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Reproducing CO_2 exchange rates of a crop rotation at contrasting terrain positions using two different modelling approaches

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ABSTRACT

In undulating landscapes erosion is largely responsible for the spatial distribution of C stocks in agricultural soils. Whether these stocks contribute to global atmospheric CO_2 concentrations as source or sink of CO_2 is under constant debate. Periodic CO_2 measurements were carried out at a hummocky ground moraine site grown with maize, fodder rye and sorghum using dynamic non-steady-state transparent and opaque chambers. Flux calculation for CO_2 was conducted using the empirical gap-filling model of Hoffmann et al. (2015b), which uses temperature and radiation to simulate ecosystem respiration (R_{eco}) and gross primary production (GPP) and to calculate net ecosystem CO_2 exchange (NEE). This model was compared with a process-based agro-ecosystem simulation model, MONICA, which was tested for its ability to simulate R_{eco}, GPP and NEE, using the empirical model as benchmark. Both models simulated GPP and R_{eco} in the same order of magnitude, with MONICA simulating a considerably higher amount of CO_2 produced by photosynthesis for maize and less deviating CO_2 produced by photosynthesis for the other crops and CO_2 consumed by respiration for all crops as compared to the empirical model. Both models largely agree in CO_2 flux patterns, but show considerable differences directly after harvest and during bare soil periods. Strengths and weaknesses of both approaches were discussed and synergies of applying both approaches in conjunction were identified in a way that (i) MONICA may act as an independent method to identify significant deviations from the optimum crop growth pattern and thus point at times during which assumptions of the empirical model for simulating NEE may be violated and that (ii) the empirical model may act as a calibration benchmark for MONICA flux simulations.

1. Introduction

In undulating landscapes erosion is the most important soil-forming process. These landscapes mostly most exhibit very heterogeneous soil properties, especially with regard to soil carbon (C) stocks (Doetterl et al., 2012; van Oost et al., 2007, 2012; Vandenbygaart et al., 2012). The consequences of the spatial distribution of C stocks for C fluxes between ecosystem compartments and CO_2 exchange with the atmosphere are mainly unknown. For this reason, the contribution of agricultural land to global atmospheric CO_2 concentrations (later referred to as [CO_2]), being either source or sink of CO_2, is under constant debate (Houghton et al., 2012; Schimel et al., 2015; Smith et al., 2012). Changes in C stocks of agricultural soils occur as a result of alterations to the balance between C input and loss. In a soil–plant system, C input is considered when CO_2 is captured from the atmosphere by plants via photosynthesis and stored in their living tissue. C is lost from the system through autotrophic respiration (R_a) of the plants and through microbial decomposition of plant tissue, when soil organic carbon (SOC) is respired again to CO_2 (heterotrophic respiration R_h). This happens in a slow, continuous process, but land use change may also trigger large peaks (Wei et al., 2014). Within the system, C is transferred from the plant to the soil by deposition of plant residues on the soil's surface or in

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the soil column as dead roots (Jones et al., 2009). Root exudates add additional C to the soil during active plant growth. In sloped landscapes, erosion and deposition may significantly alter this balance (Sanderman and Chappell, 2013; van Oost et al., 2007). However, it remains unclear at which point of the erosion–deposition process chain C sequestration or C liberation processes dominate (Berhe et al., 2007; Berhe and Kleber, 2013; Kirkels et al., 2014; Lal and Pimentel, 2008; Vandenbygaart et al., 2015).

C fluxes in and out of a soil–plant system are observed by means of concentration differences in the surrounding air (Smith et al., 2010). CO_2 concentration measurements require a skilled set-up which does not significantly alter the environmental conditions or else interferes with the processes that are subject of subsequent interpretation. Closed chambers are widely used to introduce an artificial system boundary for CO_2 exchange with the wider atmosphere (Livingston and Hutchinson, 1995). However, closed chambers also inhibit heat and moisture exchange which causes the environmental conditions in the trapped air volume to change quickly, with significant consequences for the plant's physiological behaviour (Lai et al., 2012; Langensiepen et al., 2012; Pumpanen et al., 2004). For this reason, continuous CO_2 concentration monitoring is extremely difficult and campaign-based, discontinuous data acquired by means of short-term chamber measurements prevail for flux analysis. Gap filling methods are then required to derive continuous flux series from single event data. Such methods are often based on simple empirical models, which simulate CO_2 fluxes based on temperature and radiation dynamics (Elsgaard et al., 2012; Falge et al., 2001; Hoffmann et al., 2015b; Richardson et al., 2006). These empirical models deliver not much more than a gap-free time series of what was measured and may fail in reproducing intensity and dynamics of ecosystem CO_2 fluxes, consequently misinterpreting the system's contribution to the atmospheric C budget, if plant physiological development is not well captured by adequately spaced measurement campaigns.

As an alternative, computer simulation models are available, which were constructed on the basis of biophysical processes and have been used already for decades to assess the impact of environmental conditions on plant growth as well as on water and nutrient dynamics in soil–plant–atmosphere systems (Ewert et al., 2015; Martre et al., 2015). Some of these models even allow for a deconstruction of the ecosystem C balance into its components (Abdalla et al., 2014; Abrahamsen and Hansen, 2000; Huang et al., 2009). However, these models have rarely been designed or tested at the level of the above-mentioned CO_2 fluxes, being rather used to predict environmental or management impact on more integrating variables, such as plant biomass production, yield formation or net C stocks of soils (Jandl et al., 2014; Neill, 2011; Schmid et al., 2006; Smith et al., 2012).

We compared the empirical gap-filling algorithm of Hoffmann et al. (2015b, later referred to as the empirical model) with MONICA, an established process-based agro-ecosystem simulation model (Nendel et al., 2011), using field-measured CO_2 exchange data from a field experiment investigating the C budget of maize, fodder rye and sorghum grown on different erosion-induced transient soils in the undulating landscape of North-eastern Germany. Prior to this performance test we calibrated (i) MONICA's soil part against long-term soil C dynamics in various crop rotation experiments and (ii) MONICA's crop part against the aboveground biomass data obtained from the field experiment. From the conceptual point of view, MONICA should be able to reflect the influence of site properties and weather on actual CO_2 fluxes and crop growth and successfully predict cumulative CO_2 fluxes, CO_2

