
Maintenance respiration	13.31	±1.06	10.16	±1.13	3.11	±0.39
Total gaseous output	**20.53**	**±1.79**	**13.24**	**±2.3**	**6.59**	**±0.54**
DOC leaching	~~>~~<0.01	~~±>~~±<0.01	~~>~~<0.01	~~±>~~±<0.01	~~>~~<0.01	~~±>~~±<0.01
Total leaching output	**~~>~~<0.01**		**~~>~~<0.01**		**~~>~~<0.01**	
C bud export	1.97	±0.17	0		0	
C straw export	2.75	±0.21	2.28	±0.72	0	
Total biomass output	**4.72**	**±0.38**	**2.28**	**±0.72**	**0**	
Balance	**0.46**	**±3.49**	**1.35**	**±4.74**	**2.35**	**±1.1**

4 Conclusion

We presented a two-year measurement campaign of trace gas emissions from adjacent land uses i.e~~.~~., arable land, grassland and forest ecosystems, with concurrent model development and rigorous testing through a model-data fusion.

We found high emissions of N_2O and CO_2 on our arable land sites, low emissions on grassland sites and the lowest emissions on the forest sites. These observations enable us to investigate the underlying effects of plant growth, temperature and WFPS, land use effects, seasonal patterns and management effects. Respiration amounts rise in less shaded (warmer) areas of the forest, while N_2O emissions increase ~~toward~~towards the ~~foot~~foothills of the ~~hills of~~ forest and arable land sites due to nitrogen accumulation. Highly variable N_2O emissions in ~~forest~~forests resulted in large ~~uncertainty of~~uncertainties in the model verification data~~ and was~~, which translated ~~in~~into large ~~uncertainty of~~uncertainties in the model results for ~~forest~~forests. Detailed measured data ~~of~~on soil and management allowed ~~fitting~~us to fit the biogeochemical model LandscapeDNDC to the measured soil moisture, yield and GHG emissions of CO_2 and N_2O. ~~Overall,~~A subjective conclusion about the overall model performance is ~~classified~~shown in Table 6~~.~~

: The model reproduced the measured data reasonably well in time, separated into seasons and management events. ~~Model~~The model performance was best in predicting management effects on N_2O emissions and annual CO_2 emissions for all land uses. With regard to land use, the simulations for grassland sites work best, followed by those for arable land. ~~Simulations~~The simulations for N_2O emissions on arable land outperform those for CO_2, and vice versa for grassland. Low emissions on forest sites were generally difficult to depict ~~by~~using our ~~modeling~~modelling approach.

The model-data fusion approach allowed us to ~~derive~~identify model structural deficiencies that would likely increase model performances if ~~implemented~~addressed in Landscape DNDC: ~~(1)~~ missing N_2O uptake processes; ~~(2)~~ missing NO_3^- (and potentially dissolved organic nitrogen) uptake through shallow groundwater; ~~(3)~~ missing lateral interaction ~~at~~on hillslopes due to the 1D model ~~set up~~setup.

Table 6: Overall posterior model performance of LandscapeDNDC on different land ~~use~~uses in reproducing GHG emission data. ~~Classified~~Subjectively classified into (1) good, (2) medium and (3) poor model performance in simulating reliable annual sums, seasonal patterns and ~~magnitude~~magnitudes of management events (e.g~~.~~., fertilizer application). NA = not applicable, i.e~~.~~., no forest management during ~~modeled~~modelled period from 2010-2016.

Modelled performance on each land use	N_2O emissions			CO_2 emissions		
	annual	seasonal	management	annual	seasonal	management
Arable land (A1-3)	2	1	1	1	2	3
Grassland (G1)	1	2	1	1	1	1
Forest (W1-W3)	2	2	NA	1	2	NA

Furthermore, posterior model runs allowed ~~quantifying~~ for the quantification of the magnitude and uncertainty of ~~not measured fluxes of the~~ unmeasured C and N cycle~~. Investigated~~ fluxes. The investigated forest site ~~is in general acting~~generally acts as the largest sink for C and N, with annual sequestration rates of 2.4 ± 1.1 t C ha^{-1} and 3.3 ± 2.0 kg N ha^{-1}. ~~The~~Whether the extensive grazed grassland is also acting as a sink for C with 1.4 ± 4.7 t C ha^{-1} per year remains uncertain, while the N cycle of the grassland model cannot be closed with the given settings. Shrinking N soil pools indicate a missing input, which we assume ~~from~~to be shallow groundwater with an additional N supply of ~~around~~approximately 40.9 ± 25.9 kg N ha^{-1} a^{-1}.

