NEGEM

Quantifying and Deploying Responsible Negative Emissions in Climate Resilient Pathways

Upgraded LPJmL5 version

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Executive Summary

In the IPCC Special Report on 1.5°C (SR1.5), the deployment of negative emission technologies and practices (NETPs) is emphasized as an important measure, in addition to stringent decarbonization, required to implement the Paris Agreement. The overall objective of NEGEM is the assessment of the quantitative potential, effectiveness and impacts of these NETPs in a multi-disciplinary approach taking into account the range of disciplines in the relevant sustainability, socio-political and socio-economic sciences. Following this focus on a real-world perspective, WP3 aims to evaluate sustainable potentials as well as environmental impacts, side-effects and trade-offs of large-scale NETP deployment. The analyses will build on spatially-explicit, process-based biogeochemical modelling of key environmental functions with the dynamic global vegetation model LPJmL (PIK), on the one hand, and material flows analyses and life cycle assessment (ETH, INSA, VTT), on the other hand.

Before discussing the deployment pathways for NETPs, it is crucial to assess realistic and sustainable NETP potentials. For quantitative assessment of such realistic potentials from land-based NETPS (re-/afforestation, bioenergy with carbon capture and storage (BECCS) and pyrogenic CCS (PyCCS)), state-of-the art biogeochemical modelling of the land surface is a precondition, including a consistent coupling of all relevant carbon, water, nitrogen and energy fluxes at a high temporal and spatial resolution, as well as the representation of management options such as irrigation and fertilization. The objective of the deliverable D3.1 is to report on the LPJmL model developments conducted to provide a new model version operational for NEGEM analyses. The upgraded model named LPJmL5-NEGEM integrates an enhanced phenology representation, nitrogen dynamics and the respective parametrization of woody and herbaceous types of lignocellulosic bioenergy crops that capture the key environmental functions most relevant to the NETP potential and impact assessment. The introduced processes were harmonized and tested in simulations of the global vegetation, whereas yields of lignocellulosic bioenergy crops were evaluated against an extensive dataset of spatially-explicit observations.

LPJmL5-NEGEM, as described within this report, provides an advanced modelling tool to evaluate a) the biomass-based NETP potentials constrained by environmental limits (i.e. planetary boundaries, D3.2), b) NETP interference with biosphere integrity (D3.3), c) effects of climate extremes on NETP potentials and impacts (D3.4), and d) impacts on food security and freshwater availability (D3.7).

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Introduction

Within the NEGEM project, WP3 is dedicated to the comprehensive assessment of environmental impacts, side-effects and trade-offs of large-scale deployment of negative emission technologies and practices (NETP). In the analyses at PIK supporting D3.2-D3.4, D3.7 and D3.10, the potential, environmental impacts and trade-offs of terrestrial biomass-based NETPS (re-/afforestation, bioenergy with carbon capture and storage (BECCS) and pyrogenic CCS (PyCCS)) will be quantified using an upgraded version of the terrestrial biosphere model LPJmL. Soil carbon sequestration (SCS) will not be assessed in terms of dedicated practices (i.e. sustainable tillage, cover crops, renaturation of wetlands etc.), but to a certain extent addressed by LPJmL-simulated shifts in the soil and litter carbon pools resulting from transitions between natural vegetation and the land use for biomass-based NETPs. To ensure a solid basis of model processes capturing the key environmental functions most relevant to the NETP potential and impact assessment, D3.1 focused on providing a model version operational for NEGEM analyses.

The upgraded model LPJmL5-NEGEM will be described in the following chapters. It provides an advanced assessment tool in form of spatially-explicit, process-based biogeochemical modelling for the evaluation of a) the biomass-based NETP potentials constrained by environmental limits (i.e. planetary boundaries, D3.2), b) NETP interference with biosphere integrity (D3.3), c) effects of climate extremes on NETP potentials and impacts (D3.4), and d) impacts on food security and freshwater availability (D3.7).

1 LPJmL update for WP3 analyses

The dynamic global vegetation model (DGVM) LPJmL (Lund-Potsdam-Jena managed land) is a process-based model that simulates climate and land use change impacts on the terrestrial biosphere, agricultural production, and the carbon and water cycle. LPJmL operates in daily time steps and at a spatial resolution of 0.5° x 0.5°, simulating key ecosystem processes in direct coupling with the carbon and hydrological cycles that were recently extended by the nitrogen (N) cycle in LPJmL5. Detailed descriptions and validations of the biogeochemical dynamics can be found in Schaphoff et al. (2018) and von Bloh et al. (2018).

In addition to the representation of vegetation by nine natural plant functional types (PFTs) (Sitch et al. 2003) and 13 crop functional types and managed grassland (Bondeau et al. 2007), LPJmL includes three types of fast-growing second-generation energy crops parametrized as *Eucalyptus* in tropical climates and poplar and willow in temperate climates for woody types and C4 grass for herbaceous energy crops (Beringer, Lucht and Schaphoff 2011, Heck et al. 2016). These representative bioenergy functional types (BFTs) will be used to simulate climate sensitive and management-specific yields of different feedstock types for BECCS and PyCCS in the NEGEM analyses. Furthermore, LPJmL dynamically simulates environmental processes required for the spatially explicit representation of the interacting planetary boundaries of freshwater use, N flows, land use change, and biosphere integrity that are evaluated in the analyses of environmentally limited NETP potentials and the impact assessment in WP3. As ecosystem functions are represented for both, natural and managed ecosystems, LPJmL can assess effects of transitions from natural vegetation to cultivated land, i.e. on carbon, nutrient and water flows that are particularly relevant for the WP3 impact evaluations.

Over the last decade, different versions of the model have been developed and applied to evaluate the role of natural and managed ecosystems in the Earth system, including the impacts on different planetary boundaries (Steffen et al. 2015, Ostberg et al. 2015, Jägermeyr et al. 2017, Heck et al. 2018). LPJmL4 integrates major developments like the enhanced representation of plant phenology and irrigation systems on managed land that are crucial for the simulation of biomass plantations providing feedstock for BECCS and PyCCS and for the pressures applied on environmental flow requirements, defining the planetary boundary of freshwater use. LPJmL5, which was developed in parallel to LPLmL4, does not feature these developments, but introduces N dynamics into the model (see Figure 1) allowing for a dynamic representation of the planetary boundary of the biogeochemical flow of N. In order to employ a model that could quantify negative emission potentials of re-/afforestation, BECCS and/or PyCCS in view of trade-offs with respecting planetary boundary, nature conservation goals, food and water security, as planned for the assessments in WP3, the developments of LPJmL4 and LPJmL5 needed to be consolidated. The process of generating the updated model version LPJmL5-NEGEM is described below separated into three sections: the description of merging the additional LPJmL4 features into one consolidated LPJmL5 model version (chapter 2), the report on an updated parametrization of the BFTs along the integration of the different features (chapter 3) and the examination of an approach to dynamically simulating re-/afforestation (chapter 4).

