PIXGRO: A model for simulating the ecosystem CO₂ exchange and growth of spring barley

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Received 8 October 2003; received in revised form 1 April 2005; accepted 6 April 2005
Available online 28 June 2005

Abstract

A model, PIXGRO, developed by coupling a canopy flux sub-model (PROXELNÉE; PROcess-based piXEL Net Ecosystem CO₂ Exchange) to a vegetation structure submodel (CGRO), for simulating both net ecosystem CO₂ exchange (NEE) and growth of spring barley is described. PIXGRO is an extension of the stand-level CO₂ and H₂O-flux model PROXELNÉE, that simulates the NEE on a process basis, but goes further to include the dry matter production, partitioning, and crop development for spring barley. Dry matter partitioned to the leaf was converted to leaf area index (LAI) using relationships for the specific leaf area (SLA). The canopy flux component, PROXELNÉE was calibrated using information from the literature on C3 plants and was tested using CO₂ flux data from an eddy-covariance (EC) method in Finland with long-term observations. The growth component (CGRO) was calibrated using data from the literature on spring barley as well as data from the Finland site. It was then validated against field data from two sites in Germany and partly via the use of MODIS remotely sensed LAI from the Finland site.

Both the diurnal and the seasonal patterns of gross CO₂ uptake were very well simulated ($R^2 = 0.92$). A slight seasonal bias may be attributed to leaf ageing. Crop growth was also well simulated; simulated dry matter agreed with field observed data from Germany ($R^2 = 0.90$). For LAI, the agreement between the simulated and observed was good ($R^2 = 0.80$), giving an indication that functions describing the conversion of fixed CO₂ to dry matter and the subsequent partitioning leaf dry matter and LAI simulation were robust and provided reliable estimates.

The MODIS LAI at a resolution of 1000 m agreed poorly ($R^2 = 0.45$) with the PIXGRO simulated LAI and the observed LAI at the Finland site in 2001. We attributed this to the coarse resolution of the image and/or the small size of the barley field (about 17 ha or 0.25 km²) at the Finland site. By deriving a regression relation between the observed LAI and NDVI from a higher resolution MODIS (500 m resolution), the MODIS-recalculated LAI agreed better with the PIXGRO-simulated LAI ($R^2 = 0.86$).

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PIXGRO provides a prototype model bridging the disciplines of plant physiology, crop modeling and remote sensing, for use in a spatial context in evaluating carbon balances and plant growth at stand level, landscape, regional, and with some care, continental scales. Since almost 50% of the European land surface is covered by crops, such a model is needed for the dynamic estimation of LAI and NEE of croplands.

Keywords: Crop growth modeling; Net ecosystem exchange (NEE); Remotely sensed LAI; Spring barley modeling

1. Introduction

About 50% of the land surface of Europe is covered by crops. Hence, agricultural lands have become an important part of the European ecosystems, influencing the ecosystem exchange processes including net ecosystem CO2 exchange (NEE) and other ecological functions of landscapes. To assess how agriculture affects landscape processes, it is necessary to both quantify the NEE of croplands as well as estimate crop growth, partly because the NEE depends on growth and also because crop production information is needed for making policy and economic decisions. Due to the high costs and labour requirements for extensive field data collection, models are often used as alternative or additional tools for estimating NEE. For example, PROXELNEE (Tenhunen, 2001; Reichstein, 2001; Reichstein et al., 2002) is a canopy gas-exchange model that has been used to assess the NEE for tundra and grasslands, Mediterranean shrublands, and has also been recently validated against eddy-covariance (EC) data for forests in Central and Mediterranean Europe (Falge et al., 2001; Reichstein et al., 2002).

As in the case for grasslands, crop models should facilitate both the assessment of exchange processes and crop growth, which influences NEE via changing LAI. Many crop models have been published (e.g. CERES-Wheat: Otter-Nacke et al., 1987; CERES-Maize: Jones and Kiniry, 1986; etc., see review by Ritchie, 1991) and are used extensively worldwide to simulate crop growth and yields usually at farm level. Traditionally those models have their major focus on yield simulation, while other studies focus on water and nitrogen balances (Liu and Bull, 2001; Heinemann et al., 2002; Krysanova and Haberlandt, 2002; van den Berg et al., 2002; Zhang et al., 2002). Often, many of these crop models rely on phenomenological descriptions of growth and yield, while ecophysiological consequences of growth are somewhat neglected. It is thus a major aim of this study to present a model which closes this gap by linking a well-established physically and physiologically based soil-canopy gas-exchange model (PROXELNEE; cf. Tenhunen et al., 1994; Falge, 1996; Reichstein et al., 2002, 2003) with a crop phenology and growth model (CGRO) to simulate ecosystem processes and plant growth from half-hourly to interannual time-scales. Further, it is also the aim of this study to evaluate such a coupled model in terms of its ability to upscale from point field levels to regional scales using remote sensing data.

One option for developing such a coupled model would be to combine an existing crop model with a calibrated canopy flux model such as PROXELNEE. However, experience gained from modeling mixed cropping systems indicate that the direct combination of crop models developed for individual species often results in the complex task of reconciling sub-programs designed for the same functions but programmed differently within the individual models (Caldwell and Hansen, 1993; Adiku, 1995). To avoid such difficulties, we have adopted the canopy process descriptions and programming framework currently available in PROXELNEE and added further routines that simulate dry matter accumulation, partitioning, the LAI and crop development for spring barley.

