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Rejecting hydro-biogeochemical model structures by multi-criteria evaluation

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ABSTRACT

This work presents a novel way for assessing and comparing different hydro-biogeochemical model structures and their performances. We used the LandscapeDNDC modelling framework to set up four models of different complexity, considering two soil-biogeochemical and two hydrological modules. The performance of each model combination was assessed using long-term (8 years) data and applying different thresholds, considering multiple criteria and objective functions. Our results show that each model combination had its strength for particular criteria. However, only 0.01% of all model runs passed the complete rejectionist framework. In contrast, our comparatively applied assessments of single thresholds, as frequently used in other studies, lead to a much higher acceptance rate of 40–70%. Therefore, our study indicates that models can be right for the wrong reasons, i.e., matching GHG emissions while at the same time failing to simulate other criteria such as soil moisture or plant biomass dynamics.

Software availability

Name of software: LandscapeDNDC (version 0.33.13)
Developer and contact address: Institute of Meteorology and Climate Research - Atmospheric Environmental Research (IMK-IFU), Garmisch-Partenkirchen, 82467, Germany, Tel. +49 8821-183-153
E-mail: klaus.butterbach-bahl@kit.edu, ralf.kiese@kit.edu, edwin.haas@kit.edu
Year first available: 2013
Hardware required: Desktop, Laptop or HPC
Software required: Windows, Unix or Mac
Availability and cost: An executable program can be downloaded at http://svn.imk-ifu.kit.edu/ free upon request
Program language, program size: C++, about 30 MB

1. Introduction

The main anthropogenic source of N_2O is linked to emissions from agricultural soils and vast application of organic and synthetic nitrogen fertilizers (Reay et al., 2012). The underlying processes of soil carbon (C) and nitrogen (N) cycling and emission are affected by a multitude of non-linear factors, e.g. fertilization, tillage, climate, nutrient use efficiency as well as microbial metabolism (Stehfest and Bouwman, 2006). Consequently, greenhouse gas (GHG) emissions are highly variable in space and time. This variability across spatio-temporal scales cannot be addressed by field measurement as the spatial scale is too limited (Butterbach-Bahl et al., 2013). To overcome these limitations process based models, which summarize and translate our current understanding of processes underlying the biosphere-atmosphere GHG exchange into numerical equations, have been developed. These models allow upscaling in space and time domains and they can also be applied in the framework of scenario studies and used for decision support (Wang and Chen, 2012). Nevertheless, the algorithms used in such models are simplifications and still associated with

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uncertainty since magnitude and parameterisation of many biogeochemical processes are uncertain, too (Butterbach-Bahl et al., 2013; Kraus et al., 2015).

Studies about biogeochemical model uncertainty analysis of GHG exchange processes and fluxes are still limited and differ with respect to implemented process descriptions, output targets and uncertainty sources. Lehuger et al. (2009) presented the first uncertainty analysis for a process-based biogeochemical model (CERES-EGC, a biogeochemical extension of the CERES crop model). The model output of N_2O fluxes were generated on 7 different sites with a Metropolis-Hasting algorithm, involving 15 model parameters. They found posterior model outputs with an uncertainty ranging from 13 up to 1422% for annual N_2O flux predictions. A review by Wang and Chen (2012) summarizes the few existing parametrization and uncertainty studies for soil biogeochemical models and recommend uncertainty analysis for multiple sites and the use of multiple criteria. They further suggest a development of a model library containing various model structures to facilitate comprehensive model comparison and uncertainty studies. Such a variable model structure approach was realized by Haas et al. (2013) with LandscapeDNDC (DeNitrification-DeComposition), a framework for simulation of water, C and N cycling and associate GHG emissions in terrestrial (forest, arable, grassland) ecosystems. LandscapeDNDC consists of interchangeable modules representing soil biogeochemistry e.g., scDNDC (Zhang et al., 2015) or the MeTr^x module (Kraus et al., 2015), hydrology e.g., water cycle wcDNDC or CMF (Catchment Modelling Framework; Kraft et al., 2011), vegetation and microclimate processes. C and N turnover and related soil GHG emissions are, beside the main microbiological processes, depending on soil moisture conditions (Breuer et al., 2002; Butterbach-Bahl and Dannenmann, 2011). Consequently, to achieve reliable simulation of GHG emissions, an accurate representation of the soil moisture is a key requirement (Butterbach-Bahl et al., 2013; Frolking et al., 1998; Kröbel et al., 2010). Nevertheless, in biogeochemical models soil hydrological processes are often simulated based on simple bucket approaches, i.e. water moves vertically down a profile once a certain threshold has been reached, as e.g. in the LandscapeDNDC hydrological module wcDNDC. The nonlinear partial differential Richards' equation brings the advantage of a physical based approach. The equation describes vertical unsaturated flow, capillary rise and interaction with groundwater level. The implementation has been undertaken by Haas et al. (2013) and Wlotzka et al. (2014). They tested the coupled model system for C and N cycling on virtual hillslope studies including lateral nutrient transport. For sound validation of models, simulations must be tested with various observed data representing C, N and water cycling. However, most studies investigating biogeochemical processes and associated GHG emission simulated by the DNDC model family concentrate only on the validation of a subset of model results. Studies have been published with outputs such as N_2O emissions, yields or soil temperature and moisture profiles (see literature survey of Giltrap et al., 2010) with the risk that simulated GHG emissions are right for the wrong reasons. To overcome this problem model testing should be done by taking as many different observations into account as possible. They further should be accompanied by an uncertainty analysis (Pappenberger and Beven, 2006). There is an intensive discussion about different sorts of model uncertainties and how to address them (Beven, 2015). One of the most widely used concepts for assessing model uncertainties is the Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992; Beven and Freer, 2001). GLUE has its origin in hydrological research but has been utilized in other scientific fields such as biogeochemistry or plant growth studies (Houska et al., 2014; Nylinder et al., 2011; Senapati et al., 2016; Wang and Chen, 2012).