2 Features of LPJmL5-NEGEM

LPJmL has been continuously developed and extended for a broad range of applications in recent years. To consolidate these efforts, major developments have been integrated into a new model version (LPJmL4, see Figure 1; Schaphoff et al. (2018)), including an enhanced representation of the plant phenology, which significantly improved the representation of the seasonal vegetation greenness (Forkel et al. 2014) as well as an extended irrigation module with different irrigation schemes (Jägermeyr et al. 2015). In parallel, extensive development work has been invested in the integration of N dynamics into the precursor model LPJmL3.5, resulting in LPJmL5, which simulates the terrestrial biosphere of both natural and managed, as coherently linked by its water, carbon and N pools and fluxes (von Bloh et al. 2018). In order to make LPJmL operational and reliable for the assessment of impacts and realistic potentials of negative emissions, these two distinct model branches had to be merged and consolidated, thus integrating enhanced representations of vegetation dynamics from both model versions. In the context of NEGEM, the enhanced phenology module in LPJmL4 is important as other model versions overestimated vegetation carbon which could in turn lead to overestimations of negative emission potentials through afforestation and BECCS/PyCCS. At the same time, the representation of the nitrogen cycle in LPJmL 5 is crucial to capture nitrogen limitation in forests and bioenergy plantations and resulting effects on negative emission potentials. The following section therefore first describes the relevant model developments in LPJmL4 and 5, before evaluating the merged model version LPJmL5-NEGEM in test simulations.

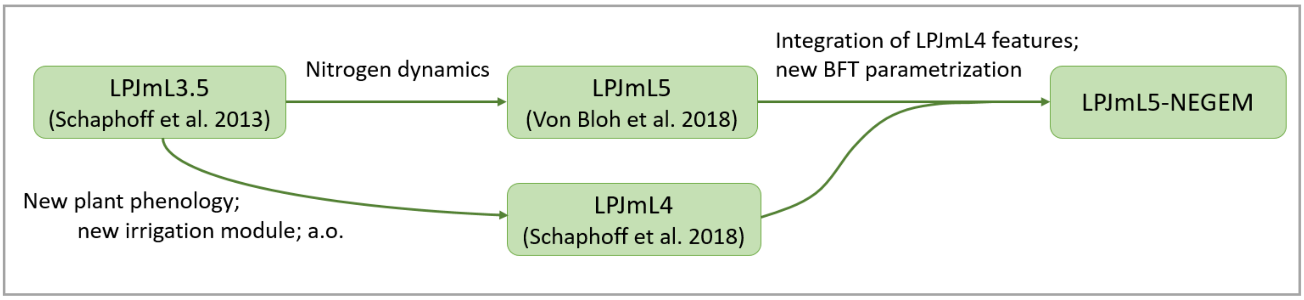


Figure 1 Schematic representation of recent model developments and their consolidation

2.1 Important recent LPJmL model developments

2.1.1 New phenology module in LPJmL4

While general carbon and water flows in the vegetation were well represented in LPJmL3.5 (Schaphoff et al. 2013), it was (like other DGVMs) limited in the representation of phenology and seasonal to decadal dynamics of vegetation greenness as observed by satellites. Addressing this deficit, an updated phenology module was integrated in LPJmL4 which takes environmental controls on phenology better into account (Forkel et al. 2014). While the former phenology module differentiated between temperature-driven summergreen PFTs, water-driven raingreen PFTs and evergreen PFTs without seasonal variation, it did not include the effects of light on phenology or the effects of water on leaf development in deciduous trees (Sitch et al. 2003). The updated phenology module in turn considers constraining effects of cold temperature, limited light, drought and heat stress by modifying the growing season index (GSI) model from Jolly, Nemani and Running (2005), an empirical phenology model that multiplies limiting effects of several environmental controls. The empirical parameters within the modified GSI model were optimized against satellite-derived fractions of absorbed photosynthetic active radiation resulting in an improved representation of spring onset and the end of the growing season in temperate and boreal forests, as well as more realistic Arctic tree line cover in high-latitude regions amongst others (Forkel et al. 2014). Adequately representing phenology is not only important for the terrestrial carbon cycle in general, as it directly influences plant/net ecosystem productivity, but also strongly influences albedo and thereby affects the climate system. With respect to NETP potentials, the improved phenology is crucial for simulating realistic potentials of re-/afforestation and biomass plantations for BECCS or PyCCS feedstock production, especially in high latitudes. Further, it enhances the simulation of climate change impacts on forests and biomass yields for different future climate pathways or climate extremes (particularly relevant for D3.4).

2.1.2 Implementation of the nitrogen cycle in LPJmL5

Building on and refining existing modelling implementations of N dynamics (Gerber et al. 2010, Smith et al. 2014, Parton et al. 2001), LPJmL3.5 was extended with the terrestrial N cycle for an enhanced representation of nutrient limitations in plant productivity. While von Bloh et al. (2018) provide a detailed description of modelled pools and fluxes, we shortly describe major processes and their relevance for the analyses in NEGEM in this section.

Both photosynthesis and respiration rate are influenced by N availability in LPJmL5, thus accounting for N dependant plant growth and ecosystem productivity. Accordingly, the water-limited photosynthesis rate is reduced if the corresponding N demand cannot be fulfilled by N uptake (see Figure 2a). Based on Smith et al. (2014), plant N-uptake in turn depends on soil mineral N-concentration, fine root mass, soil properties and plant demand for N. Upon N stress, more biomass is allocated to the roots to improve nutrient uptake. Besides a detailed representation of plant nutrient cycling and allocation (see Figure 2b), comprehensive soil N dynamics are implemented in LPJmL5. The two main reactive forms of N in soils, NO_3^- and NH_4^+, as well as N within soil organic matter are represented by distinct pools, which receive inputs through atmospheric deposition, fertilization, decomposition of plant biomass and biological N fixation. Following Parton et al. (2001), Gerber et al. (2010), and Schaphoff et al. (2013) amongst others, N within these pools is subject to transformation processes (mineralization, Immobilization, nitrification, plant uptake) and can be lost to the atmosphere via denitrification or volatilization and leaching of soil NO_3 to the groundwater. This does not only allow the assessment of agricultural N management on plant productivity, but also on N pollution through leaching.

The implementation of the N cycle into LPJmL5 represents a major improvement regarding a holistic representation of relevant processes within the terrestrial earth surface. Simulating N limited plant growth is argued to be important for future projections of plant productivity under climate change scenarios, as neglecting nutrient limitation might lead to overestimating CO_2 fertilization effects on plant growth upon elevated atmospheric CO_2 concentrations (e.g. Kolby Smith et al. 2016). In the context of NEGEM, it thus allows for an enhanced representation of carbon stored in forest plantations and achievable yields on bioenergy plantations under future climate scenarios. Also, as WP3 aims at assessing NETP impacts on and potentials within critical environmental limits as delineated by the planetary boundary framework (D3.2), LPJmL5 provides the methods to dynamically calculate impacts of fertilized bioenergy plantations on N flows, e.g. by assessing additional N leaching to groundwater. This could be an important measure for evaluating the scenario-specific status of the planetary boundary for N flows.