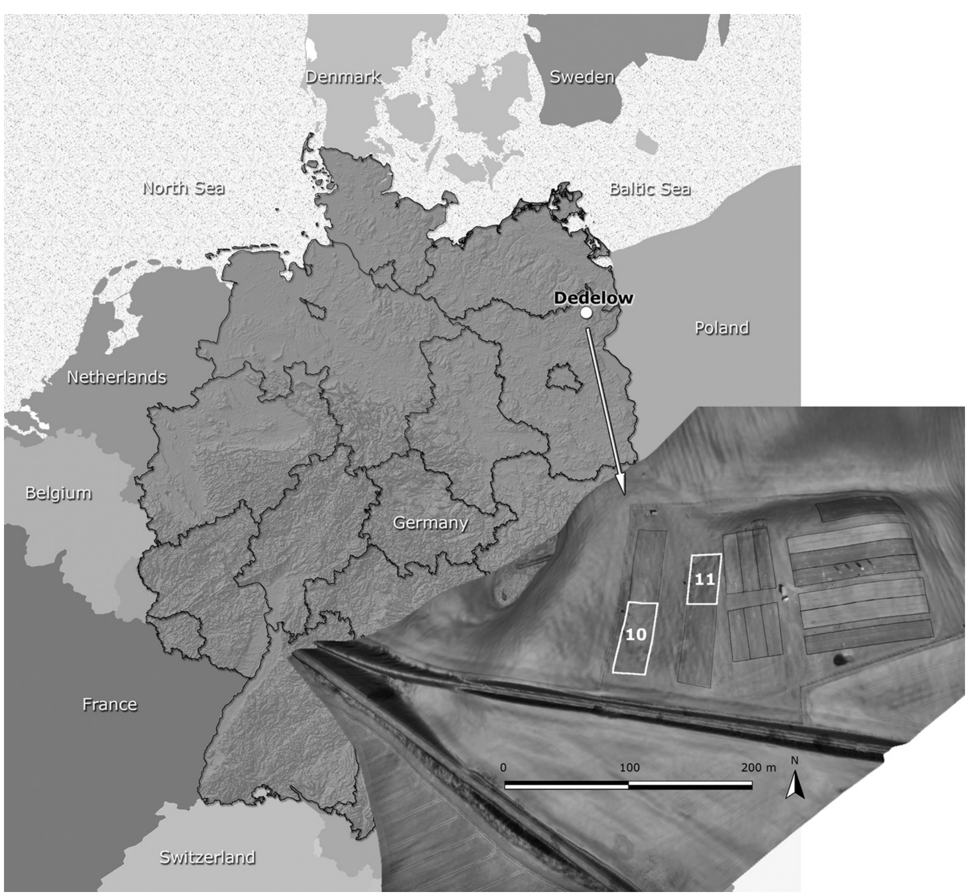

Fig. 1. The CarboZALF experimental site in north-eastern Germany.

budgets and biomass yields at two different landscape positions: hill slope and syncline. In this exercise, we show how MONICA reproduces net ecosystem exchange (NEE) as gross primary production (GPP)–R_a–R_h of the maize–fodder rye–sorghum rotation. The aim of this exercise is (i) to investigate the strengths and weaknesses of both approaches and (ii) to identify promising synergies of applying both approaches in conjunction. It is hypothesised that MONICA may act as an independent method to identify considerable changes in the crop growth pattern and thus point at times during which assumptions of the empirical model for simulating NEE may be violated. Vice versa, the empirical model may act as a calibration benchmark for MONICA flux simulations.

2. Materials and methods

2.1. Site description

The experimental field site is located in the Uckermark, NE Germany, a hummocky ground moraine landscape (Fig. 1; 53°23N, 13°47E, 50–60 m asl). Between 1992 and 2012, an average annual rainfall of 485 mm and a mean annual air temperature of 8.6 °C were recorded by the ZALF Experimental Field Station in Dedelow (www.zalf.de). Climatic conditions are characterised by large inter-annual variability of precipitation, whereas no temporal trend can be detected in decadal rainfall or temperature.

The study area shows a complex soil pattern mainly influenced by relief and type of parent material, e.g. sandy to marly glacial and glacio-fluvial deposits. Along a natural catena, Haplic or Stagnic Luvisols show at knolls and slopes and Mollic Gleysols and Eutric Histosols at footslopes and depressions (soil classification according to the World Reference Base, FAO, 2014). Centennial human activities, especially land use and amelioration, led to a significant change in soil and site conditions, mainly by water and tillage erosion. Consequently, eroded soils, such as Calcaric Regosols and Calcic Luvisols, developed at hilltops and upper to mid-slope positions. Colluvic Regosols influenced either by groundwater or return flow in the upper 2 m cover footslopes and small depressions (kettle holes). Soils affected by erosion meanwhile cover 80% of the arable land, soils which are unaffected by erosion only 20% (Deumlich et al., 2010; Sommer et al., 2008). The CarboZALF-D experimental site was selected for being representative for the regional ground moraine landscape. Plots include non-eroded (Albic Cutanic Luvisol), moderately (Calcic Cutanic Luvisol) to strongly eroded soils (Calcaric Regosol) as well as groundwater-influenced, colluviated soils (Endogleyic Colluvic Regosol). A crop rotation of silage maize (*Zea mays* L.)–winter fodder rye (*Secale cereale* L.)–sorghum (*Sorghum bicolor* L.) was grown from 2010 to 2012. The same amounts of mineral fertiliser were applied to all plots: 160 kg N ha^{-1} in the form of calcium ammonium nitrate (74% NH_4NO_3 and 26% $CaCO_3$). In this paper, we present results from the slope position (moderately eroded, plot 11) and the depression (colluviated, plot 10) for 2010 and 2011.

2.2. Field measurements

2.2.1. Environmental controls

Half-hourly values of air temperature (20 cm height), soil temperatures (2, 5 and 10 cm depth), photosynthetically active radiation (PAR), and precipitation were continuously recorded by a climate station installed at the site. Additionally, plot-specific air and soil temperatures were manually measured simultaneously with CO_2 flux measurements. Plot-specific half-hourly air and soil temperature models were derived from correlations between the respective climate station temperature records and plot-specific manual temperature data.

2.2.2. CO_2 flux measurements

Periodic CO_2 measurements were carried out at three permanently installed soil collars (0.75 × 0.75 m) at each plot using dynamic flow-through non-steady-state transparent (NEE; light transmission of 86%) and opaque (ecosystem respiration—R_{eco}) chambers (Anthony et al., 1995; Drösler, 2005) attached to an infrared gas analyser (Li-820, Lincoln, NE, USA). Full-day CO_2 measurement campaigns with repeated (30–50) individual chamber measurements (closure time 3–5 min) were conducted regularly every 4–6 weeks from 05/2010 to 05/2012, for a total of 18 and 21 full campaigns per plot 10 and 11, respectively. Further details on CO_2 measurement methodology are given in Hoffmann et al. (2015b).