With an aim to use PIXGRO at landscape and regional scales, its validation would also require landscape scale data in addition to point field measurements. There is evidence indicating that pertinent spatially distributed information on vegetation such as the leaf area, chlorophyll content, and the above-ground biomass may be derived from satellite imagery using the vegetation Indices (NDVI, EVI) (Puredorj et al., 1998; Huete et al., 2002) or inversion of radiative transfer models. An additional aim of this study is, therefore, to explore the possibility of using the MODIS satellite products as a further independent source of data for validating PIXGRO.
2. Materials and methods

2.1. Net ecosystem CO₂ exchange

At the highest hierarchical level, the PIX-GRO model consists of two coupled sub-models (Fig. 1): PROXEL-NEE (PROcess pXEL net ecosystem exchange model) and CGRO (Crop GROwth). PROXEL-NEE describes the physical and physiological canopy and soil processes, while CGRO describes the plant growth processes and phenological development. PROXEL-NEE simulates the short-term dynamics of whole-ecosystem CO₂ and H₂O exchange as a function of prescribed meteorological conditions and ecosystem properties (Reichstein, 2001; Reichstein et al., 2002). PROXEL-NEE has two main process levels; namely the canopy and soil processes. Canopy processes include the canopy carbon balance (photosynthesis and respiration) and canopy water balance (transpiration). The simulated soil processes are the soil water balance, soil heat balance and soil CO₂ efflux. A soil water-dependent signal (gfac; see Table 1) regulates leaf
stomatal conductance and hence controls photosynthesis and transpiration rates via a feedback.

The simulation of canopy gas exchange is based on earlier works of Caldwell et al. (1986) and the further improvements made by Sala and Tenhunen (1996) and Reichstein (2001). The canopy is assumed to comprise a number of horizontal homogeneous layers for which the leaf-level gas exchange can be computed and summed to give whole canopy gas exchange. The computation of the leaf-level photosynthesis follows Farquhar and von Caemmerer (1982) as modified for practical field applications by Harley and Tenhunen (1991). In brief, the gross photosynthesis rate, \( P_{\text{gross}} \) (\( \mu \text{mol} \text{ m}^{-2} \text{ s}^{-1} \)) is given by

\[
P_{\text{gross}} = \frac{\Gamma^*}{c_1} \min(w_c, w_j)
\]

where \( w_c \) and \( w_j \) are the maximum RUBISCO enzyme and electron transport-dependent carboxylation rates, respectively (both \( \mu \text{mol} \text{ m}^{-2} \text{ s}^{-1} \)); \( \Gamma^* \) the CO2 compensation point and \( c_1 \) the internal CO2 concentration (\( \mu \text{l} \text{l}^{-1} \), i.e. ppm) and the function \( \min \) selects the minimum of \( w_c \) and \( w_j \). The \( w_c \) is dependent on \( c_i \) according to a Michaelis–Menten equation with a maximum \( V_{c, \text{max}} \). Also the \( w_j \) depends on the flux density of the photosynthetically active radiation absorbed by the leaf. The key parameters describing the \( w_j \)-light function are the light use efficiency and the maximum electron transport capacity \( J_{\text{max}} \). The parameterization of the photosynthesis model requires information on canopy geometric structure (leaf area index, leaf angles, leaf width, etc.), leaf optical properties (absorbance, transmittance, reflectance) and leaf physiological properties (\( V_{c, \text{max}} \), \( J_{\text{max}} \)-light use efficiency, etc.). The data for estimating the parameter values were obtained from a CO2 flux experiment conducted on spring barley, the test crop, at an eddy-covariance tower site in 2001 at Jokioinen, Finland, described in detail in Section 2.2. However, leaf-level physiological data were not available for spring barley at the Jokioinen site, so we applied a generic parameterization for C3-grass canopies based on general knowledge (Nobel, 1991; Jones, 1996) and unpublished data from a German barley site (Falge, unpublished). The subsequent parameterization procedure involved the input of the observed leaf area index from Jokioinen into PROXEL_NEE and inversion of the model, enabling the estimation of the carboxylation and electron transport capacities at 25°C (\( V_{c, \text{max}} \), \( J_{\text{max}} \)) according to Reichstein et al. (2003). The inverse parameter estimation was performed by minimizing the sum of squared residuals between observed and modeled gross primary productivity using the nlinsq procedure (Levenberg–Marquardt algorithm) in the software.

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Table 1

<table>
<thead>
<tr>
<th>Module</th>
<th>Parameter definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Gamma^* ) (( \mu \text{mol} \text{ m}^{-2} \text{ s}^{-1} ))</td>
<td>Electron transport capacity at 25°C</td>
<td>80.2</td>
</tr>
<tr>
<td>( V_{c, \text{max}} ) (( \mu \text{mol} \text{ m}^{-2} \text{ s}^{-1} ))</td>
<td>Carboxylation capacity at 25°C</td>
<td>38.2</td>
</tr>
<tr>
<td>( c_1 ) (( \mu \text{mol} \text{ m}^{-2} \text{ s}^{-1} ))</td>
<td>Respiratory capacity at 25°C</td>
<td>2.0</td>
</tr>
<tr>
<td>( \Delta H_{\Gamma^*} ) (( \text{J mol}^{-1} ))</td>
<td>Activation enthalpy of electron transport</td>
<td>45000</td>
</tr>
<tr>
<td>( \Delta S_{\Gamma^*} ) (( \text{J mol}^{-1} \text{K}^{-1} ))</td>
<td>Activation entropy of electron transport</td>
<td>643</td>
</tr>
<tr>
<td>( \Delta H_{V_{c, \text{max}}} ) (( \text{J mol}^{-1} ))</td>
<td>Activation enthalpy of dark respiration</td>
<td>64000</td>
</tr>
<tr>
<td>( \Delta S_{V_{c, \text{max}}} ) (( \text{J mol}^{-1} \text{K}^{-1} ))</td>
<td>Activation entropy of carboxylation</td>
<td>55000</td>
</tr>
</tbody>
</table>

For detailed information of additional generic parameters see Tenhunen et al. (1990), Falge (1996), and Reichstein (2001).