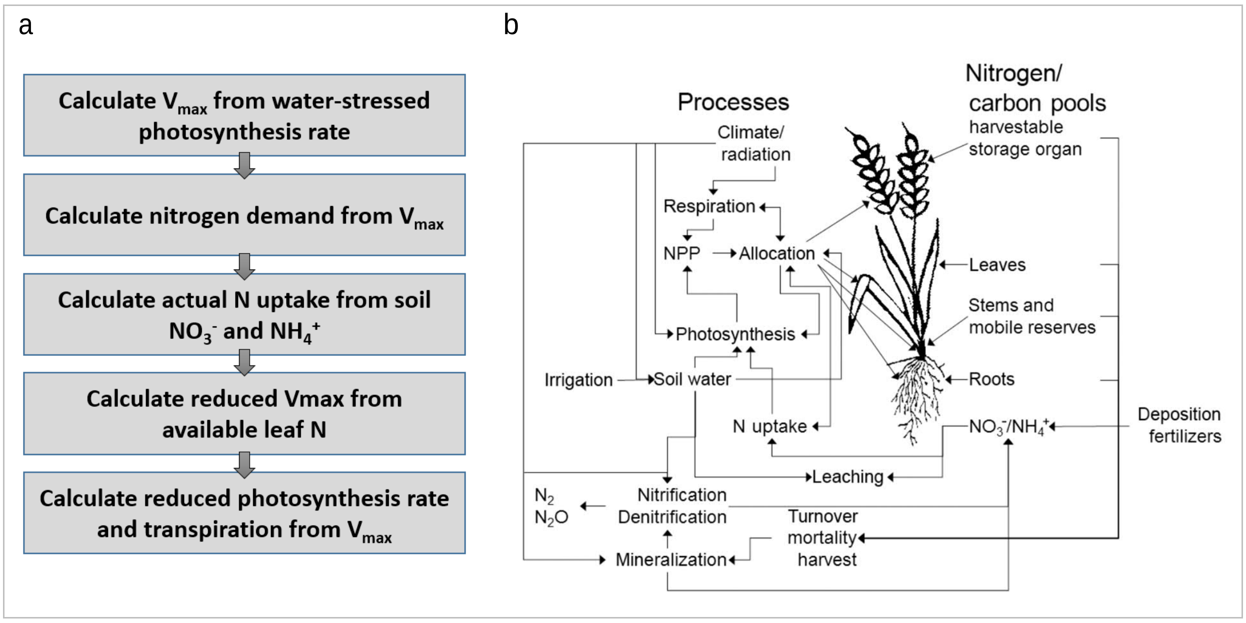


Figure 2 (a) Schematic representation of the nitrogen-limited photosynthesis rate in LPJmL5, V_{max} = maximum carboxylation capacity; (b) Nitrogen pools and fluxes as well as associated processes for the example of crops. Figures reproduced from von Bloh et al. (2018).

Besides direct effects on simulated NETP potentials, the implementation of the N limitation may also improve the representation of global patterns of absolute yield levels on cropland. Whereas in LPJmL3.5 and 4 regional differences in crop yields have to be calibrated via a scaling of the maximum leaf area index (LAImax), the harvest index, and the factor for scaling leaf-level photosynthesis to stand level (see Fader et al. 2010), the differing crop productivity levels between intensively and extensively managed regions can now be largely reproduced by the model itself (von Bloh et al. 2018). While this enhanced representation of N limitation effects on crop yields does not affect NETP potentials directly, it does influence interactions between the food system and NETP potentials, which will be studied during a later stage of the NEGEM project (D3.7).

However, capturing management induced ranges of N limitation requires a well-informed fertilizer input, not only for the time period of interest but also for the preceding time to simulate either N-depleted or -enriched soils. For example, applying a static fertilizer input, as used for the introduction of LPJmL5 in von Bloh et al. (2018), showed that the correlation of simulated crop yields with FAO yield statistics may improve under N limitation for some crops and countries but also significantly worsen for others. As data on fertilizer is, however, not fully available on a global scale, especially for historic time periods, deriving a fertilizer input from available data (e.g. Elliott et al. 2015 for the year 2000) will require well-justified assumptions on the historic development of fertilizer use. Subsequently, this input data will then need to be validated against FAO statistics.

2.2 Consolidating LPJmL4 and LPJmL5

As both modelling branches, LPJmL4 and LPJmL5, feature developments enhancing the representation of vegetation dynamics that are of crucial importance to the analyses planned for D3.2 – D3.4 and D3.7, the versions were merged into a version LPJmL5-NEGEM. Integrating the developments described above into a version operational for the assessment of realistic NETP potentials required a number of test simulations (see settings below) for debugging, checking for double-accounting and eliminating erroneous interferences between processes. Further, the parametrization of plant functional types needed to be harmonized in order to allow efficient establishment and growth under both the new limiting functions for phenology and N limitation.

While the integration of N dynamics is relevant for a number of LPJmL-supported analyses in WP3 (i.e. forest growth, management ranges for biomass plantations, climate extremes), it introduces uncertainties through the dependency on solid fertilizer input data wherever yields of food crops are subject to the assessment (i.e. D3.7: impact on food security and freshwater availability). Therefore, LPJmL5-NEGEM is programmed to optionally exclude N dynamics and operate in a “LPJmL4-like” mode (LPJmL5-NEGEM-Ccycle). For each research question and respective analysis, we will choose whether we require insights from N limitation opting for LPJmL5-NEGEM-CNcycle or if a solid representation of food crop yields with LAI calibration to FAO statistics is needed (LPJmL-NEGEM-Ccycle), as long as no reliable fertilizer input data has been generated.

2.3 Testing LPJmL5-NEGEM

2.3.1 General carbon cycle dynamics in LPJmL5-NEGEM

Given the challenges in consolidating model versions, we tested whether the integration of LPJmL4 features into LPJmL5 affected the general carbon cycle dynamics using a stable version of LPJmL5-NEGEM. Therefore, we ran a simulation with dynamic historic land use, driven by a transient climate input from 1901 to 2005. The climate input was derived fromobserved monthly temperature and precipitation from the CRU TS3.23 dataset (University of East Anglia Climatic Research Unit; Harris and Jones 2015) and radiation data based on reanalysis data from ERA-Interim (Dee et al. 2011). Historic land use change was based on HYDE3 (Klein Goldewijk and van Drecht 2006), which provides relative changes in cropland and pasture extent from 1700 until 2005. For agricultural fertilization, we used a static historic fertilization input based on Elliott et al. (2015).

Results for the final stable version of LPJmL5-NEGEM indicate that both global NPP and soil carbon density are well within the range of observation-based estimations and GPP is marginally above the upper range of respective estimates found in literature (see Table 1). Whereas LPJmL4 simulations overestimated global vegetation carbon compared to literature ranges (see Schaphoff et al. 2018), the global sum is in comparison underestimated in LPJmL5-NEGEM. Reasons for that could involve the combination of limiting factors of phenology and N, but it should be further investigated to understand why the carbon accumulation should be affected differently than the productivity. Yet, LPJmL5-NEGEM performance is in the range of previous model versions (see Schaphoff et al. 2018, von Bloh et al. 2018). While global literature estimates can serve for contextualization of simulated results, but notice that they are subject to significant uncertainties.

Table 1 Simulated global carbon fluxes -net primary productivity (NPP), gross primary productivity (GPP) and pools (soil and vegetation carbon) and comparison to literature estimates. limN refers to a scenario with static historic fertilization rates. Results are averaged for 1996-2005.