2.3. CO_2 flux calculation and gap filling: the empirical modelling approach

Flux calculation for CO_2 was based on the ideal gas equation, accounting for chamber volume and area, air pressure, and average air temperature during the measurement. Flux calculation, separation into R_{eco},GPP, and NEE as well as subsequent gap filling between measurement campaigns was conducted using the *R* script of Hoffmann et al. (2015b). Measurements <30 s were rejected and measurements >1 min were shortened by a death band of 10% at the beginning and end, respectively (Kutzbach et al., 2007). For each measurement, the final flux rate was selected from all potential flux rates generated by a moving window approach using a stepwise algorithm, numerous quality criteria and the Akaike information criterion (AIC; for details see Hoffmann et al., 2015b). For R_{eco}, gap filling between measurement campaigns was performed using campaign-specific temperature-dependent Arrhenius-type models by Lloyd and Taylor (1994). GPP fluxes were calculated by subtracting modelled R_{eco} fluxes from measured NEE fluxes, and then modelled using campaign-specific hyperbolic PAR-dependent models (Elsgaard et al., 2012; Michaelis and Menten, 1913; Wang et al., 2013). Average measured flux rates were used if no significant fit was achieved for campaign-specific R_{eco} or GPP models. Half-hourly NEE values were calculated from modelled R_{eco} and GPP fluxes (Drösler, 2005; Hoffmann et al., 2015b), and cumulated from May 1st to April 30th of the following year. Negative values represent a C gas flux from the atmosphere to the ecosystem; positive values a flux from the ecosystem to the atmosphere. The uncertainty of the annual CO_2 exchange was quantified using a comprehensive error prediction algorithm described in detail by Hoffmann et al. (2015b).

2.4. CO_2 flux simulation: the process-based modelling approach

2.4.1. Model description

The MONICA model (Nendel et al., 2011) is a complete mechanistic agro-ecosystem simulation model, which was designed to simulate crop growth as well as water and nitrogen dynamics in crop and soil for applied purposes. The carbon algorithms allow for simulations of the effects of climate and management on long-term organic matter dynamics in soil and, in turn, feedback signals to soil physical properties and conditions for crop production.

Crop growth description follows a generic approach, based on the SUCROS model (van Keulen et al., 1982). Daily net dry matter production by photosynthesis and respiration is driven by global radiation and temperature. [CO_2] affects the crop's maximum photosynthesis rate (Mitchell et al., 1995) and stomatal resistance (Yu et al., 2001), which in turn influences transpiration. Maintenance respiration R_m is calculated separately for day and night periods. It is satisfied with priority from assimilates provided by photosynthesis. Thereafter, growth respiration R_g limits the biomass growth increment. Maintenance and growth respiration are summarised in the daily output of the model as R_a, conceptually including dark respiration $R_d = R_m$ in the absence of light and photorespiration $R_p = R_m + R_g$. Assimilates are assigned to the different organ compartments according to a partitioning matrix, dependent on the crop development stage. Crop development, in turn, is calculated from a thermal sum (degree-days) and modified, when appropriate, for each stage by day length and vernalisation (Kersebaum, 1995). Crop growth is limited by water and N stress. Water stress is indicated by the ratio of actual-to-potential transpiration and a crop-specific threshold value which defines the crop's sensitivity to drought. Water and nitrogen (N) uptake is calculated from the potential evaporation and crop N status, depending on the simulated root distribution, as well as the availability of water and N in different soil layers (Kersebaum, 1995). The concept of critical N concentration in plants as a function of crop biomass (Greenwood et al., 1990) is applied to assess the impact of N shortage.

The calculation of organic matter turn-over in soil is based on the routines used in the DAISY model (Hansen et al., 1991). Soil C dynamics are described by three pairs (slow or rapid decomposition) of conceptual pools (soil organic matter, soil microbial biomass and added organic matter). Decomposition rate coefficients are both temperature- and moisture-dependent, and reflect the environmental conditions of the simulated site; decay and respiration rates of soil microbial biomass are further influenced by soil clay content. Efficiency parameters determine the loss of CO_2 during microbial turnover processes, which is summarised in the daily output as heterotrophic respiration R_h.

2.4.2. Model calibration: soil parameters

MONICA (Nendel et al., 2011) contains the largely unaltered soil organic matter turn-over routine of the DAISY model (Hansen et al., 1991). DAISY has been previously tested against a range of long-term experiments, demonstrating its overall ability to reproduce long-term soil organic matter dynamics across different soils and climates (Smith et al., 1997). In order to calibrate MONICA to the conditions of the field experiment, the model was additionally tested against a long-term crop rotation experiment in Müncheberg (Ellerbrock et al., 1999), which is located 95 km south of the site of the gas exchange experiment, in the same agro-environmental zone. The selected crop experiment was an unfertilised rotation of winter wheat, silage maize, winter rye, linseed, potato, spring barley and pea on a sandy soil, for which top soil organic carbon (SOC) measurements were available every second year. A global inverse calibration procedure was carried out, using the Nash-Sutcliffe Modelling Efficiency (EF, Nash and Sutcliffe, 1970) and the mean absolute error (MAE, Willmott and Matsuura, 2005) as a performance indicator. The following test against the short-term CO_2 gas exchange was executed on the basis of this calibration.

2.4.3. Model calibration: crop parameters

MONICA has been calibrated to predict the growth of maize, also under elevated [CO_2], and intensively tested for its ability to predict yields in uncalibrated situations in Germany (Nendel et al., 2011) and across four sites in different agro-environmental zones (Bassu et al., 2014). In this case, a minor calibration was carried out to better match above-ground biomass for the maize grown under sufficient water supply in the terrain depression, including thermal time to emergence since the maize in the experiment emerged erratically due to remaining pre-crop maize stubbles impeding seed contact with the soil and thus proper moisture supply to the seed. For rye, MONICA has been calibrated and tested against data from Germany only (Nendel et al., 2011). No further calibration was pursued. Sorghum has been parameterised using data from a German cross-site experiment for energy cropping systems (Glemnitz et al., 2015) and additionally adjusted for above-ground biomass simulation using data from the current experiment.

2.4.4. Model set-up

Information used as input for the simulation included daily weather (radiation, minimum and maximum air temperature, precipitation, relative air humidity, wind speed), soil characteristics (texture, SOC, horizon boundaries) and annual minimum and maximum depth of the groundwater table.