In this study, we are interested in the benefits of a physically based process description over a conceptual approach in simulating soil water dynamics within a biogeochemical model. We follow the philosophy that complex models should be identifiable (low parameter uncertainty) and accurate (good agreement with observation data). Further, a model should be able to simulate various observation data concurrently and close to reality, especially when dealing with highly non-linear process interactions like in hydro-biogeochemical systems. To asses only such model runs, we perform a multi-criteria evaluation of different model structures and quantify their underlying uncertainties. This study combines the following points:

(1) We utilized a comprehensive, high quality, long-term dataset from a grassland study site in Linden, Germany (Jäger et al., 2003), which was established in 1998. Data of trace gas emission (N_2O, CO_2, cumulative CO_2 and N_2O), plant growth (biomass, cumulative biomass), and soil hydrology (soil moisture) was taken to evaluate the models.
(2) We established four model structures, by combining two varieties of the LandscapeDNDC biogeochemical modules with two soil moisture routines, resulting in the four model set-ups scDNDC/wcDNDC, scDNDC/CMF, MeTr^x/wcDNDC and MeTr^x/CMF.
(3) We reduced the parameter space of modules involved in GHG emission processes (e.g. decomposition, ammonification, nitrification and denitrification) through a stepwise sensitivity analysis.
(4) We run a multi-criteria GLUE for each model combination to find behavioural parameter sets and select appropriate model structures based on this assessment. Formally, we use a posteriori model rejection framework by selecting only those model structures that meet predefined objective functions (Vaché et al., 2004). The method is designed to detect and locate potential model and measurement errors. Our accepted model runs pinpoint such errors and help to analyse the data.

2. Methods

2.1. Model description

LandscapeDNDC is a simulation framework for terrestrial ecosystem models (Grote et al., 2009; Haas et al., 2013) with a modular structure allowing the easy and efficient combination and coupling of different modules describing different processes in ecosystem compartments, i.e. mathematical descriptions of microclimate, water cycle, plant physiology and soil biogeochemical processes. The modules are an abstract representation of the ecosystem. LandscapeDNDC defines six ecosystem compartment: canopy air chemistry, canopy and soil microclimate, vegetation physiology, vegetation structure (only for forest applications), water cycle and soil biogeochemistry. Every of this ecosystem compartments is represented by different modules, see Table 1 and Fig. 1 for details. In this study, we test different combinations of two soil biogeochemistry modules (scDNDC and MeTr^x) and two water cycle modules (wcDNDC) and CMF in order to quantify model structure related uncertainty and to test validity of model structures. The different module combinations result in four model set-ups of the LandscapeDNDC framework, which are in the following referred to as scDNDC/wcDNDC, scDNDC/CMF, MeTr^x/wcDNDC and MeTr^x/CMF. For the plant physiology and microclimate, for all model set-ups we selected grasslandDNDC (Molina-Herrera et al.,