* These parameters determine the temperature response of the respective capacities in parenthesis.
package PV-WAVE that relies on IMSL algorithms (Visual Numerics Inc., 2001). In contrast to Reichstein et al. (2003), no seasonal variation in the parameters was introduced. The parameter estimation was performed on data where leaves were fully developed (Julian Days 190–210) and involved 648 half-hourly data points. Standard errors for the parameters were computed according to classical statistical assumptions (Draper and Smith, 1981), and were very low, i.e., less than 5% of the parameter values. But the standard errors are probably underestimated since residuals of eddy-covariance data are usually not independent. The complete parameterization is shown in Table 1.

2.2. Estimation of gross primary production (GPP) from eddy-covariance data

One important diagnostic variable of the PROXEL NEE sub-model is the canopy gross carbon uptake (GPP) determined by the canopy photosynthesis model as $P_{\text{gros}}$ (Eq. (1)). Since plant growth depends on the amount of fixed carbon, it is important to separately evaluate the GPP simulated by the PROXEL NEE component against measured flux data. The flux data were obtained from the Tower site in Finland (Table 2). Details of the experiment may be obtained from Lohila et al. (2004). In brief, a 17-ha site in Jokioinen, southern Finland ($60^\circ 53.932^\prime N, 23^\circ 30.861^\prime E, \text{elevation 104 m}$) was plowed in autumn 2000 and harrowed in spring 2001, after which spring barley ($H. vulgaris$ L., “Inari”) was sown on May 25 with a row spacing of 0.13 m. At sowing, the field received 42.5 kg N/ha, 15 kg P/ha and 25 kg K/ha. During barley growth, the CO$_2$ and energy fluxes were measured at a height of 3.0 m using the micrometeorological eddy-covariance method. The instrumentation included an SWS-211 (Applied Technologies, Inc.) three-axis sonic anemometer and a LI-6262 (Li-Cor, Inc.) CO$_2$/H$_2$O analyzer. The heated inlet tube for the LI-6262 was 5.6 m in length and a flow rate of 6-l/min was used. The EC data acquisition was carried out by a Lab-View based program BARFLUX. Generally, the instrumentation and the data processing procedures for the estimation of half-hourly fluxes followed Aurela et al. (1998) and Tuovinen et al. (1998). The night-time CO$_2$ fluxes at air temperatures between 10 and 15 $^\circ C$ under well-watered conditions were related to friction velocity ($u^*$). These fluxes increased with $u^*$ at low $u^*$, and saturated at higher friction velocities. Based on a fitted function:

$$F_c(u^*) = F_{c \text{ max}}(1 - e^{-k u^*}) (2)$$

where $F_c$ is the observed CO$_2$ flux, $u^*$ the friction velocity, $F_{c \text{ max}}$ the saturated $F_c$ (when $u^*$ is not limiting), $k$ the exponential parameter, at least 95% of the maximum night-time CO$_2$ flux was reached at friction velocities above 0.2 m/s ($k$ always $>15$ s/m). Consequently, all eddy-covariance data with $u^* < 0.2$ m/s were excluded from the analysis, since it is likely that under these conditions, storage and advection can alter gas fluxes through the boundary layer.

Ancillary meteorological measurements taken during the study include air temperature and humidity at canopy level (0.20 m) and at 2.5 m ($\text{Vaasala HMP230}$), net radiation, global radiation, reflected global radiation, photosynthetic photon flux density (PPFD) and 

<table>
<thead>
<tr>
<th>Site name</th>
<th>Year</th>
<th>Country</th>
<th>Data type</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>Canopy process</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jokioinen</td>
<td>2001</td>
<td>Finland</td>
<td>CO$_2$ flux, NEE</td>
<td>Calibration/validation</td>
</tr>
<tr>
<td>Growth</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deutenhausen$^a$</td>
<td>1992</td>
<td>Germany</td>
<td>LAI Leaf Stem</td>
<td>Grain TDW</td>
</tr>
<tr>
<td>Jokioinen</td>
<td>2001</td>
<td>Finland</td>
<td>LAI Leaf Stem Grain</td>
<td>TDW Calibration/validation</td>
</tr>
<tr>
<td>(Scheeßel)</td>
<td>2001</td>
<td>Germany</td>
<td>LAI Leaf Stem</td>
<td>–</td>
</tr>
<tr>
<td>(Weidenfelde)</td>
<td>2001</td>
<td>Germany</td>
<td>LAI Leaf Stem</td>
<td>–</td>
</tr>
<tr>
<td>Jokioinen</td>
<td>2001</td>
<td>Finland</td>
<td>MODIS (1000 m) LAI</td>
<td>–</td>
</tr>
<tr>
<td>Jokioinen</td>
<td>2001</td>
<td>Finland</td>
<td>MODIS (500 m) NDVI</td>
<td>–</td>
</tr>
</tbody>
</table>

TDW: total dry weight.