2.5. Comparing the models

Both approaches were compared relative to each other, using standard performance indicators. The mean bias error (MBE, Addiscott and Whitmore, 1987) summarises the average error of model predictions and should tend to zero. The MBE neither measures the magnitude of errors nor the correspondence between observations and predictions, but it identifies over- or under-predictions by the model. In contrast, the mean absolute error (MAE, Shaeffer, 1980) measures the average magnitude of prediction errors, but does not indicate the direction of deviations. MAE can be normalised by dividing by the mean of the observations, yielding the normalised mean absolute error

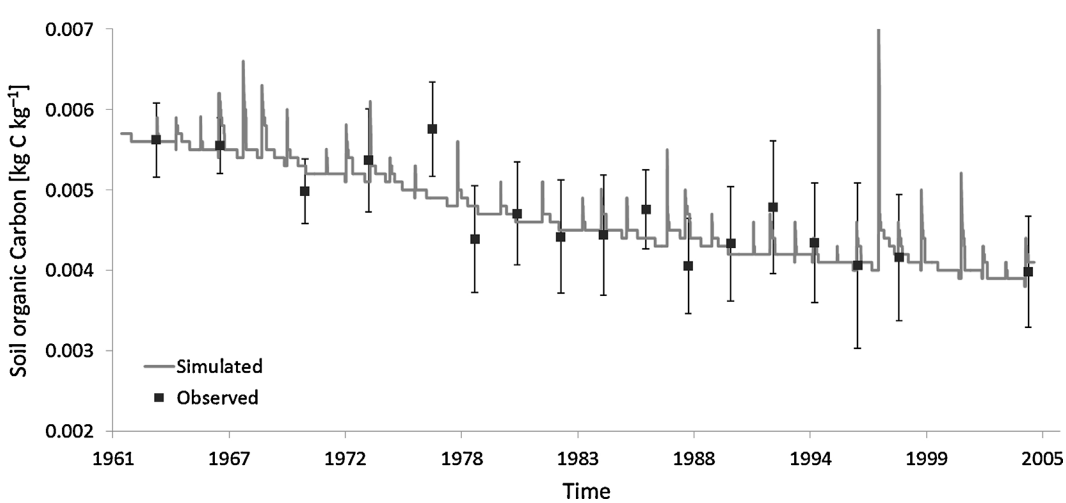

Fig. 2. Results of a global inverse calibration of MONICA against a long-term crop rotation experiment. Dots: observed soil organic carbon concentrations in 0–0.3 m soil depth at the 'Müncheberg V140' experiment (unfertilised treatment). Lines: simulated soil organic carbon concentrations using MONICA.

(nMAE). Finally, the root mean square error (RMSE) is calculated to allow the data to be compared with earlier modelling exercises in which RMSE was frequently used. RMSE is very sensitive to outliers and is also dependent on the size of the data set, which is why it has lost its popularity. The modelling efficiency ME (Nash and Sutcliffe, 1970) is a common indicator based on the correlation between the observed and predicted values, ranging from $-\infty$ to 1. Optimum ME equals 1 and a value of zero indicates that the model is no better estimator than the observed mean.

3. Results

3.1. Calibrating the process-based model against a long-term soil organic carbon experiment

In a global inverse calibration procedure using the experimental data of the 'Müncheberg V140' long-term crop rotation experiment, adjusting the decomposition rate of the slowly decomposing soil organic carbon pool from 4.3×10^{-5} (Bruun et al., 2003) to 3.3×10^{-5} delivered the best simulation performance (Fig. 2). EF for this simulation was 0.55 and the MAE was 0.30 g C kg^{-1}, corresponding to a normalised MAE of 6.4%.

3.2. Calibrating the process-based model against carboZALF above-ground biomass data

Above-ground biomass was simulated by MONICA as a precondition for proving its ability to produce reasonable CO_2 gas exchange rates, since plant CO_2 exchange is closely related to plant biomass development. Only slightly adjusted, MONICA simulates above-ground biomass of all three crops grown in the terrain depression, where water supply has always been sufficient for growth, with only minor deviations (Fig. 3, top). MONICA has not been calibrated further to match growth at the slope position where groundwater table is deeper and water not fully supplied to the crop during short periods. Here, we observe an overestimation of maize and rye growth, and a slight underestimation of sorghum growth (Fig. 3, bottom). Overall MAE was 0.81 t dry matter ha^{-1} in the depression (nMAE 6.0%) and 2.05 t ha^{-1} on the slope (nMAE 21.0%).

3.3. Simulation of the carboZALF gas exchange data

The simulations of both model approaches (empirical and process-based) are compared against each other, assuming that at the dates of the field measurement campaigns the empirical model – directly relying on 30–50 individual chamber measurements – represents a true measured value of daily CO_2 exchange (Figs. 4 and 5). Both models simulate GPP and R_{eco} in the same order of magnitude, with MONICA showing a more than acceptable performance in terms of the correlation-based indicator EF, but a less convincing performance with respect to the difference-based indicators MAE and MBE (Table 1). MONICA simulated a considerably higher amount of CO_2 produced by photosynthesis of maize (+32% in the depression and +42% at the slope), while for fodder rye (+19% and +24%) and sorghum (–5% and –4%) the deviation was much less (Table 2). The simulation of CO_2 consumed by respiration was in general less deviating from results of the empirical model for all crops (maize: 0% and +5%, fodder rye: –20% and –17%, sorghum: –17% and –15%, Table 2). However, the values add up in a way that NEE simulation accumulates to more than double the value predicted by the empirical model over the whole crop rotation (115% and 133%, Table 2), for which mainly the low model performance for maize accounts.

Both models largely agree in pattern during periods where growth conditions were suboptimal (Figs. 4 and 5). For maize, MONICA simulates higher GPP rates than the empirical model throughout the season (Fig. 6). For rye and sorghum, MONICA simulates episodically lower GPP rates than the empirical model, coinciding with periods of drought stress hampering plant growth. The patterns differ most (i) directly after harvest, when MONICA simulates still significant respiration rates which originate from the immediate onset of plant residue decomposition in soil (Fig. 7) while the empirical model does not, and (ii) during bare soil