	Literature estimates	*LPJmL5-NEGEM limN*
Vegetation Carbon (Gt C)	437-453 (1)	372
Soil Carbon (Gt C)	1952-2752 (1)	2106
GPP (Gt C/yr)	115 - 131 (2), 113-125 (3)	134
NPP (Gt C/yr)	44-64 (1)	63

(1) Carvalhais et al. (2014), (2) Beer et al. (2010), (3) Jung et al. (2011)

2.3.2 Representation of N limitation in LPJmL5-NEGEM

To test the ability of LPJmL5-NEGEM to represent N limitation in plant growth, gross primary production from the simulation with static historic fertilization input based on Elliott et al. (2015) described in section 2.3.1 (*limN*) was compared to a scenario with unlimited N supply (*unlimN*), implemented through high atmospheric deposition rates in each grid cell.

When comparing the gross primary production (GPP) computed in the *unlimN* and *limN* simulations, the removal of N limitation becomes evident in the higher GPP in most regions, especially in the boreal zone, indicating that boreal ecosystems are strongly nutrient limited (see Figure 3). On the other hand, no or marginal increases in GPP are simulated for *unlimN* in dry regions, where other factors such as water availability strongly limit plant growth (von Bloh et al. 2018). The pattern is similar to nutrient limitation as simulated with LPJmL5 in von Bloh et al. (2018), indicating that merging LPJmL4 with LPJmL5 did not negatively affect the model's ability to represent N limitation.

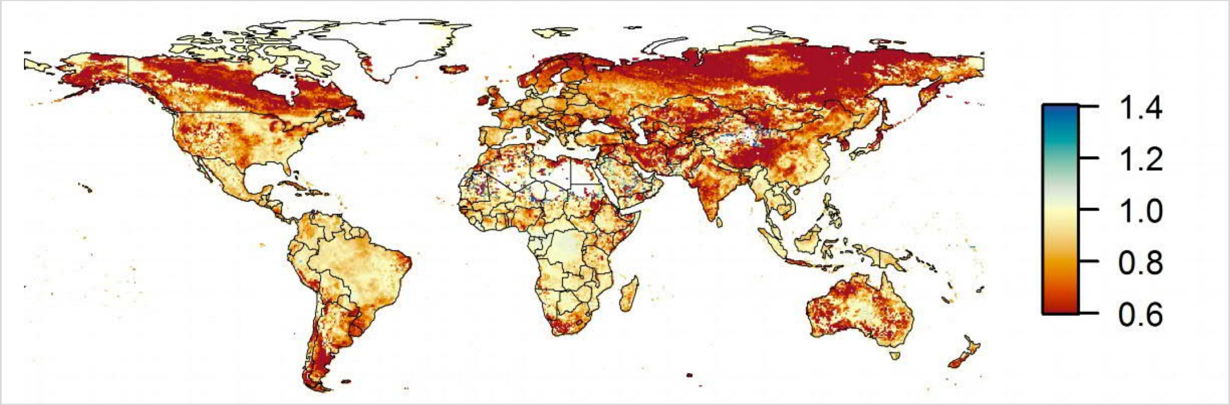


Figure 3 Relative change in GPP in a scenario with unlimited N supply (unlimN) in comparison to a scenario with static historic fertilization input (limN). Numbers above one indicate decreases in unlimN in comparison to limN; numbers below one indicate increases in GPP in unlimN. Results are averaged for the years 1996-2005.

3 Parametrization of bioenergy plantations in LPJmL5-NEGEM

The representation of lignocellulosic bioenergy crops in the process-based vegetation model LPJmL5-NEGEM simulating the plant growth, water and fertilization requirements on biomass plantations is crucial to the assessment of the potentials and impacts of biomass-based NETPs. Therefore, each step of consolidating the major features of LPJmL4 and LPJmL5 was followed by the parametrization of the BFTs required due to the introduction of additional parameters for the enhanced representation of phenology (4.2.1) and N dynamics (4.2.2).

As lignocellulosic bioenergy crops have been subject to intensive optimization through breeding and management, it is important to update the observational data in order to capture these optimizations for the validation of the BFT parametrization. We obtained a recently published comprehensive dataset compiling observational data on yields from lignocellulosic bioenergy crops (Li et al. 2018) that provides a substantial improvement over the dataset used in prior parametrizations in terms of quantity, time periods, geographical distribution and details on irrigation and fertilization (4.1.1).

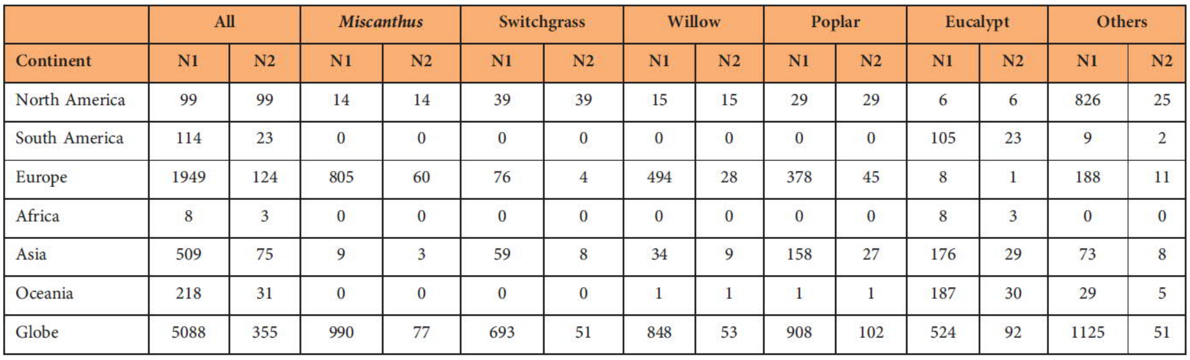
3.1 Observational dataset of bioenergy crops

3.1.1 Suitability of a yield dataset for lignocellulosic bioenergy crops from Li et al. 2018

In 2018, a very comprehensive yield dataset for major lignocellulosic bioenergy crops was published compromising 5,088 entries of data from 257 published studies which cover 355 geographic sites in 31 countries (Li et al. 2018, see Table 2 for the regional distribution of entries and sites). 3,963 of these entries belong to miscanthus, switchgrass, willow, poplar or eucalypt – the five major bioenergy crop types which are represented by three bioenergy functional types in LPJmL. While a number of meta-analysis and reviews have been published before, they often compromise only one crop type (Miguez et al. 2008, e.g. Arnoult and Brancourt-Hulmel 2015, Lewandowski et al. 2003) and/or include a considerably lower amount of experimental sites/publications (Searle and Malins 2014, Laurent et al. 2015). For comparison, the majority of data used for the previous parametrization of bioenergy plantations in LPJmL3.5 was based on a review from (Searle and Malins 2014), and only data from 52 field studies were included (Heck et al. 2016).

The dataset compiled by Li et al. (2018) thus represents the most comprehensive current yield dataset for second generation bioenergy crops, owing to their systematic and reproducible literature search in the Web of Science and the China Knowledge Resource Integrated Database complemented by references of 60 review or meta-analysis studies. Importantly, the dataset additionally links each observed biomass yield with the corresponding information on species, climate conditions as well as management conditions such as fertilization, irrigation, rotation length and planting density amongst others, providing suitable data for validating management-specific growth dynamics of the different second-generation energy crops in LPJmL5-NEGEM.