Current land use in this catchment is dominated by forests (37%) and arable land (35%), whereas grassland sites (11%) are mainly distributed along the stream. ~~Under~~From the viewpoint of climate~~-~~-smart landscapes, the measured data ~~suggests~~suggest the benefit of forests in a landscape, ~~having~~as they have the ~~least~~fewest GHG emissions. Riparian zones can act as sinks of N~~,~~ but only during the vegetation period and during times when roots have access to groundwater. Arable land use produces high amounts of N_2O, ~~but~~ not throughout the year, but rather, in spring after fertilizer application.

Potential interactions of land use ~~pattern~~patterns cannot be quantified with the current one~~-~~-dimensional model approach. However, the dataset could be used in future studies to quantify the nitrate uptake of riparian zones in more detail, e.g~~.~~., by coupling LandscapeDNDC to a hydrological model, as done by ~~Klatt et al. (2017)~~Klatt et al. (2017). Such a model setup would also allow ~~an~~for upscaling in space, e.g~~.~~., for the generation of GHG inventories or an analysis of more detailed management scenarios in time.

Code availability

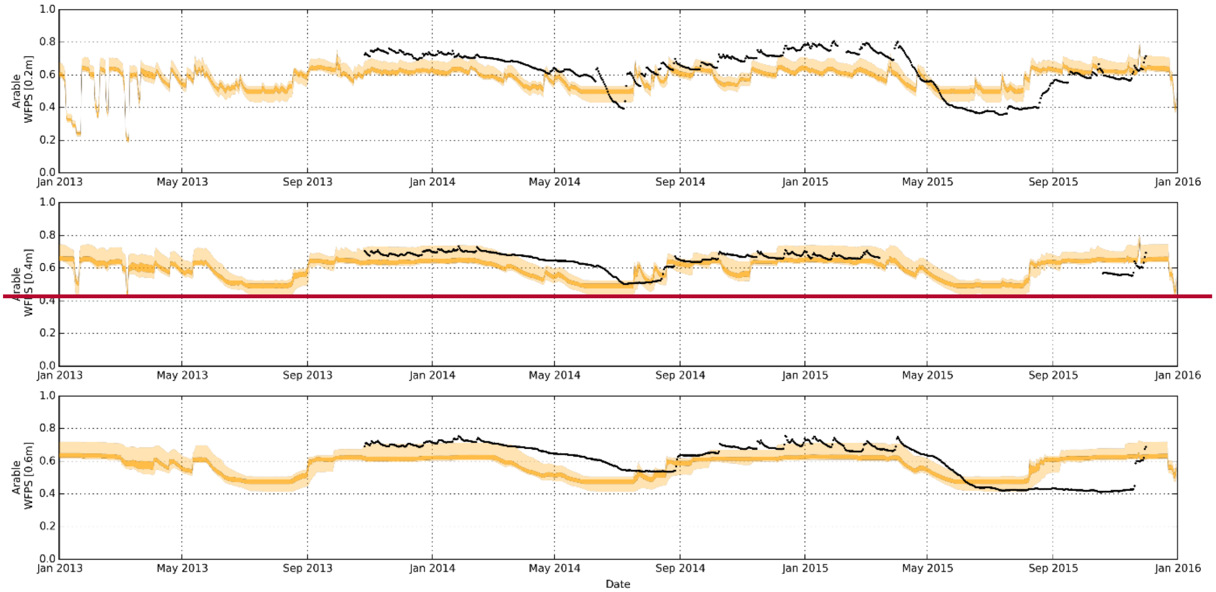
The LandscapeDNDC framework is free available upon request from www.~~svn~~ldndc.imk-ifu.kit.edu