$^a$ Source: Schröder (1999).
reflected PPFD (Licor LJ-190SZ). The data were collected with a Vaisala QL1 data logger as 30-min averages. While eddy-covariance directly measured only the net ecosystem exchange (NEE), the data can be split into gross carbon uptake (GPP) and the ecosystem respiration \( R_{\text{eco}} \) via the general equation:

\[
\text{GPP} = \text{NEE} - \text{R}_{\text{eco}}
\]  

\( \text{NEE} \) is the photosynthesis minus the ecosystem respiration, \( \text{R}_{\text{eco}} \). Night-time data that passed the above-mentioned quality criteria were taken as valid estimates of ecosystem respiration. Subsequently, for consecutive 14-day periods, a non-linear regression model according to Lloyd and Taylor (1994)

\[
R_{\text{eco}}(T_{\text{air}}) = R_{\text{eco}}(T_{\text{ref}}) \exp \left( \frac{1}{T_{\text{air}}} - \frac{1}{T_{\text{ref}}} \right)
\]

was fitted to the observations of night-time ecosystem respiration \( R_{\text{eco}} \) versus air temperature \( T_{\text{air}} \), where \( R_{\text{eco}}(T_{\text{ref}}) \) is the estimated respiration at reference temperature \( T_{\text{ref}} \), \( E_c \) is an activation energy-like parameter that determines the temperature sensitivity and \( T_0 \) is the temperature where respiration ceases.

In accordance with previous studies (Reichstein et al., 2002; Subke et al., 2003), we fixed \( T_{\text{ref}} \) and \( T_0 \) at 10 and \(-46.02 \) °C, respectively (cf. Lloyd and Taylor, 1994), and allowed \( E_c \) and \( R_{\text{eco}}(T_{\text{ref}}) \) to vary. Due to noise in the eddy-covariance data, the parameters could not be estimated for all periods. If the standard error of the parameter estimate was larger than a heuristic threshold of 30% of the estimate the estimation was rejected, and the parameters were interpolated linearly from the last and the next valid 14-day period. The ecosystem respiration was then estimated from the half-hourly air temperature \( T_{\text{air}} \) according to the regression equation of each 14-day period. Finally, the GPP could be estimated according to Eq. (3). Missing data were filled with an algorithm described in Falge et al. (2001).

2.3. Growth, partitioning, LAI and plant development

The CGRO component module is shown in Fig. 1 as part of PIXGRO. It is structured in a manner similar to that adjacent to natural ecosystems (executed in parallel when PIXGRO is used in landscape applications). The simulated LAI from CGRO is passed to the PROXELNEE canopy process module and the computed fixed C fluxes are returned to CGRO, which then simulates crop growth.

Dry matter accumulation rate is simulated from the hourly gross photosynthesis, \( P_{\text{gytn}} \) (\( \mu \)mol CO2/m2 h; see Eq. (1)) after conversion to gross carbohydrate production rate, \( P_{\text{g}} \) (g CH2O/m2 h) and the latter reduced by plant respiration losses. Respiration modeling has attracted the interest of many scientists. A detailed review of the past 30-year progress on the modeling of respiration can be found in Amthor (2000).

For lack of data for detailed respiration modeling, we use the simplest framework, which divides the whole-plant respiration into (i) maintenance and (ii) growth or canopy gross fractions. McCree (1970) proposed that the canopy gross respiration may be estimated as a fixed proportion (about 25%) of the gross photosynthesis while an additional 1.5% of the existing plant biomass is also lost as maintenance respiration. In this study, a temperature-dependent maintenance respiration, \( R_{\text{ma}} \) (g CH2O/g tissue h) is calculated according to Jones (1991) as:

\[
R_{\text{ma}} = k_m \exp(b(T_{\text{air}} - 25))
\]

with \( k_m \) being the respiration rate at 25 °C (g CH2O/g tissue h), \( b \) a constant and \( T_{\text{air}} \) is the hourly air temperature (°C). A conversion efficiency, \( E \) (g tissue/g CH2O), which also accounts for the growth respiration (Jones, 1991) is used to convert the gross photosynthesis rate to dry matter accumulation rate. The net crop dry weight growth rate, \( dW/dt \) (g tissue/m2 h) is thus:

\[
\frac{dW}{dt} = E(P_{\text{gytn}} - R_{\text{ma}}W)
\]

where \( W \) is the total plant dry weight.