Table 2 Regional distribution of yield data entries (N1) and geographic sites (N2) across world regions for different lignocellulosic bioenergy crops. Reproduced from (Li et al. 2018).



	All		*Miscanthus*		Switchgrass		Willow		Poplar		Eucalypt		Others	
Continent	N1	N2	N1	N2	N1	N2	N1	N2	N1	N2	N1	N2	N1	N2
North America	99	99	14	14	39	39	15	15	29	29	6	6	826	25
South America	114	23	0	0	0	0	0	0	0	0	105	23	9	2
Europe	1949	124	805	60	76	4	494	28	378	45	8	1	188	11
Africa	8	3	0	0	0	0	0	0	0	0	8	3	0	0
Asia	509	75	9	3	59	8	34	9	158	27	176	29	73	8
Oceania	218	31	0	0	0	0	1	1	1	1	187	30	29	5
Globe	5088	355	990	77	693	51	848	53	908	102	524	92	1125	51

3.1.2 Scope and limits of the dataset

While many geographic regions are covered by the dataset, the yield entries are strongly concentrated on the northern hemisphere (Northern America, Europe and China) and a lack of data especially in Africa and South America can be noticed (see table 2), partly due to scarce research on bioenergy yields in these regions (Li et al. 2018).

Since the systematic literature search was conducted in the end of 2016, this dataset accounts for biomass yield measurements up to the year, 2016. With a mean sampling year of 1999 and most data entries from field measurements between 1986 and 2012, the dataset integrates recent findings. Given the dynamic research area on second generation bioenergy cultivation, it will be important to regularly revalidate bioenergy parametrization in LPJmL once updated yield datasets are available.

3.1.3 Exploring effects of irrigation and fertilization on observed yields

In conjunction with biomass yield measurements, Li et al. (2018) compiled detailed information on irrigation and fertilization. In case information was available, the dataset includes information on whether the field plot was irrigated and/or fertilized or not. In case of irrigation or fertilization, the dataset additionally comprises the amount of irrigation and fertilization (differentiated according to different elements). Understanding the effects of irrigation and fertilization on yields is important for a good representation of bioenergy yields in LPJmL depending on the management conditions. LPJmL5-NEGEM can both prescribe varying N fertilization amounts for bioenergy plantations, as well as the geographic distribution of irrigation schemes (surface, drip and sprinkler irrigation with corresponding efficiencies, for a detailed description see Jägermeyr et al. (2015). This dataset can thus serve as a reference for parametrizing the yield sensitivity of different bioenergy crop types to fertilization. For further assessments, the information on fertilization amounts could provide a basis for generating a literature-based fertilization input for the model, reflecting field practices. Similarly, the observed irrigation practices could be compared to the water requirements for bioenergy plantations simulated in LPJmL.

3.2 Parametrization process: challenges, results and validation

In all LPJmL versions prior to LPJmL5-NEGEM, the BFTs have never been validated with such a comprehensive dataset of yield observations as described in 3.1. Yet, as the potential feedstocks for biomass-based negative emission technologies play an important role in the realistic assessment of biogeochemical potentials of land-based negative emission technologies, we tested the major updates of LPJmL5-NEGEM against this most recent and extensive dataset. As the major developments of the enhanced representation of phenology and N dynamics introduced new parameters for the simulated plant and crop functional types, the BFTs also required parametrization for these processes, as described in the following.

For the evaluation of the model results, we compared the yields reported in Li et al. (2018) from different observation periods to the average BFT yields simulated by LPJmL for 1992-2007 driven by the CRU TS3.23 dataset (University of East Anglia Climatic Research Unit; Harris and Jones 2015). Rainfed and irrigated biomass plantations of herbaceous and woody BFTs were simulated globally, wherever biophysical conditions were suitable for the specific plant growth. For maps depicting simulated potentials of rainfed yields of herbaceous and woody BFTs see Figure 4. Covering at least two 8-year harvest cycles for the woody biomass plantations, the simulated yields were averaged over 16 years and compared to the observed yields of poplar, willow, Eucalyptus, switchgrass and miscanthus on the experiment sites located in the respective grid cell. The management variations in the observational data result in a range of yields for each site and may source from different breeding, soil preparation, fertiliser and irrigation management, crop spacing, sapling sizes or harvest routines. In LPJmL, management uncertainty is limited to irrigation management in versions without N dynamics and extended to fertilizer use for LPJmL5 versions. To depict the management uncertainty, we show the minimum and maximum yields of the observational data and the LPJmL simulations as error bars in Figures 5 and 6 for each LPJmL grid cell with corresponding observational data and compare the mean values of these extremes.

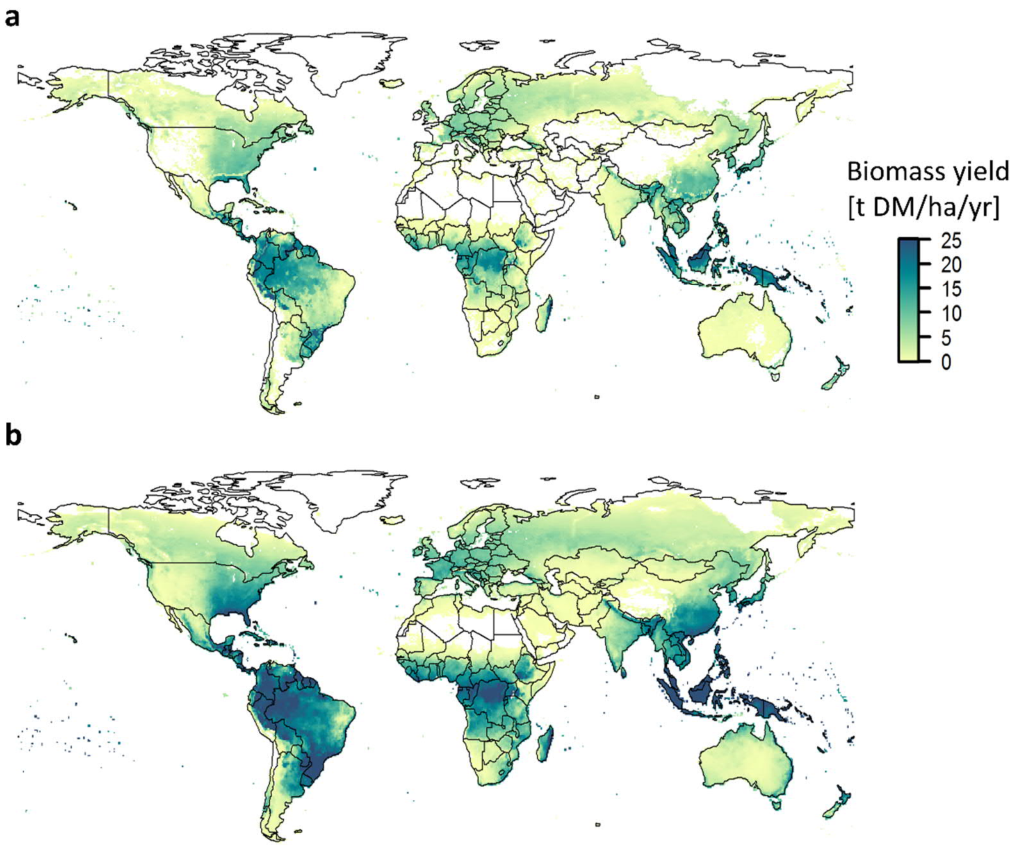


Figure 4 Potentials of rainfed woody (a) and herbaceous (b) yields as simulated with LPJmL5-NEGEM without coupling to the nitrogen cycle. Yields were averaged for 1992-2007 to cover two 8-year harvest cycles for simulated woody short rotation coppice plantations.