The SPOTPY tool, used for model-data fusion, is free and open source and is available from www.pypi.python.org/pypi/spotpy

Data availability

All measured data ~~is~~are free available upon request from www.fb09-pasig.umwelt.uni-giessen.de:8081

Appendices



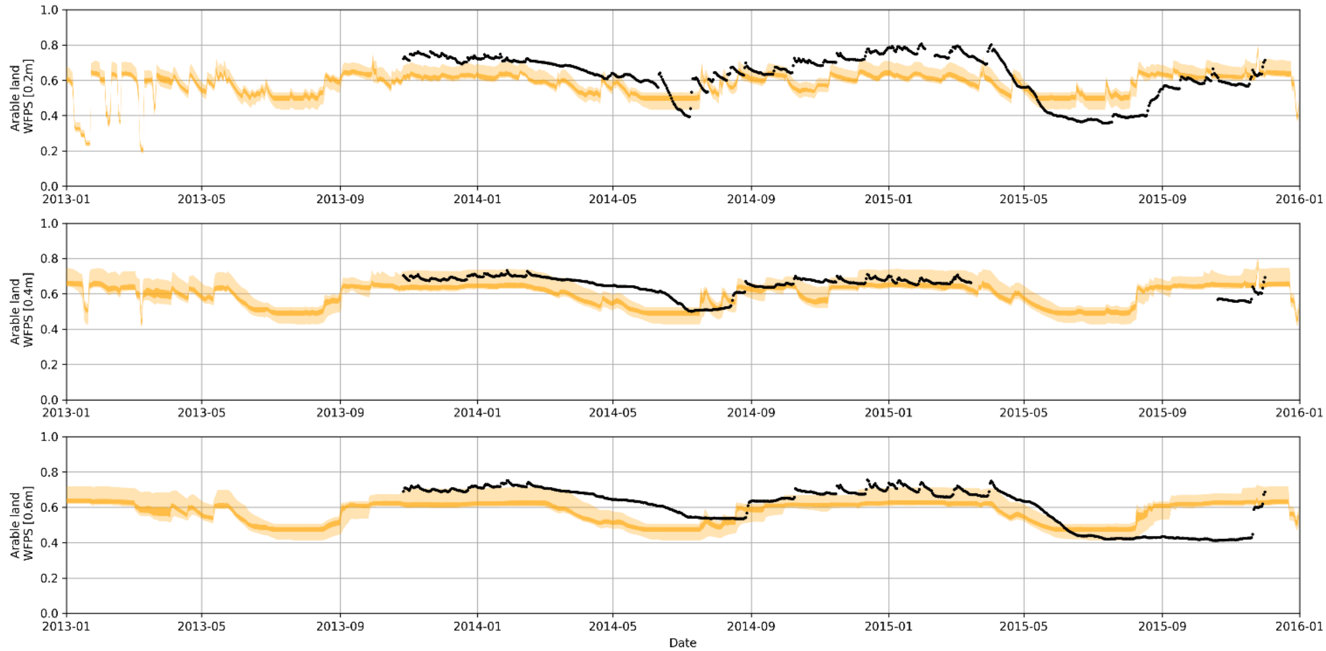


Figure A1: Modeled WFPS on arable land in different depths. RMSEs ranging from 0.0774 to 0.1194% WFPS [0.2m], 0.0511 to 0.0955% WFPS [0.4m] and 0.0921 to 0.1193% WFPS [0.6m].