The net hourly growth is partitioned to leaves, stems, roots, and – where appropriate – to the grain. The values of the partitioning coefficients change with the stage of the crop development (Table 3). Until the end of vegetative growth, biomass is partitioned to leaves, stems and roots. Thereafter, biomass produced is partitioned mainly to reproductive structures. If we denote the partition coefficient as \( \eta \), then the rate of weight gain for the various plant organs can be calculated as:

\[
\frac{dW_o}{dt} = \eta \frac{dW}{dt}
\]

\( dW_o \)
Table 3: Values and definition of some key CGRO parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_m$ (g CH$_2$O/g tissue h)</td>
<td>Maintenance respiration constant</td>
<td>0.0006</td>
</tr>
<tr>
<td>$b$</td>
<td>Maintenance respiration constant</td>
<td>0.0693</td>
</tr>
<tr>
<td>$E$ (g tissue/g CH$_2$O)</td>
<td>Growth respiration/conversion factor</td>
<td>0.70</td>
</tr>
<tr>
<td>SLA (cm$^2$/g)</td>
<td>Specific leaf area</td>
<td>200</td>
</tr>
<tr>
<td>$T_b$ (°C)</td>
<td>Base temperature</td>
<td>0</td>
</tr>
<tr>
<td>$V$</td>
<td>Leaf area senescence factor</td>
<td>0.001</td>
</tr>
<tr>
<td>Crop stage (°Cd)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1. Sowing</td>
<td>76</td>
<td></td>
</tr>
<tr>
<td>2. Emergence</td>
<td>614</td>
<td></td>
</tr>
<tr>
<td>3. Flowering</td>
<td>791</td>
<td></td>
</tr>
<tr>
<td>4. Grain fill</td>
<td>1424</td>
<td></td>
</tr>
<tr>
<td>5. Maturity</td>
<td>1600</td>
<td></td>
</tr>
</tbody>
</table>

$\eta$ Partition coefficient dependent on plant organ and crop stage

<table>
<thead>
<tr>
<th>Organ</th>
<th>Crop stage</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Leaf</td>
<td>0.00</td>
</tr>
<tr>
<td>Stem</td>
<td>0.00</td>
</tr>
<tr>
<td>Roots</td>
<td>0.00</td>
</tr>
<tr>
<td>Grain</td>
<td>0.00</td>
</tr>
</tbody>
</table>

where the subscript ‘p’ denotes plant organ (leaf, stem, root and grain). Biomass partitioned to the roots is converted to root length and distributed over a dynamic root zone which extends downwards at a constant velocity from emergence to flowering. The distribution of the root length density with depth follows the proposal of Adiku et al. (1996), whereby more root length density is assigned to zones with higher initial root mass but a logistic function reduces the additional root length density assigned to a zone when the density approaches a preset maximum. The increase in leaf area is obtained by converting dry matter partitioned to the leaves via the specific leaf area (SLA, cm$^2$/g) and expressed as the leaf area index:

$$\text{LAI} = \frac{\text{SLA} \times W_1}{10000} - V$$

where $10000$ converts from cm$^2$ to m$^2$ and $V$ is a loss term to account for leaf senescence (which commences normally after flowering). The LAI is then passed to the canopy process routine to calculate CO$_2$ fixed for the next time step.

To simulate plant development, we assume that the plant has five stages namely, sowing (Stage 1), emergence (Stage 2), flower development (Stage 3), grain formation (Stage 4), and maturity (Stage 5). The duration of each stage is determined by pre-set thermal time, GDD (°Cd) calculated from:

$$\text{GDD} = \sum_{i=1}^{n} (T_{av} - T_b) t$$

where $T_{av}$ is the daily average temperature, $T_b$ is a base temperature, and $t = t_i$ and $r = \eta_i$ are the initial and final times (days), respectively, for the duration of a given stage. Values of some key CGRO parameters are given in Table 3.

Initial data for calibrating CGRO were obtained from a spring barley experiment conducted at Deutenhausen, Germany in 1992 and published by Schneider (1999). Data sources are listed in Table 1. Further calibration and fine-tuning of the parameter values was achieved using data from Jokioinen, Finland, during the CO$_2$ flux experiment described above. During the growth of spring barley, the leaf area index was measured weekly with a LAI-2000 Plant Canopy Analyser (LI-COR, Inc, NE) from six points located within 100 m from the measurement tower. Plant biomass was harvested six times by clipping all plants from two
0.25 m² plots, oven drying the samples at 40 °C and weighing them.

2.4. Validation data sources

2.4.1. Field data

Field data for validating PIXGRO were obtained from two sites in Germany. The two sites, Schoenlind and Weiherhoefen, lie within the Upper Eger basin near Weissenstadt in Franconia and are about 3 km from each other. Sections of spring barley fields grown by farmers in 2001 were rented by the Department of Ecology, University of Bayreuth, Germany, soon after emergence and subsequently sequentially sampled (in triplicate) at 2-week intervals throughout the growing season. The harvested materials were separated into leaves and stems and sub-samples of the leaves were used to determine the leaf area with a leaf area meter (Model Li 3100). The remainder of the harvest material was used to determine the above-ground matter after oven drying at 75 °C for 2 days. Meteorological data during the growth period were obtained from two stations in the basin: (i) Voitsumura, which was very close to Schoenlind, and (ii) Waldstein, which was about 2 km north of Weiherhoefen. The two stations are maintained by the Bayreuth Institute for Terrestrial Ecosystem Research (BITOEK), University of Bayreuth. The data collected include the air temperature, solar radiation, soil temperature, relative humidity, precipitation, and wind speed at hourly time step. In our simulations, data for Voitsumura were used for Schoenlind and those from Waldstein for Weiherhoefen.

2.4.2. Remote sensing data

The Moderate Resolution Imaging Spectro-radiometer (MODIS) data 2001 were obtained for the Finland site and used as an additional validation data source. The MODIS level 3, 16-day maximum-value composite of NDVI images and products for 500 and 1000 m meter resolution were used in this study. The vegetation product uses MODIS Terra surface reflectance, corrected for molecular scattering, ozone absorption, and aerosols.