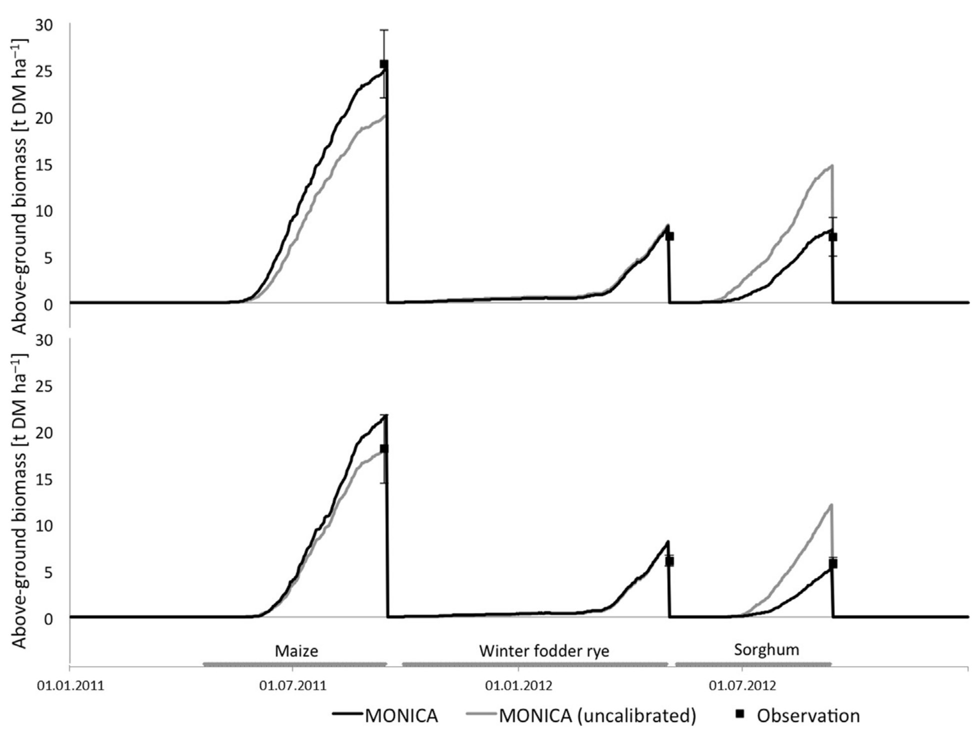

Fig. 3. Observed (dots) and simulated above-ground biomass of a crop rotation grown in a terrain depression (top) and on a hill slope (bottom).

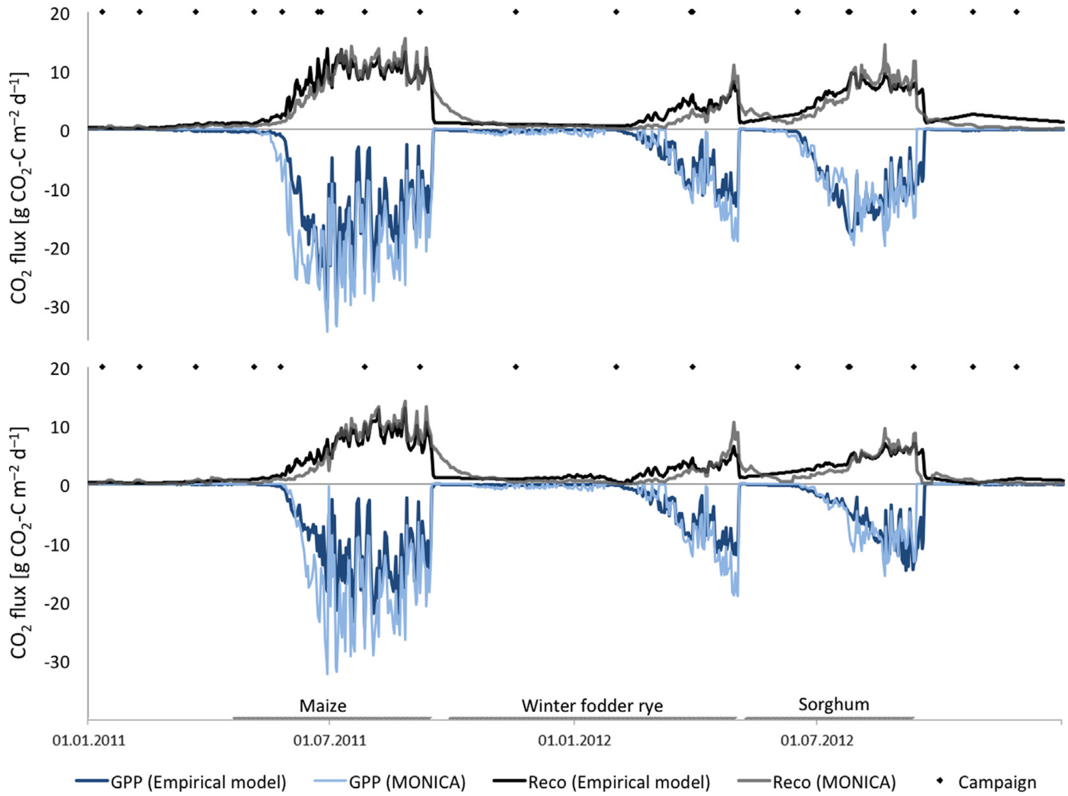

Fig. 4. CO_2 fluxes of gross primary production (GPP; blue coloured lines) and ecosystem respiration (R_{eco}; grey coloured lines) of a plant–soil system at two contrasting terrain positions as simulated using an empirical model (dark coloured lines) and the process-based agro-ecosystem model MONICA (light coloured lines). Top: depression; bottom: hill slope; ◆: campaign dates of high-frequency CO_2 flux measurements.

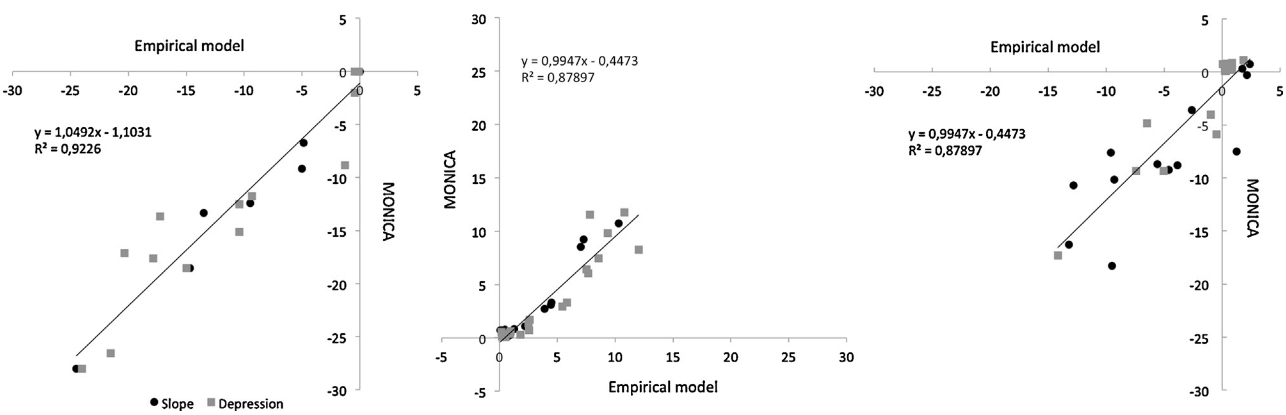

Fig. 5. Scatterplots of simulated GPP (left), R_{eco} (centre) and NEE (right) as produced by the MONICA vs. aggregated measured values at the campaign dates.