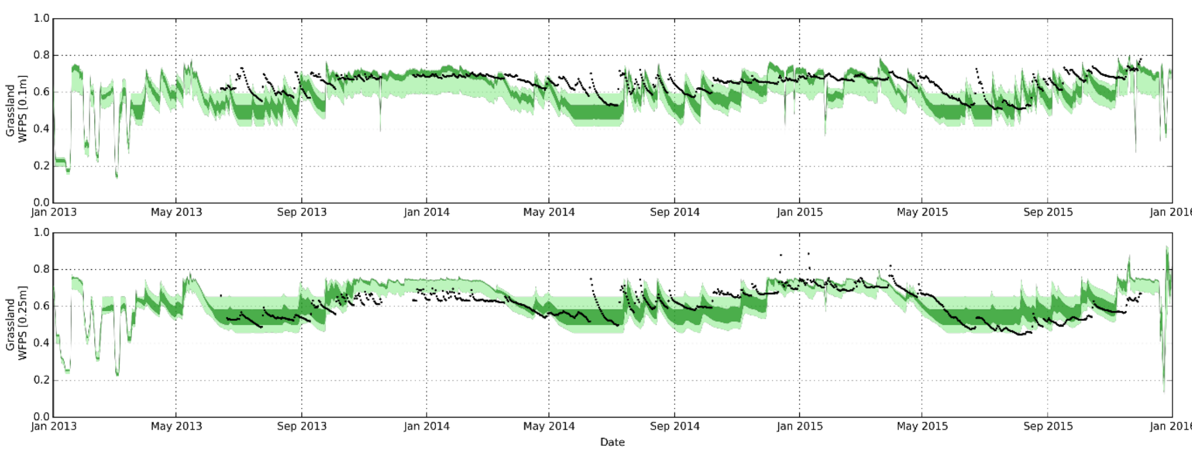


Figure A2: Modeled WFPS on grassland in different depths. RMSEs ranging from 0.043 to 0.1481% WFPS [0.1m] and 0.056 0.1069% WFPS [0.25m].

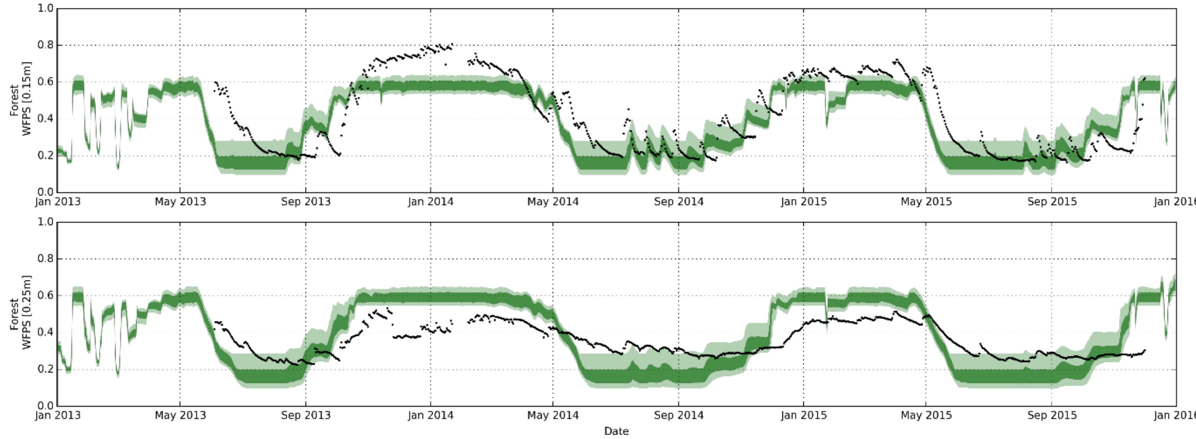


Figure A3: Modeled WFPS on forest in different depths. RMSEs ranging from 0.0817 to 0.1324% WFPS [0.15m] and 0.0812 to 0.1606% WFPS [0.25m].