First, we downloaded from the MODIS web site the 1000 m resolution LAI and compared this directly with the PIXGRO-simulated LAI. Secondly, the reflectance in bands 1 (620–670 nm) and 2 (841–876 nm) for a higher resolution MODIS (500 m) was used to calculate the normalized difference vegetation index (NDVI) as:

\[
NDVI = \frac{\rho_{\text{NIR}} - \rho_{\text{red}}}{\rho_{\text{NIR}} + \rho_{\text{red}}}
\]  

where \(\rho_{\text{NIR}}\) and \(\rho_{\text{red}}\) are the surface bi-directional reflectance factors for their respective bands. In a number of studies, it has been shown that the LAI correlates well with the NDVI (Knyazikhin et al., 1998) or with a simple ratio, SR (\(SR = \text{NIR}/R\); Chen, 1999). In this study we express the relation between SR and NDVI as:

\[
SR = \frac{1}{1 - NDVI}
\]

The maximum NDVI value composite (MVC) approach minimizes the effect of cloud cover and variability in atmospheric optical depth. Although the MVC procedure eliminates most cloudy pixels, some MVC products contain residual cloud contamination that could adversely affect our analysis. To further reduce effects of cloud contamination and atmospheric interference in seasonal NDVI time series, we applied the best index slope extraction (BISE) technique (Viovy et al., 1992) to reduce the noise and smooth the time series.

3. Results and discussion

3.1. Gross CO₂ uptake

The flux component of the coupled PIXGRO model simulates well the diurnal dynamics of gross CO₂ exchange on an hourly scale, driven mainly by the available energy (global radiation). On weekly to seasonal scale, the correspondence is more related to the leaf area development of the crop (Fig. 2). There is a slight diurnal hysteresis, with the model underestimating fluxes in the morning, but overestimating in the afternoon. This could be attributed, to differences in water status of the plants, which is not dynamically modeled here. Despite the generally good model-data agreement, the model tends to underestimate fluxes at the beginning of the season, while it overestimate fluxes at the end of the season.

This relatively small but clear seasonal bias is also depicted in Fig. 3 where daily flux integrals are shown.
Fig. 2. Average diurnal curves (a, b, e, f) of simulated (GPPmod) and “observed” (GPPeddy) gross carbon uptake, and meteorological conditions (c, d, g, h) (global radiation, W/m²; air temperature, °C; and vapour pressure deficit, hPa) at four times during the crop growth period (four stages of LAI development). The observed data are from the spring barley site at Jokioinen.
Possible reasons for this are that a constant physiological activity expressed as $V_{\text{c max}}$ is not appropriate (cf. Reichstein et al., 2002; Wilson and Hanson, 2003) or that we do not account for shading of the leaves through emerging flowers, that reduces the available energy. Nevertheless, at half-hourly and daily scale the overall model-data coincidence (Fig. 4) is remarkable and close to what can be expected when comparing to eddy-covariance data that has an inherent random sampling error (Moncrieff et al., 1996).

Neural network approaches showed that usually root mean squared errors of more than $1/\text{H}^2\text{mol m}^{-2}\text{s}^{-1}$ have to be expected (Wijk and Bouten, 1999; Papale and Valentini, 2002).

3.2. Simulation of the dry matter accumulation and partitioning

The CGRO component also simulated dry matter accumulation and partitioning quite well as shown for the time course of the simulated and observed above-ground dry weight for Jokioinen, Schoenlind, and Weisbergen in Fig. 5a–c, respectively. At Jokioinen, the observed total dry weight increased gradually from sowing following a sigmoid pattern and attained a final weight of about 1.0 kg m$^{-2}$ (Fig. 5a). The total dry weight was quite well simulated by CGRO, with the simulated curve falling generally within error bars. The final simulated total dry weight (0.9 kg m$^{-2}$) was lower than the observed but was within 10% error range.

The simulation of dry matter partitioning was quite good at the early stages of crop development, but there were discrepancies at the later stages. For leaf, the final observed dry weight was about 0.11 kg m$^{-2}$ while the model simulated 0.20 kg m$^{-2}$. It should, however, be noted that observed dry matter was about 0.16 kg m$^{-2}$ earlier on Day 190, suggesting that some leaf material was lost from the field by the end of the growth period. In its current state, CGRO simulates leaf senescence by reducing the green leaf area but not loss of leaf dry matter, hence the inability of the model to capture decreasing trends in biomass. In this regard, further improvement of CGRO may be necessary.

Stem dry weight was quite well simulated even though the model somewhat under-predicts the final stem weight by about 20%. Grain development commenced from Day 190 and rose sharply to a final grain
dry weight of about 0.60 kg/m². The model captured the trend of grain development but under-predicts the final grain weight (0.46 kg/m²) by about 20%. Despite these discrepancies, CGRO captures the general patterns of dry matter accumulation and partitioning of spring barley quite well.

Fig. 5b shows the simulated and observed aboveground total dry weight for spring barley at Schoenlind. As for Jokioinen, the observed total dry weight increased with time and attained a final weight of 0.80 kg/m². The pattern of dry matter accumulation was well simulated by CGRO and much of the simulated curve was within the standard error range of the observed. The final simulated dry weight was somewhat lower than the observed but was within a 10% error range. The observed dry matter accumulation rate at Weiherhoefen (Fig. 5c) was slow during the initial stages of crop development but showed a very rapid rise (from about 0.1 to 0.6 kg/m²) within a short period of 10 days (Day 170–180). Further, growth beyond this stage was minimal and the final dry weight was about 0.70 kg/m². Although the model simulated the initial growth quite well, it was unable to simulate the rapid rise in dry weight from Day 170 to 180. The model sim-
ulated a fairly constant growth between Day 170 and 200 and a somewhat reduced growth at the final stages leading to a final dry weight of about 0.80 kg/m².