3.2.1 Impact of the new phenology scheme on BFT yields

Comparing BFT yields simulated in the former LPJmL3.5 version to the observations reported in the Li et al. (2018) dataset showed that the model overestimates biomass yields of the BFTs considerably without the substantial developments included in LPJmL4 (Figure 5). As experiences with the simulation of the natural vegetation in LPJmL3.5 have shown that productivity was overestimated for many biomes due to neglection of phenology-limiting effects of cold temperature, heat, light and water stress (Forkel et al. 2014), we considered the simplistic representation of phenology and green leaf status as a main factor for this overestimation in LPJmL3.5. Thus, we tested the performance of LPJmL5-NEGEM in terms of BFT yield representation against the observational dataset applying the limiting phenology functions of LPJmL4 and the adapted parameters for the BFTs in line with their natural archetype, i.e. the tropical broadleaved evergreen tree for Eucalyptus, the temperate broadleaved summergreen tree for willow and poplar and the tropical C4 grass for the herbaceous BFT, representing miscanthus and switch grass. In LPJmL5-NEGEM, the phenology status of the BFTs is resultantly defined as a function of cold-temperature, warm-temperature, short-wave radiation and water availability, as developed by Forkel et al. (2014) (see section 3.1.1) with BFT-specific slopes and inflection points of the limiting functions, as well as change rates of the limitation from the actual predicted day to the previous day for each limiting function (see Table 3). The latter aims to avoid abrupt phenological changes because of changing weather conditions.

Table 3 Parameters slope (=slope of limiting function), base (=inflection point of limiting function) and tau (=change rate of the limiting function from actual to previous date) of the four functions for phenology defined for the three second-generation bioenergy functional types (BFTs) represented in LPJmL5-NEGEM adapted from Schaphoff et al. (2018) and Forkel et al. (2014).

Limiting function	Parameter	BFT tropical tree	BFT temperate tree	BFT grass
Cold-temperature	slope	1.01	0.2153	0.91
	base [°C]	8.3	5	6.418
	tau	0.2	0.2	0.2
Warm-temperature	slope	1.86	1.74	1.47
	base [°C]	38.64	41.51	29.16
	tau	0.2	0.2	0.2
Light	slope	77.17	58	64.23
	base [Wm^{-2}]	55.53	59.78	69.9
	tau	0.52	0.2	0.4
Water	slope	5.14	5.24	0.1
	base [%]	4.997	20.96	41.72
	tau	0.44	0.8	0.17

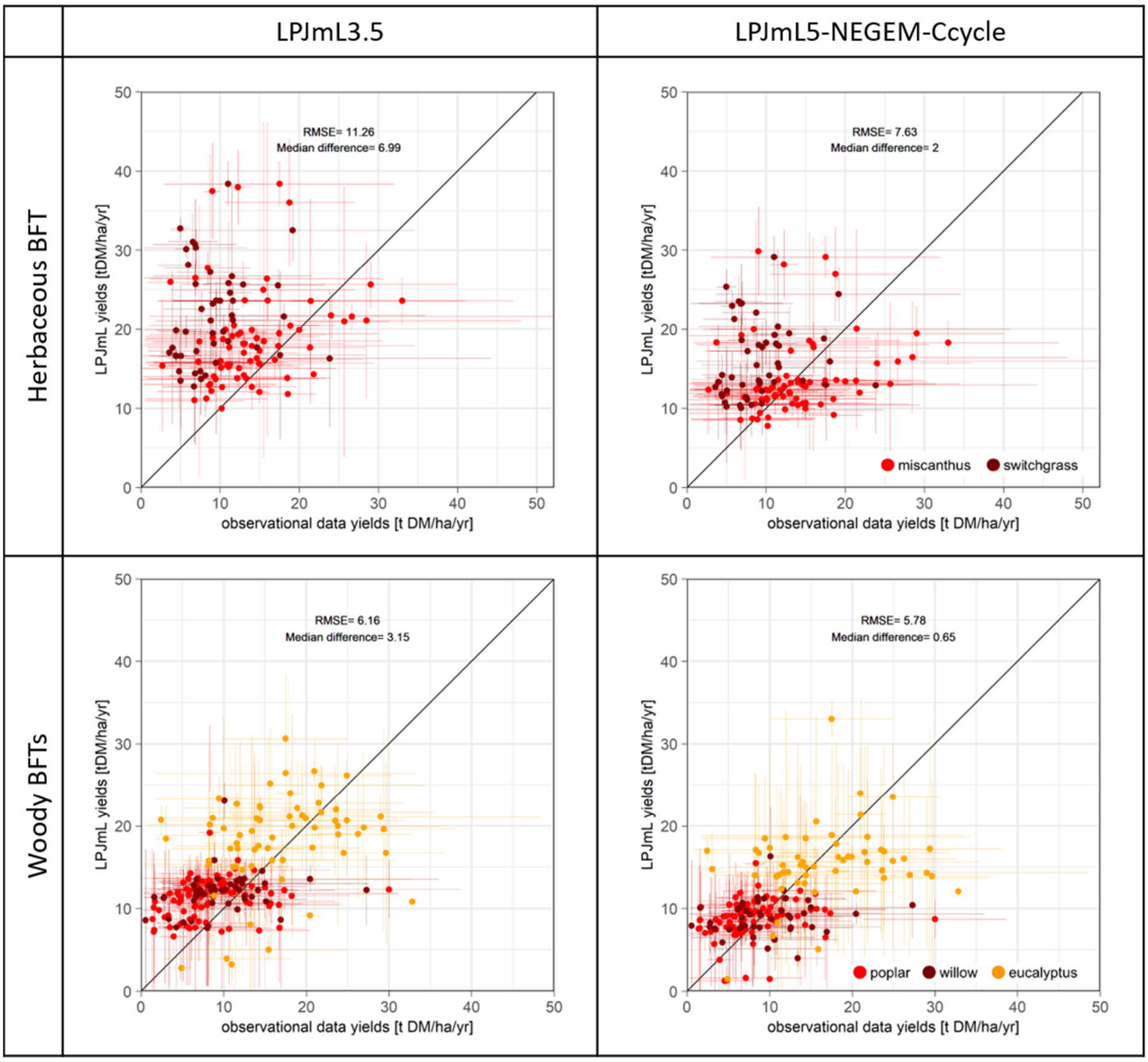


Figure 5 Scatterplots of observed and LPJmL-simulated BFT yields in the respective grid cell for different model versions. Model uncertainty is derived from simulations with and without irrigation (average 1992-2007), whereas observation uncertainty reflects dependencies on plantation management. LPJmL5-NEGEM-Ccycle was employed as the updated version LPJmL5-NEGEM excluding nitrogen dynamics resulting in a better fit to the observed yields compared to the LPJmL3.5 version.