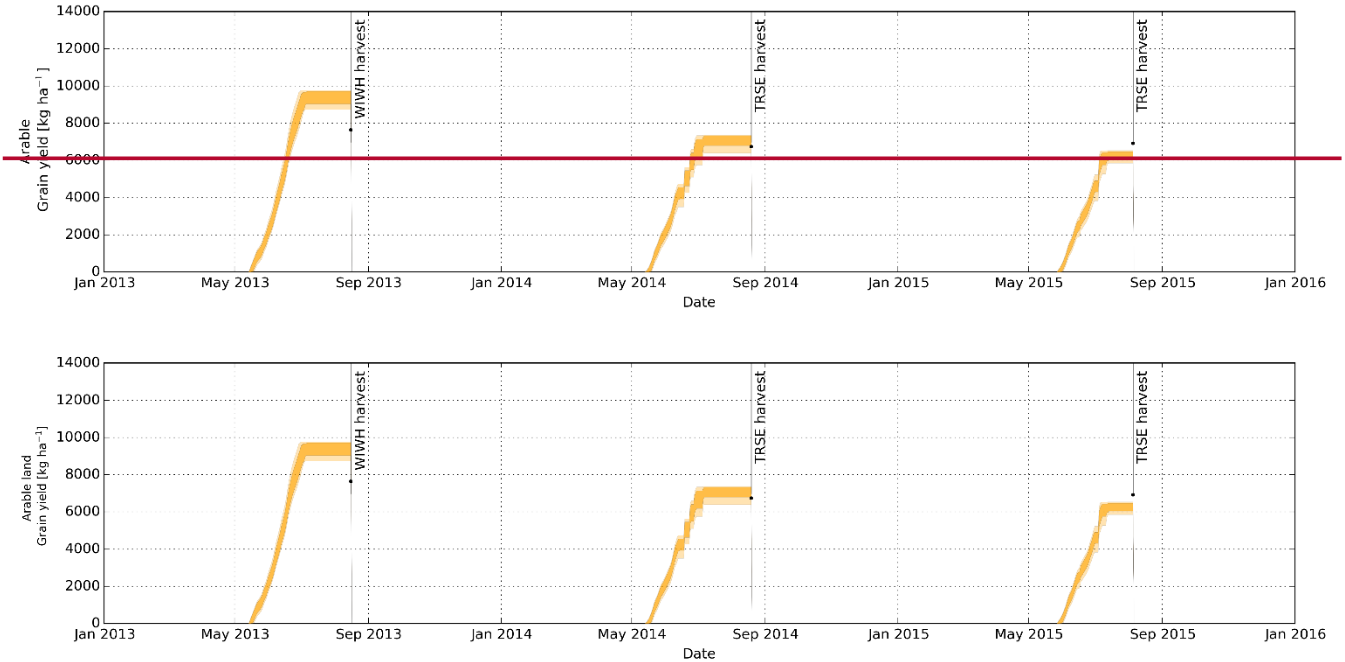


Figure A4: Modeled dry weight grain yield on arable land use. WIWH = Winter wheat, TRSE = Triticum secale. RMSEs ranging from 1125.7 to 2529.2 kg ha^{-1}.

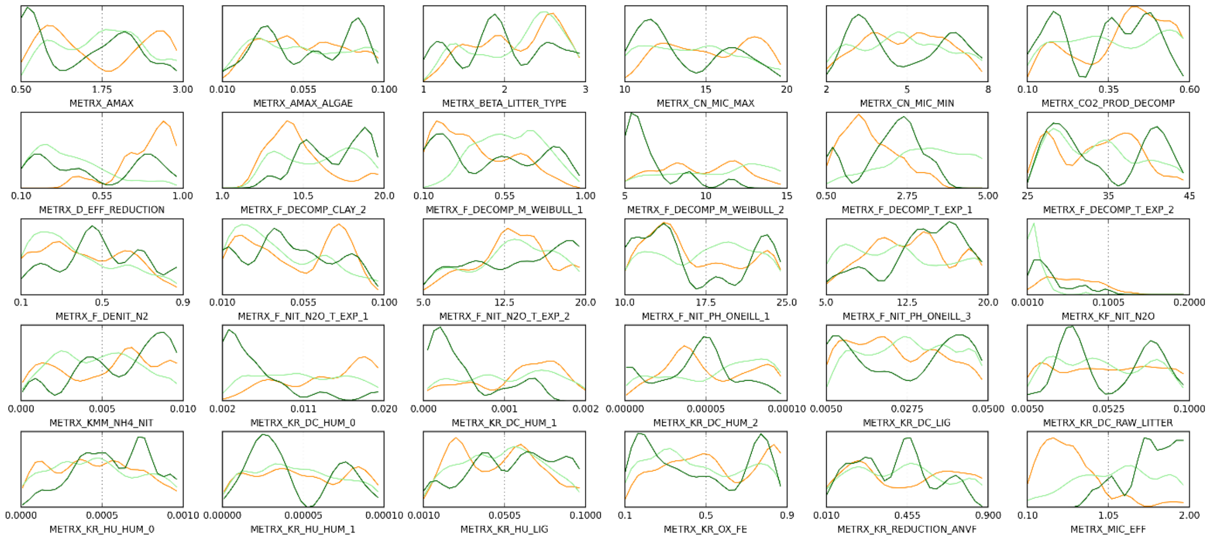


Figure A5: Posterior parameter distribution of the LandscapeDNDC module MeTrx. Orange line = arable land, light green line = grassland, dark green line = forest model set up.