Table 1
Performance of MONICA in simulating GPP, R_{eco} and NEE, using the simulated daily values from the empirical model as benchmark.

		n	MAE	MBE $g\,CO_2\text{-}C\,m^{-2}\,d^{-1}$	RMSE	nMAE	EF
GPP	Depression	14	2.77	1.66	3.48	0.26	0.83
	Slope	11	1.59	1.39	2.28	0.24	0.91
	Both sites	25	2.25	1.54	3.01	0.25	0.87
R_{eco}	Depression	19	1.33	0.74	1.71	0.29	0.80
	Slope	16	0.80	0.14	0.94	0.28	0.90
	Both sites	35	1.09	0.47	1.41	0.29	0.85
NEE	Depression	19	2.42	1.94	3.55	0.75	0.52
	Slope	16	1.48	1.08	2.17	0.84	0.73
	Both sites	35	1.99	0.78	1.55	3.00	0.61

Table 2
Comparison of GPP, R_{eco} and NEE simulations across the complete crop rotation and its components as produced by the empirical model and MONICA for two contrasting terrain positions [g CO_2-C m^{-2}].

		Depression			Slope		
		GPP	R_{eco}	NEE	GPP	R_{eco}	NEE
Fallow 1.1.2011–20.4.2011	Emp. Model	−12 ± 2	53 ± 3	41 ± 4	−2 ± 1	37 ± 4	36 ± 5
	MONICA	0	34	−4	0	35	35
	Difference	−12	19	44	−2	2	0
Maize 21.4.2011–29.9.2011	Emp. Model	−1653 ± 79	1113 ± 60	−540 ± 106	−1272 ± 35	838 ± 41	−441 ± 52
	MONICA	−2183	1105	−1079	−1806	879	−937
	Difference	530	8	539	534	−41	496
Winter rye 30.9.2011–08.5.2012	Emp. Model	−518 ± 15	396 ± 16	−122 ± 26	−478 ± 10	364 ± 39	−114 ± 40
	MONICA	−613	316	−298	−594	302	−292
	Difference	96	80	176	116	62	178
Sorghum 9.5.2012–31.12.2012	Emp. Model	−978 ± 47	889 ± 60	−89 ± 76	−578 ± 164	546 ± 32	−32 ± 164
	MONICA	−925	742	−183	−555	462	−94
	Difference	−53	147	94	−23	84	61
Total 1.1.2011–31.12.2012	Emp. Model	−3161 ± 143	2451 ± 139	−710 ± 212	−2330 ± 211	1785 ± 116	−552 ± 261
	MONICA	−3721	2197	−1526	−2955	1678	−1287
	Difference	560	254	814	625	107	735

periods, when the empirical model interpolates between only few measurement campaigns while the process-based model continues simulating the ongoing microbial activity and organic matter turnover in the soil.

4. Discussion

Both modelling approaches reproduce reasonable CO_2 exchange rates in the range of the measured values, although at a small temporal resolution considerable differences are noted for individual CO_2 fluxes. Observed CO_2 fluxes originate from short-term (seconds to minutes) measurements and the temporal scaling to produce daily values to compare with the daily time step simulations of the process-based model requires empirical models, whose performance is put to test at the same time. However, apart from the drivers temperature and radiation considered in the empirical model, the other main drivers of ecosystem CO_2 exchange, i.e. plant biomass and soil moisture, can be considered stable for the duration of a single day. Hence, for the actual day of measurement, the daily CO_2 exchange rate derived by

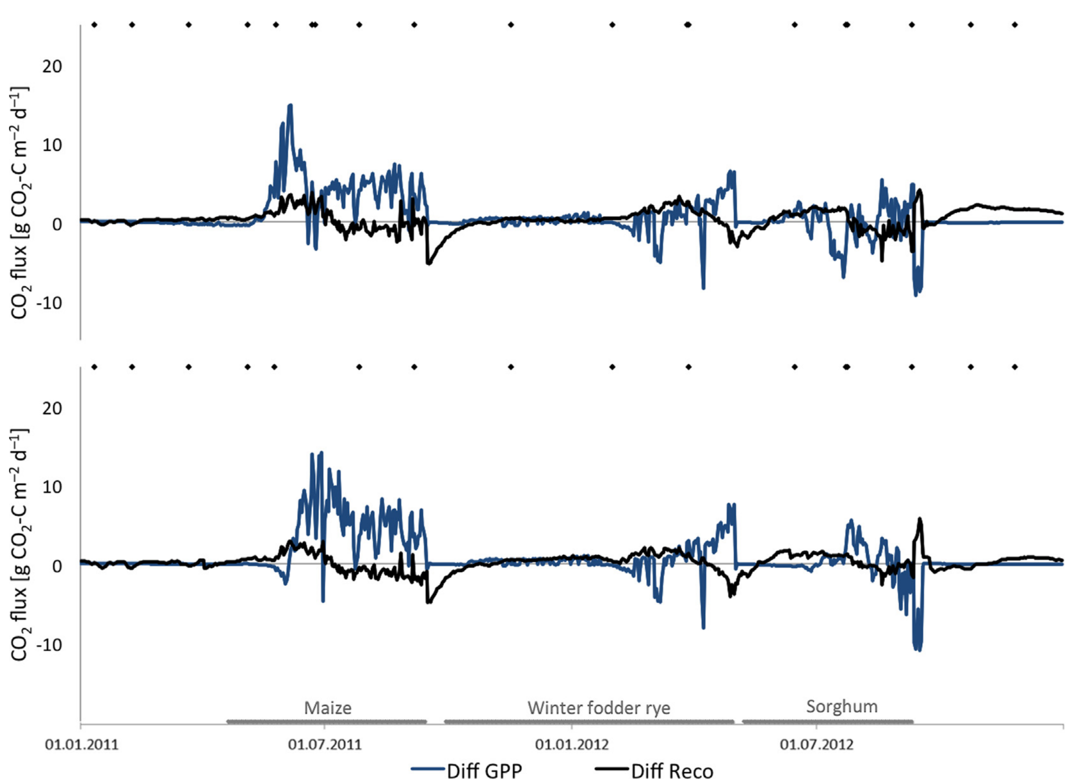

Fig. 6. Difference between two simulations of CO_2 fluxes of gross primary production (GPP; blue line) and ecosystem respiration (R_{eco}; black line) of a plant–soil system at two contrasting terrain positions using an empirical and a process-based agro-ecosystem model. Top: depression; bottom: hill slope; ◆: campaign dates of high-frequency CO_2 flux measurements.