To isolate the effect of integrating the advanced phenology limiting functions, we compared the BFT yields simulated in LPJmL3.5 against LPJmL5-NEGEM running without the coupling to the N cycle, hereafter called LPJmL5-NEGEM-Ccycle. Due to the improved representation of spring onset and the end of the growing season, as already reported for the simulation of the natural archetypes in Forkel et al. (2014), the profound overestimation of BFT yields in LPJmL3.5 could effectively be reduced (Figure 5). For LPJmL versions not including the N dynamics, it has been argued before that the simulated BFT yields might be higher than the observed yields due to the lacking representation of N limitation in these model versions (Heck et al. 2016). However, this argument should not dominate the reasoning as the processes of these model versions were validated against observations or other model approaches of the real-world which is certainly exposed to N limitation (for the extensive validation of LPJmL4, see Schaphoff et al. (2018)).

3.2.2 Parametrization of the herbaceous BFT for LPJmL5-NEGEM with nitrogen dynamics

LPJmL5-NEGEM allows the modeler to decide whether N dynamics should be simulated depending on the processes relevant to the research question. Therefore, the herbaceous BFT as the most promising future source of bioenergy feedstock (Laurent et al. 2015, Arnoult and Brancourt-Hulmel 2015), was parametrized for LPJmL5-NEGEM with N dynamics and compared to the observational dataset. Some key parameters of the natural archetype for the herbaceous BFT (plant functional type: C4 grass) were adapted to N limitation effects on transpiration to meet the global and local transpiration fluxes in the extensive validation process conducted for LPJmL5 in von Bloh et al. (2018). As there is no data available on these fluxes at a global scale for dedicated biomass plantations, we rely on the changes that were required for the parametrization of the natural archetype and incorporate them for the BFTs assuming that N limitation affect evapotranspiration of grasses similarly. These adapted parameters include a higher canopy conductance, which is in the range of values reported in Barnard and Bauerle (2013), and increased evapotranspiration rates to meet global and local evapotranspiration fluxes as validated against EDDY flux tower measurements (Falge et al. 2017, von Bloh et al. 2018) as well as parameters required for N low dynamics (see Table 4). In the calculation of the plant's N demand, we consider a store of labile N to buffer fluctuations between N demand and supply from the soil mineral N pool. Thus, the N demand is increased by the factor of k_{store} - 1.3 for grasses according to Smith et al. (2014). Further, the actual uptake of N is determined by this demand as well as soil mineral N concentrations, fine root mass, soil temperature and porosity. The maximum N uptake rate per unit of fine root mass is set to 5.1 gN $kgC^{-1}d^{-1}$ for crops and grasses following Smith et al. (2014). According to the PFT-specific turnover rates for leaves and fine roots, N is shifted from the living biomass to the litter pool. While the corresponding amount of carbon is moved into the litter pools, not all of the associated N is disposed of but remains in the plant. Thus, we assume that 30% of the N in grasses cannot be recovered before turnover (von Bloh et al. 2018).

Table 4 List of BFT-specific parameters (maximum nitrogen uptake rate Nup;root, increase in nitrogen demand kstore, nitrogen recover fraction at turnover kturn, minimum canopy conductance gmin, maximum water transport capacity Emax) used in the LPJmL5-NEGEM model.

parameter	$N_{up;root}$	k_{store}	k_{turn}	g_{min}	E_{max}
unit	gN kgC^{-1}	--	%	mm s^{-1}	Mm day^{-1}
Herbaceous BFT	5.1	1.3	30	0.8	8

The new parametrization of the herbaceous BFT in simulations, including N dynamics, was tested in a number of test runs identifying errors sourced by merging BFT-specific functions of LPJmL4 and LPJmL5. A stable version of LPJmL5-NEGEM was eventually be established after eliminating water balance errors due to double accounting of the water demand for irrigated stands and crop failures caused by an erroneous interference of intercropping systems with the herbaceous BFTs.

To evaluate the performance of herbaceous BFTs in LPJmL5-NEGEM, including the coupling with the N cycle (LPJmL5-NEGEM-CNcycle) we compared the simulated yields to the miscanthus and switchgrass yields of the observational data from Li et al. (2018). In these simulations the management range could be broadened by assumptions on fertilizer use resulting in a minimum featuring no fertilization nor irrigation and a maximum characterized by unlimited fertilizer and water supply. The mean value of these extremes computed by LPJmL5-NEGEM-CNcycle were again compared to the mean value of the lowest and highest yields reported for test sites in the respective cell. With N-deficient soils representing the conditions for minimum yields in the model simulations, the lower bound of the management uncertainty was significantly lower. As the majority of experiment sites were tested for exposure to similarly non-optimal conditions, the mean values representing the total management range show an improved match compared to the prior LPJmL versions (Figure 6). However, the extreme case of absolute absence of fertilization and irrigation throughout the whole planting and growing of biomass plantations is barely represented in the data compiled by Li et al. (2018). Thus, the herbaceous BFT yields of more than half of the locations compared here are underestimated by LPJmL5-NEGEM-CNcyle. It can further be noted, that most locations with underestimated yields cultivated miscanthus, whereas switchgrass yields are rather overestimated in LPJmL5-NEGEM. This observed pattern can thus also be explained with the fact that both miscanthus and Switchgrass are represented within the herbaceous BFT in LPJmL, although miscanthus yields are typically higher (Li et al. 2018). Whereas the current parametrization of the herbaceous BFT in LPJmL represents a compromise between Switchgrass and miscanthus yields, improvements in representing yields of herbaceous lignocellulosic crops might be achieved by separating the parametrization of the two species.