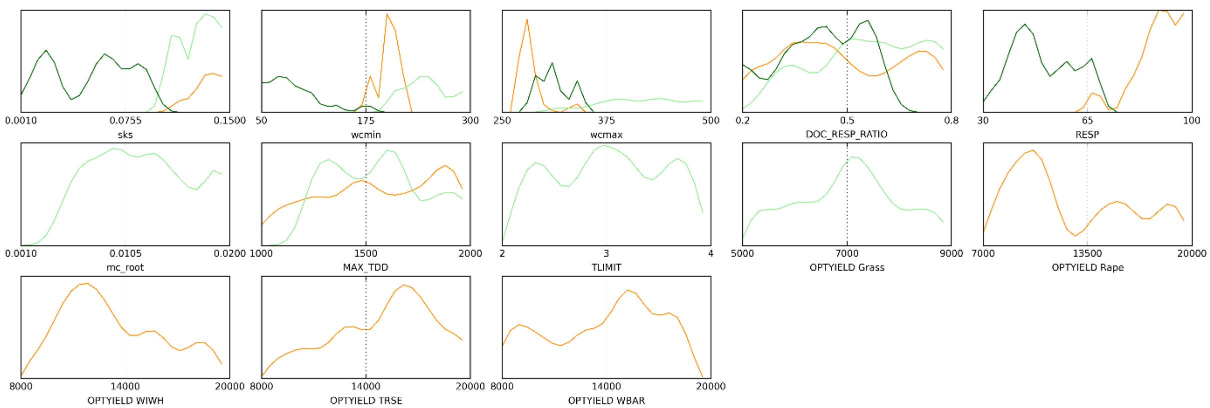


Figure A6: Posterior parameter distribution of the LandscapeDNDC modules wcDNDC and physiology. Orange line = arable land, light green line = grassland, dark green line = forest model set up.

Table A1: Input parameters for all investigated LandscapeDNDC modules with uniform distribution for Latin Hypercube Sampling. FASY = Fagus sylvatica, PERG = Perennial grass.

module	parameter name	Description	min	max
wcDNDC	sks_arable	Value of soil layer for saturated hydraulic conductivity	0.1	0.2
wcDNDC	sks_grassland	Value of soil layer for saturated hydraulic conductivity	0.1	0.15
wcDNDC	sks_forest	Value of soil layer for saturated hydraulic conductivity	0.1	0.1
wcDNDC	wcmin_arable	Wilting point of soil layer	170	220
wcDNDC	wcmin_grassland	Wilting point of soil layer	200	300
wcDNDC	wcmin_forest	Wilting point of soil layer	40	200
wcDNDC	wcmax_arable	Field capacity of uppermost soil layer	270	350
wcDNDC	wcmax_grassland	Field capacity of soil layer	300	500
wcDNDC	wcmax_forest	Field capacity of soil layer	270	350
physiology	DOC_RESP_RATIO_FASY	Ratio of root exudates related to root growth respiration	0.1	0.6
physiology	RESP_FASY	Factor determining plant respiration	30	70
physiology	DOC_RESP_RATIO_PERG	Ratio of root exudates related to root growth respiration	0.2	0.8