The comparison of simulated and observed (observed data from validation data sets only) is shown in Fig. 5d. It may be concluded ($R^2 = 0.90$) from the spread of data points around the 1:1 line that the model does not show any consistent bias.

3.3. Simulation of LAI

Fig. 6a shows the time course of the measured and simulated LAI for spring barley grown at Jokioinen, Finland. The observed LAI rose from about 0.3 m²/m² in early June (Day 164) to a peak of 4.5 m²/m² by mid July (Day 200) and declined thereafter to about 0.2 m²/m² in late August (Day 230). Simulated LAI generally followed the observed, rising from 0.3 m²/m² to a peak of about 3.8 m²/m² and declining to about 1.5 m²/m². Although following similar trends as the observed, the simulated LAI slightly but consistently under-predicted the LAI and reached a peak earlier than the observed. On the other hand, the simulated LAI declined less-sharply than the observed.

The time course of observed and simulated LAI for the validation data sets is shown in Fig. 6b and c. The observed LAI at Schoenlind (Fig. 6b) followed a bell-shape. LAI increased gradually from about 0.6 (Day 155) to a peak of 3 m²/m² and remained quite steady at this value for almost 20 days (Days 180–200) before...
declining to about 1.5 m²/m² (Day 210). The model simulated quite correctly the pattern of LAI development with much of the simulated curve falling within the error bars. The simulated LAI attained a peak of 3.5 m²/m² and the decline was somewhat faster than observed.

The pattern of LAI at Weiherhoefen site was somewhat skewed towards the later stages of development. The rate of development was rather slow at the initial stages but increased very sharply between Days 180 and 200, followed by a rapid decline to about 1.0 m²/m² by Day 215. Model simulation was not very accurate although the general pattern was reflected. The peak LAI simulated was about 4.5 m²/m², which was quite lower than the observed value of 6.0 m²/m². Despite the discrepancies, a general comparison between the simulated and observed (observed data from the validation sites only) gives an $R^2 = 0.82$ (Fig. 6d), indicating quite a good agreement between the simulated and the observed.

3.4. Remotely sensed LAI data

Fig. 7 shows the time course of PIXGRO-simulated LAI, the direct downloaded MODIS (1000 m) LAI, and the observed LAI for Jokioinen, Finland in 2001. The MODIS LAI followed the general rise and fall pattern commonly observed, but was initially higher than the observed and PIXGRO-simulated LAI, and the rise was very slow until about Day 200. Thereafter, the MODIS-LAI rose sharply from 2 to 4 m²/m² followed by a rapid decline to about 1.0 m²/m². This pattern of the MODIS-LAI failed to reflect the observed and the agreement with PIXGRO was poor ($R^2 = 0.45$). Therefore, we deemed this data set as inappropriate for validating PIXGRO. The failure of the downloaded MODIS (1000 m)-LAI to simulate the observed LAI or PIXGRO LAI may be attributed to two main reasons. First, the barley field was only about 0.25 km², while the MODIS data of pixel size 1 km² was far larger. This would imply that the image could include other vegetation types (grassland and needle leaf forest) leading to mixed pixels.

Secondly, the MODIS-LAI algorithm employed to convert the MODIS spectral reflectance to LAI (see Knyazikhin et al., 1998), may not be entirely valid for the site in question. Due to these drawbacks we derived the NDVI for the higher resolution MODIS (500 m resolution) data (not shown). The time course of the NDVI shows a better resemblance to the observed LAI (Fig. 6a) even though the NDVI starts to rise earlier.
than the emergence of the spring barley, apparently as a result of background reflection of the soil. Further, we derived the relation between the observed LAI and the simple ratio, SR (Eq. (11)) as shown in Fig. 8a, which gave a good fit ($R^2 = 0.73$). Using this regression equation and the MODIS (500 m)-SR, a new MODIS-LAI was calculated and compared with PIXGRO simulation. The agreement improved ($R^2 = 0.86$; Fig. 8b), but most of the data points were above the 1:1 line, indicating that either MODIS consistently underestimated the LAI or the PIXGRO overestimated the LAI. However, given that PIXGRO generally simulated well the LAI at the Jokioinen site, then it appears that some further improvement of the MODIS derived LAI is necessary.

4. General discussion

Numerous and diverse models that simulate eco-physiological response of vegetation and/or crop growth have been published during the last decades, raising the question whether another model should be developed and added to this group. One reason for the proliferation of models is the difficulty in applying detailed ecosystem models at landscape scales or to a variety of landscape elements, e.g., landscapes comprise a patchwork of heterogeneous sites with different characteristics. The difficulty to meet this demand for a satisfactory set of parameters as well as input data to execute models in such situations has led to the emergence of numerous empirical models to address specific issues, such as crop evapotranspiration (e.g. BOWET: Mirschel et al., 1995), water and nitrogen dynamics (e.g. CANDY: Franko et al., 1995) and soil water balance, or nitrogen and biomass dynamics (e.g. AGROSYM: Schultz and Mirschel, 1995). In most of these cases, crop growth has been treated through empirical descriptions of state variables such as crop height or biomass, using piecewise linear equations which have limited potential for extrapolation. In other cases, semi-empirical methods have been used to simulate crop growth, based on the radiation use efficiency (RUE, g (dry matter)/MJ (intercepted radiation)) of Monteith (1977), or via phenomenological description as provided by light-response curves. Although practical, these models are not able to respond to elements of climate change such as increased CO2. The use of the empirical or lumped RUE methods for the purposes outlined in our study is very limited.