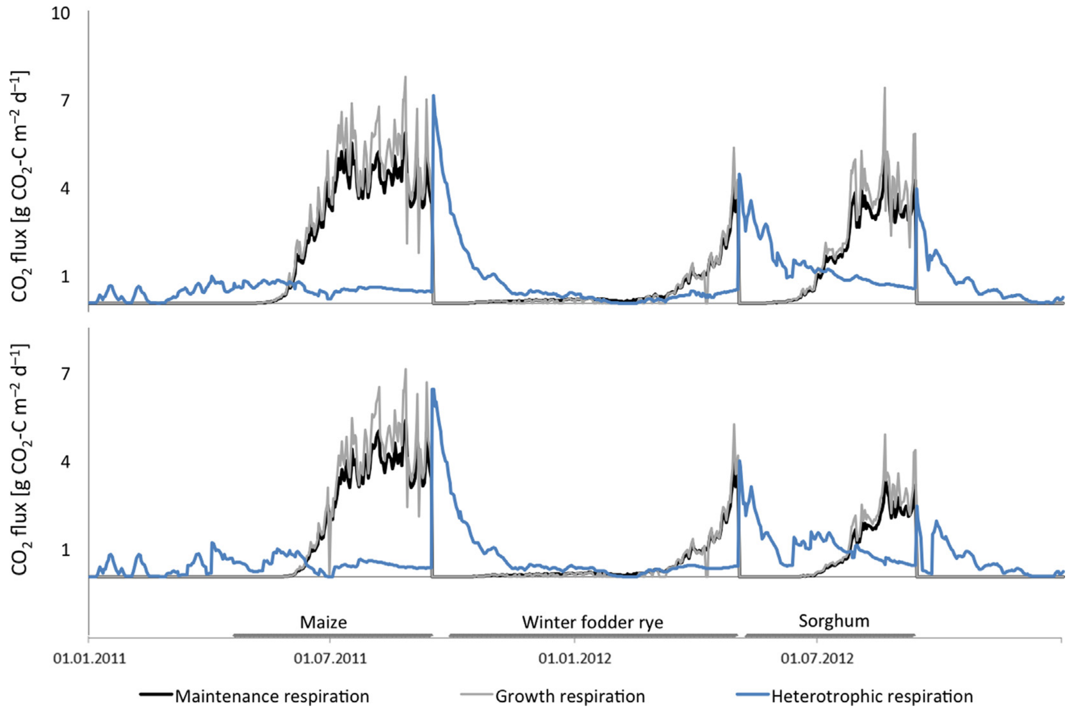

Fig. 7. Demonstration of the additional information contributed by a process-based agro-ecosystem model to the analysis of CO_2 fluxes originating from ecosystem respiration: separation of maintenance respiration (black line), growth respiration (grey line) and heterotrophic respiration (blue line) of a simulated plant–soil system. Top: terrain depression, bottom: hill slope.

temperature- and radiation-dependent empirical modelling based on 30–50 chamber measurements can be assumed as being representative of true CO_2 exchange rates. For the purpose of model comparison, the empirical data from the actual measurement campaigns can thus be used as reference to evaluate the MONICA estimates, while the true CO_2 exchange rates during the gap-filling periods are unknown and no reference level is available.

4.1. Gap-filling method

The empirical model of Hoffmann et al. (2015b) was developed as a gap-filling method in order to produce a continuous time series of CO_2 gas exchange data for a soil–plant system based on periodic chamber measurements. While gap-filling of CO_2 flux data based on temperature (R_{eco}) and radiation (NEE) is generally accepted (Moffat et al., 2007), the linear interpolation of empirically modelled CO_2 exchange rates between consecutive measurement campaigns relies on the inherent assumption of linear biomass development. Depending on the time period between two consecutive measurement campaigns, this assumption may be violated in times of rapid plant development such as often noted during shoot elongation, potentially underestimating plant photosynthetic activity and thus GPP when interpolation spans longer periods unsupported by measurements. Campaign frequency should therefore be increased in times of rapid plant growth, or plant biomass introduced as an empirical modelling parameter. In addition, empirical temperature- and radiation-dependent models often cannot be fitted when the diurnal temperature or PAR variability is small, resulting in average CO_2 exchange rates being extrapolated over several weeks. This applies especially to the winter period, in which either no crop was planted or low temperatures allowed only very reduced biological activity. However, although the relative error of the empirically derived CO_2 exchange rates may be large, particularly during periods of low activity insufficiently supported by measurements, this difference is assumed neglectable in absolute terms. These issues have previously been recognised and addressed by Hoffmann et al. (2015b), who therefore included both a calibration and a validation procedure in their empirical approach to quantify the uncertainty arising from inappropriate campaign spacing as well as lacking model fit. While the former procedure analyses discrepancies between measured and simulated half-hourly flux data using goodness-of-fit indices, the latter evaluates the effects of campaign spacing on the CO_2 flux estimates by omitting data entire measurement campaigns from the final empirical model via leave-one-out cross-validation. The overall quality of CO_2 exchange data estimated with the campaign-based empirical approach is therefore highly dependent on the frequency and the spacing of the CO_2 measurement campaigns in relation to the respective crop and its development.

4.2. Process-based simulation

In contrast to the empirical model, a process-based simulation model delivers a time series of flux rates in which every data point has the same weight, as there is no difference between supporting points and calculated values. During times of limited crop growth or absence of a crop, a process-based model produces values of similar accuracy, well reflecting the response of soil microbial activity and, if applicable, gas transport processes through the soil to environmental conditions. For doing so, however, the process-based model needs to be able to reproduce (i) soil organic matter decomposition, (ii) crop phenology, and (iii) crop growth the best possible, since these factors – especially the timing of crop growth – are conditions sine qua non for crop-related gas exchange simulations.

For the first precondition, it was ensured by means of calibration that MONICA assumes soil organic matter decomposition rates which agree with long-term data obtained from the same agro-climatic zone. The test against the ‘Müncheberg V140’ long-term SOC data set revealed that SOC decline was 23.3% slower than assumed by the original parametrisation, which represented the

SOC dynamics from the Askov long-term experiment in Denmark (Bruun et al., 2003). The Askov soils are sandy loam soils, while at Müncheberg loamy sands prevail. Hints exists that in sandy soils decomposition of soil organic matter is slower (Bimüller et al., 2014) and model parameters derived from finer textured soils may not perform sufficiently well (Heumann and Böttcher, 2004). With regard to measured and simulated R_h, the decomposition of the slow pool (recalcitrant soil organic matter) is not assumed to contribute significantly to the CO_2 emission from soil. This test and calibration procedure is merely seen as a demonstration of MONICA simulations of short-term soil CO_2 production being well in agreement with long-term SOC dynamics. Short-term organic matter turnover (e.g. plant residues) has been sufficiently tested for the DAISY model before (Müller et al., 2003).