physiology	MC_ROOT_PERG	Maintenance respiration coefficient of roots	0.001	0.02
physiology	MAX_TDD_PERG	Temperature degree days for full plant development	1200	2000
physiology	OPTYIELD_PERG	Optimum yield of crops and grasses	5000	9000
physiology	TLIMIT_PERG	Temperature limit for plant growth	2	4
physiology	DOC_RESP_RATIO_arable	Ratio of root exudates related to root growth respiration	0.2	0.8
physiology	MAX_TDD_arable	Temperature degree days for full plant development	1000	2000
physiology	RESP_arable	Factor determining plant respiration	30	100
physiology	OPTYIELD_rape	Optimum yield of Rape	7000	20000
physiology	OPTYIELD_WIWH	Optimum yield of Winter Wheat	8000	20000
physiology	OPTYIELD_TRSE	Optimum yield of Triticale	8000	20000
physiology	OPTYIELD_WBAR	Optimum yield of Winter Barley	8000	20000
METRX	METRX_AMAX	Maximum microbial death rate	0.5	3
METRX	METRX_AMAX_ALGAE	Maximum decay rate of alga	0.01	0.1
METRX	METRX_BETA_LITTER_TYPE	Exp. fac. of litter decomposition red. depend. on lignin conc	1	3
METRX	METRX_CN_MIC_MAX	Maximum allowed C:N ratio for microbes	10	20
METRX	METRX_CN_MIC_MIN	Minimum allowed C:N ratio for microbes	2	8
METRX	METRX_CO2_PROD_DECOMP	Instantaneously production of CO2 during decomposition	0.1	0.6
METRX	METRX_D_EFF_REDUCTION	Reduction factor for gas diffusion	0.1	1
METRX	METRX_F_DECOMP_CLAY_2	Factor for clay dependency of decomposition	1	20
METRX	METRX_F_DECOMP_M_WEIBULL_1	Factor for water filled pore space dependency of decomposition	0.1	1
METRX	METRX_F_DECOMP_M_WEIBULL_2	Factor for water filled pore space dependency of decomposition	5	15
METRX	METRX_F_DECOMP_T_EXP_1	Factor for temperature dependency of decomposition	0.5	5
METRX	METRX_F_DECOMP_T_EXP_2	Factor for temperature dependency of decomposition	25	45
METRX	METRX_F_DENIT_N2	Factor determining amount denitrified nitrogen goes to N2	0.1	0.9
METRX	METRX_F_NIT_N2O_T_EXP_1	Factor for temp. depend. of N2O prod. during nitrification	0.01	0.1
METRX	METRX_F_NIT_N2O_T_EXP_2	Factor for temperature dependency of N2O production	5	20
METRX	METRX_F_NIT_PH_ONEILL_1	Factor for pH dependency of nitrification	10	25
METRX	METRX_F_NIT_PH_ONEILL_3	Factor for pH dependency of nitrification	5	20
METRX	METRX_KF_NIT_N2O	Maximum fraction of nitrified NH4 that goes to N2O	0.001	0.2
METRX	METRX_KMM_NH4_NIT	Michaelis-Menten const. for NH4 depend. of nitrification	0.00001	0.01
METRX	METRX_KR_DC_HUM_0	Decomposition constant of recalcitrant young humus	0.002	0.02
METRX	METRX_KR_DC_HUM_1	Decomposition constant of recalcitrant old humus	0.00005	0.002
METRX	METRX_KR_DC_HUM_2	Decomposition constant of recalcitrant old humus	0.000001	0.0001
METRX	METRX_KR_DC_LIG	Decomposition constant of lignin	0.0005	0.05
METRX	METRX_KR_DC_RAW_LITTER	Decomposition constant of raw litter	0.005	0.1
METRX	METRX_KR_HU_HUM_0	Rate constant for humification of labile humus to recalcitrant young humus	0.000001	0.001
METRX	METRX_KR_HU_HUM_1	Rate constant for humification of recalcitrant young humus to recalcitrant old humus	0.000001	0.0001
METRX	METRX_KR_HU_LIG	Rate constant for humification of lignin	0.0001	0.1
METRX	METRX_KR_OX_FE	Rate constant of iron oxidation	0.1	0.9
METRX	METRX_KR_REDUCTION_ANVF	Decomposition reduction due anaerobicity	0.01	0.9
METRX	METRX_MIC_EFF	Microbial carbon use efficiency	0.1	2

Author contribution

T. Houska, L. Breuer and R. Kiese designed and managed the experiments. D. Kraus and T. Houska performed the simulations. T. Houska prepared the manuscript with contributions from all co-authors.

Competing interests

The authors declare that they have no conflict of interest.

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