While such specific and tailored models may work in particular situations, it seems reasonable that models of greater generality in application should be preferred to address a wide range of environmental issues. PIXGRO is designed to overcome these limitations, simulating both vegetation to atmosphere exchanges and crop growth. To date, such coupled canopy gas-exchange-crop growth models are generally lacking, even though they offer a framework for large scale applications, avoiding the need to rely on different models for individual tasks. The generic physiologically based canopy process description and the common description of soil processes in PIXGRO make the framework applicable for the simulation of many plant species, once the appropriate parameter values have been determined.

Furthermore, with the view to use PIXGRO later at landscape or regional scales (which may span several thousand square kilometers), we have kept the model structure simple and the number of state and auxiliary variables to a minimum, since computing time and storage space may become critical. In PIXGRO, only few routines are used to simulate crop growth and partitioning. For example, assimilate allocation to organs was achieved by using simple partitioning coefficients, which vary only with stage of development. In some other models, leaf area simulation is based on complex temperature functions that describe leaf appearance (Warrington and Kanemasu, 1983), while in others, growth and resource partitioning are based on detailed descriptions of canopy architecture and competition between individual organs for assimilate (e.g. GRAAL: Drouet and Pagès, 2003).

Undoubtedly, more detailed process descriptions could lead to more accurate simulation results, but the parameterization and validation also become more difficult. The inclusion of such details in landscape-scale models is a major hurdle, so that currently, some trade-off between model complexity and scale is necessary. In this study, the simple approach to simulate assimilate partitioning and LAI gave reasonable results for spring barley and also enabled the execution of PIXGRO with computation times of a few seconds per year and site.

A major limitation in the development of coupled canopy process and growth models has been the lack of appropriate validation data. The eddy-covariance method has proved to be very useful for the evaluation
of forest canopy gas-exchange models (e.g. Baldocchi, 1997; Williams et al., 1998; Reichstein et al., 2002).

However, surprisingly, eddy-covariance methods have not found widespread application for the evaluation of crop gas-exchange and growth models. Here, we show the value of these data for the evaluation of our crop model when complemented with ancillary data that relates to the state variables of the growth model. The agreement between the observed and simulated was quite good. The growing need to evaluate the effects of agriculture on the landscape and regional balances of carbon and water makes it imperative to popularize the eddy-covariance methods among crop modeling researchers. In a landscape or regional context, eddy-covariance data represent only point information. For the validation of landscape-scale models, spatially distributed data are required. Here we showed the value of remote sensing data from the MODIS/Terra sensor for such a task. It does appear, however, that image resolution is an important factor for reliable data estimation. Many croplands are patchy, with different crops grown on adjacent parcels of land. Coarse-resolution remotely sensed data, therefore, may include a number of different vegetation types in one pixel. To minimize the problem of mixed pixels, higher resolution images are more appropriate for croplands. Further, the derivation of robust relations between the plant parameters (e.g. LAI) and spectral characteristics are necessary for many crop types to facilitate the estimation of crop growth attributes. Further research is required in this area.

5. Conclusion

A combined canopy flux and crop growth model, PIXGRO was developed, for simulating gas fluxes from croplands as well as simulating crop growth, partitioning, LAI and development at landscape scales. This model integrates detailed biophysical descriptions of canopy energy/gas exchange at half-hourly time-scales with phenological and growth processes and, thus, offers the chance for multi-dimensional and across-temporal-scale evaluation. Consequently, this study is one of the few examples where a crop model was validated both against eddy-covariance CO₂ exchange data, against biomass, and leaf area index data both from ground observation and remote sensing. It has been shown that it is possible to simulate diurnal and seasonal dynamics of canopy CO₂ exchange of spring barley with generic parameters in a mechanistic model. At a resolution of 1000 m, the downloaded MODIS LAI did not agree well with the PIXGRO-simulated LAI at the Jokioinen site in Finland. However, by deriving a relation between the MODIS (500 m)-NDVI and observed LAI, the recalculated-LAI agreed better with the PIXGRO-simulated LAI. Generally, higher resolution satellite data would be preferable for validating crop models. The results indicated that our approach to develop a landscape-level model, PIXGRO, capable of simulating the NEE, vegetation growth, LAI, yield and development was largely successful. Further, the use of remotely sensed data as additional validation data source makes PIXGRO a prototype model that attempts to bridge several disciplines leading to a comprehensive model that can be used to investigate landuse-ecosystem interactions at landscape scales.

Acknowledgements

The Senior Author wishes to thank the Alexander von Humboldt Foundation, Germany for providing him with Post-doctoral Fellowship. Support from the Department of Plant Ecology, University of Bayreuth, Germany (GLOWA and CARBOEUROFLUX projects) and from the Nordic Centre for Studies of Ecosystem Carbon Exchange and its Interaction with Climate System (NECC) are gratefully acknowledged.

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