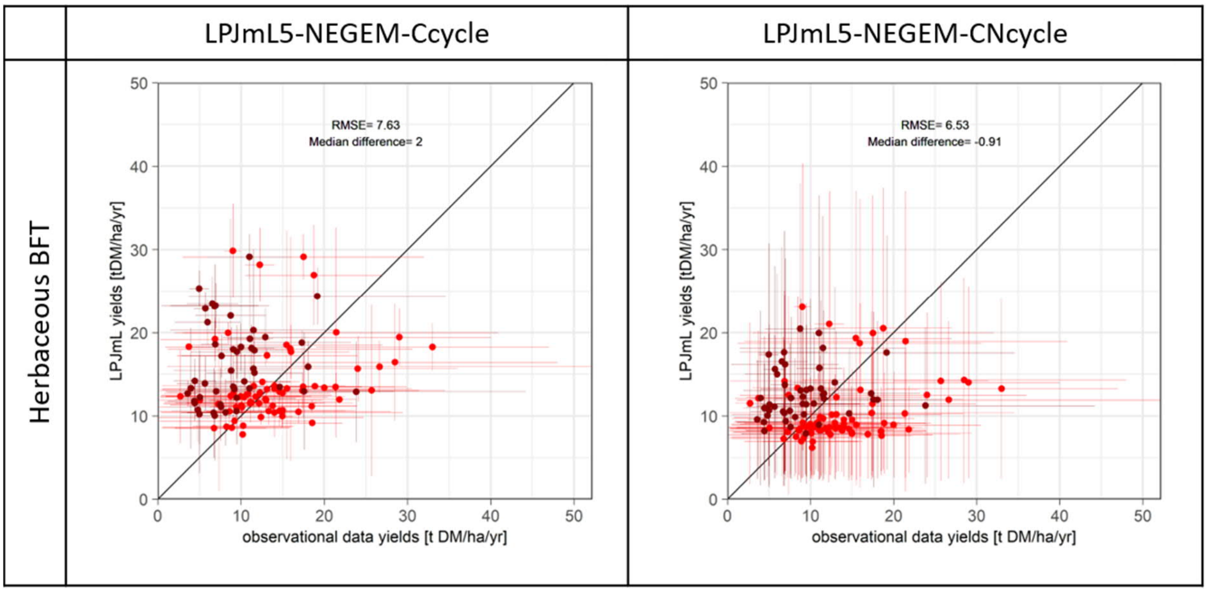


Figure 6: Scatterplots of observed and LPJmL-simulated BFT yields in the respective grid cell for different model versions. Model uncertainty is derived from a simulated minimum featuring no fertilization nor irrigation and a maximum characterized by unlimited fertilizer and water supply (average 1992-2007), whereas observation uncertainty reflects dependencies on plantation management. LPJmL5-NEGEM-CNcycle was employed as the updated version of LPJmL5-NEGEM including nitrogen dynamics.

4 Representation of re-/afforestation in LPJmL5-NEGEM

Afforestation is currently not dynamically modelled in LPJmL as a distinct process, but is represented by the regrowth of natural vegetation wherever human cultivation of crops or pasture is withdrawn. This results in a longer establishment phase of forests in the model than would be expected from reforestation or afforestation projects where succession and competition dynamics are suppressed by planting young trees. A coherent representation of re-/afforestation in or derived by LPJmL5-NEGEM simulations is, however, crucial to the assessment of land-based negative emission potentials within environmental constraints. We thus evaluated two approaches to this representation, which were assessed for their compatibility with LPJmL5-NEGEM.

First, we considered a post-processing method that derives the carbon stored in soil, litter and vegetation biomass in the re-/afforested forests from mature natural forests simulated in LPJmL. This approach would however cause trade-offs with LPJmL's direct and consistent coupling with the carbon, water and N cycle. As an example, higher growth rates in forest plantations would have dynamic impacts on the water and N cycle as well, which cannot be captured by static post-processing factors. Since the direct and consistent coupling with the carbon, water and N cycle in complex vegetation dynamics is the explicit strength of LPJmL5-NEGEM, we decided to discard this approach.

Next, we considered using a dynamic representation of re-/afforestation in LPJmL instead. For this, we could obtain the re-/afforestation module by Braakhekke et al. (2019) developed for the IMAGE application of LPJmL. However, the approach required an in-depth examination to evaluate its efficiency to simulate the processes required to support the analyses planned in D3.2, D3.3, D3.4 and D3.7 as well as the compatibility with LPJmL5-NEGEM. Results of this examination are presented in the following.

The module simulates planted forests intended for carbon sequestration using three dedicated functional types in temperate, tropical, and boreal climates (Braakhekke et al. 2019). The definition of parameters for these functional types followed an optimization to fit target growth curves. Combining field observations and model estimates for equivalent natural forests, these curves represent the development of stemwood carbon in typical plantations.

We find that the assumptions on planting density, carbon use efficiency and vegetation carbon turnover times (vegetation carbon to NPP ratio) in Braakhekke et al. (2019) are well justified by both practices reported for re-/afforestation in the literature and dynamics simulated for the natural archetypes. Furthermore, a clear advantage is that the key parameters required for the integration in LPJmL5-NEGEM are already defined according to the target growth curve optimization. All processes are tested within the LPJmL model framework, thus allowing for high compatibility with LPJmL5-NEGEM. Yet, the module was developed based on an LPJmL version neither including the advanced phenology representation nor the N dynamics. Thus, the optimization towards target growth curves must be repeated for the parameters describing the phenology limiting functions and the key parameters for the N flows. Discussions within the modelling community concluded that the GENOUD algorithm (Mebane Jr. and Sekhon 2011) provides the most suitable structure to derive this set of optimal parameters as it combines a genetic algorithm with a gradient search approach and has successfully been applied for former calibrations in LPJmL adding consistency in parameter optimization (Braakhekke et al. 2019, Forkel et al. 2014).

In their application of the re-/afforestation module, Braakhekke et al. (2019) demonstrated a clearly improved representation of observed stemwood carbon growth rates in forest plantations compared to simulated natural regrowth, while the model still underestimated it compared to observations. The correlation with observed data might, however, be enhanced by revisiting this calibration including the limiting functions of phenology and the

N dynamics featured in LPJmL5-NEGEM. This development effort is considered appropriate, as the substantial improvement of representing the carbon uptake of planted forests as reported by Braakhekke et al. (2019) should be captured: according to their simulations, the re-/afforestation of 650 Mha land over 85 years results in an additional carbon uptake of 48 Gt C for planted forests compared to 37 Gt C for natural regrowth. Dynamically modelling the enhanced carbon accumulation along with the respective water and N flows would not only allow for an enhanced representation of NETP potentials of re-/afforestation in LPJmL5-NEGEM, but would also improve the impact assessment of forest plantations, regarding increasing and decreasing pressures on planetary boundaries (D3.2), specifically for the boundary of freshwater use and the biogeochemical flow of N.

5 *Conclusions and further steps*

The aforementioned model developments provide a solid base for the WP3 assessment of the potential, environmental impacts and trade-offs of terrestrial biomass-based NETPs (re-/afforestation, BECCS, PyCCS) in the context of interacting planetary boundaries. Important LPJmL4 features such as the updated phenology module and an enhanced irrigation module were merged into LPJmL5, which includes the N cycle, resulting in LPJmL5-NEGEM. Further, the parametrization of BFTs was updated and validated within this upgraded model version using a recent extensive observational dataset on bioenergy yields. Depending on the application scenario, options for analysis in LPJmL5-NEGEM and further steps comprise:

(i) In- or exclusion of N dynamics depending on the interest of the assessment (i.e. effects of fertilization on bioenergy plantations on the planetary boundary for N flows or focus on interference with the food sector for which LPJmL5-NEGEM-Ccycle without consideration of N flows provides a better representation of calorie production in the absence of solid fertilizer input data)

(ii) Assessment of herbaceous BFT yields under N limitation where relevant

(iii) Additional parametrization of woody BFTs under N limitation where the research question requires it

(iv) Development of an integrated afforestation module in LPJmL5-NEGEM for an extended analysis beyond plantations.

The LPJmL5-NEGEM upgrade and analysis options thus provide an advanced modelling tool for the WP3 assessment, including the evaluation of biomass-based NETP potentials constrained by environmental limits (i.e. planetary boundaries for N flows, freshwater use and land system change), NETP interference with biosphere integrity, effects of climate extremes on NETP potentials and impacts, and impacts on food security and freshwater availability.

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