The second precondition for a successful reproduction of measured CO_2 gas exchange rates is an accurate representation of crop phenology. Process-based crop models, such as MONICA, calculate crop phenology, including seedling emergence, based on environmental conditions and may fail in doing so. In the case of the presented experiment, MONICA assumed earlier emergence of maize as observed in the field, since the conditions that hampered undisturbed emergence could not be introduced to the model due to the respective algorithms not being implemented. By means of parameter adjustment (thermal time until emergence) MONICA was forced to simulate maize emergence later in order to better match the observed emergence date.

The third precondition is the accurate simulation of plant biomass and also here crop models could do wrong, especially if the model has been calibrated to different genotypes or different environments (Bassu et al., 2014; Martre et al., 2015). Crop modelling at larger scales or under scenario conditions may accept larger deviations since the use of several temporal or spatial replicates may help reducing uncertainty. In fact, quantifying the uncertainty may be one of the goals of model predictions (Asseng et al., 2013). In case of the reproduction of plot-scale crop growth, even minimal errors may lead to refusal of the result, especially if errors in crop growth simulation entail even larger errors in subordinate analyses. This also applies to the simulation of CO_2 exchange rates, which largely depends on the simulation of crop growth.

4.3. Site effects and other influencing factors

For the sites under investigation, the terrain position has a significant effect on crop growth (Hoffmann et al., 2015a), which is mostly due to differences in water supply at the slope and in the syncline, the latter collecting water from subsurface flow and run-off from the circumjacent slopes and exhibiting shallower groundwater table (Hook and Burke, 2000; Manning et al., 2001; Priyashantha et al., 2007). Only in cases of excess rainfall, the water supply in the depression can produce adverse growth conditions due to O_2 deficiency in the root zone (Grant, 2004). For crop models not considering groundwater levels, the risk of failure in simulating crop growth at such sites is particularly high (Kersebaum and Nendel, 2014). In addition to this, erosion-induced differences in SOM contents exhibit correlating differences in natural nutrient supply via SOM mineralisation. While crop models often consider this circumstance with respect to nitrogen, there may be considerable effects of other nutrients (P, K, Mg and micro-nutrients) which currently available models do not account for.

All in all, there seem to be many factors related to accurate modelling of soil organic matter decomposition, crop phenology, and crop growth that could overthrow uncalibrated simulation attempts. The application of a process-based model without prior calibration may therefore lead to substantial miscarriage of C balance calculations. However, in studies where detailed plot-scale CO_2 flux simulations are not required to derive more general statements, the uncertainties introduced by the crop growth algorithms may be considered neglectable.

4.4. Comparison of the two models

Depending on the research question, the lack of prediction accuracy of a process-based model may be more than compensated by the additional information on C flux components provided by the process-based model compared to empirical models. Field CO_2 measurements can only directly measure R_{eco} and NEE, from which the empirical model then derives a complete time series of GPP. A sophisticated process-based model can separate different C fluxes, such as maintenance (R_m) and growth (R_g) respiration, also specific to individual plant organs. Using MONICA, even the contribution of root respiration can be simulated as a separate contribution to what is measured as bulk soil respiration, originating from respiring roots and microorganisms and from CO_2-producing extracellular enzyme activity (Blankinship et al., 2014). Restrictively, it has to be added that most process-based agro-ecosystem models have not yet been sufficiently parameterised at this level of detail and derive root respiration from root biomass using an organ-specific respiration rate. Moreover, the transfer of C compounds from the plant to the soil via exudates prior to their decomposition in the rhizosphere is rarely implemented in such models (Personeni et al., 2007; Toal et al., 2000). In the current example, MONICA simulates an immediate onset of crop residue decomposition after harvest, resulting in a CO_2 peak already on the following day. Again, conceptual simplifications in the model limit the reproduction of the timing of plant tissue decomposition, neglecting that microbes require some time to colonise dead plant material before notable decomposition commences. MONICA assumes all above- and below-ground plant residues being in the soil immediately after harvest and neither physical nor biochemical constraints for immediate degradation. This is why MONICA differs most significantly from the empirical model during the short period right after harvest. However, as no ploughing or other soil preparation took place immediately following harvest and incorporated the harvest residues into the soil, the empirically derived time series is assumed to be more realistic for this period.

A second period of considerable inter-model differences is noted during winter, when biological and biochemical activity is greatly reduced due to low temperatures, and the presence or absence of a crop has only a negligible absolute effect on CO_2 exchange rates. As a result of lacking model-fit and resulting linear interpolation, the values simulated by the empirical model show extremely low variability during winter and are almost constant after the harvest of sorghum. In contrast, MONICA simulates a more responsive flux series which reflects the – albeit small – existing diurnal variability of temperatures and hence microbial activity, and thus seems more realistic. However, both approaches simulate very low winter CO_2 exchange rates and, even though the deviation between both simulations is large relative to the mean of prediction, it is almost neglectable in the context of the seasonal CO_2 exchange.

5. Conclusion

The two modelling approaches differ in scope, which is why a performance comparison does not bring up a champion. Teaming up, both approaches do contribute to the analysis of CO_2 exchange measurements for a plant–soil system with their specific strengths: the empirical model by filling gaps between and temporal scaling of campaign-based short-term CO_2 measurements and the process-based model in interpreting subordinate, non-measured C fluxes and spatial scaling of CO_2 exchange dynamics. Information about plant development and the resulting dynamics of ecosystem CO_2 exchange derived from MONICA could be integrated with the measured data to support the empirical model when campaign spacing cannot be intensified for technical reasons or data is lacking in certain periods. While MONICA itself may not be suitable to simulate and capture differences in the ecosystem CO_2 exchange of individual plots, such as different soil preparation or fertilisation treatments, the temporally dynamic data from MONICA could complement the empirical modelling approach to generate improved plot-specific CO_2 and C budgets.

Another possible path ahead towards an improved tool for calculating regional C budgets on the basis of simulations could be the use of MONICA after a calibration against CO_2 flux simulations produced by the empirical model. Such calibration would then include respiration and photosynthesis parameters, going beyond the set of parameters usually touched in a calibration procedure (Rötter et al., 2012; Specka et al., 2015). MONICA already demonstrated its potential in reproducing a similar pattern as the benchmark model and further calibration may put MONICA in the position to be used for independent simulations of CO_2 fluxes in agro-ecosystems in future studies. However, some parts of the C cycle represented in MONICA should be subject to further validation, which includes below-ground C export from the crop to the soil and organ-specific photosynthesis and respiration. For a more general prediction of the impact of changing environmental conditions on the C budget of an agro-ecosystem MONICA may already be declared fit for purpose.

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