Identification of vegetation and soil carbon pools out of equilibrium in a process model via eddy covariance and biometric constraints

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Abstract

Assumptions of steady-state conditions in biogeochemical modelling are often invoked because knowledge on the development status of the modelling domain is generally unavailable. Here, we investigate the role of vegetation pool sizes on nonequilibrium conditions through model-data integration approaches for a set of sites using eddy covariance CO2 flux data. The study is based on the Carnegie–Ames–Stanford Approach (CASA) model, modified (CASAG) in order to evaluate the sensitivity of simulated net ecosystem production (NEP) fluxes to vegetation pool sizes. The experimental design is based on the inverse model optimization of different parameter vectors performed at the measurement site level. Each parameter vector prescribes different simulation dynamics that embody different model structural assumptions concerning (non)steady-state conditions in vegetation and soil carbon pools. We further explore the potential of assimilating biometric constraints through the cost function for sites where in situ information on aboveground biomass or wood pools is available. The integration of biometric data yields marked improvements in the simulation of vegetation C pools compared to single constraints with eddy flux data. Overall, it is necessary to relax both vegetation and soil carbon pools for consistency with the observed data streams. Multiple constraints approaches also leads to variable model performance among the different experimental setups and model structures. We identify and assess the limitations of various model structures and the role of multiple constraints approaches for tackling issues of equifinality. These studies emphasize the need for establishing consistent data sets of fluxes and biometric data for successful model-data fusion.

Keywords: carbon pools, CASA model, equifinality, model-data integration, multiple constraints, net ecosystem production, steady-state assumption

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Introduction

Recent advances in global carbon cycle research have emphasized the significance of biosphere–atmosphere interactions. Understanding and quantification of carbon cycle-climate system feedbacks are key for reducing uncertainty in prognostic modelling (e.g., Friedlingstein et al., 2006; Bonan, 2008; Heimann & Reichstein, 2008).

Biogeochemical modelling approaches are required to address these topics, and observational data should lay the foundations for identifying modelling structures and constraining parameterizations (O’Neill & Melnikov, 2008). Model-data integration studies have contributed significantly to these issues through inverse modelling approaches from local to global scales (e.g., Knorr & Katge, 2005; Scholze et al., 2007; Lauvaux et al., 2008).

In biogeochemical modelling, the lack of information on current states or past-history of the ecosystem within the modelling domain often leads to a priori assumptions of equilibrium states for estimating initial condi-
tions of carbon (C) pools (Odum, 1969). Initialization routines consist of iterative model runs repeating climate conditions until equilibrium, or steady state, when biosphere–atmosphere net C exchanges approach zero at the annual scale; these can be followed by transient runs where climate transitions and management practices are prescribed (Morales et al., 2005). The steady-state assumption for the ecosystem carbon cycle has been challenged (e.g., Lugo & Brown, 1986; Cannell & Thornley, 2003; Luysaert et al., 2008) and its limitations in modelling approaches emphasized (Pietsch & Hasenauer, 2006; Wutzler & Reichstein, 2007).

Moreover, the implications of the steady-state assumption for inverse modelling approaches applied to nonsteady-state ecosystems have been previously reported (Carvalhais et al., 2008). To reach steady state, the long-term C pools are incremented until ecosystem C influx and efflux is balanced and quasi-neutral net fluxes define the initial conditions of the model optimization. Consequently, the optimization of parameters governing fluxes that depend on the magnitude of C pools may lead to compensatory biases and limit the model ability to mimic the observed fluxes. Following an empirical approach, the steady state was relaxed via one specific parameter \( \eta \) that scaled the soil pools following the spin-up to equilibrium, creating an imbalance in net ecosystem fluxes by adjusting the soil carbon pools. This improved the model’s ability to simulate the observations - the model performance - but also resolved biases in estimates of parameters that control the responses of net primary production (NPP) and heterotrophic respiration \( (R_{hi}) \) to temperature and water availability. The implications of nonsteady-state conditions for model-data integration approaches were explicitly related to the initial condition problem through soil C pools, although disequilibrium in live vegetation C pools can also be a key factor (Luo et al., 2001; Santaren et al., 2007; Schaefer et al., 2008). Vegetation C pools contribute to ecosystem carbon fluxes directly through autotrophic respiration \( (R_A) \) and indirectly through C transfers to the soil and litter pools – supplying the substrate for \( R_{hi} \).

The accumulation of C in vegetation pools with slow turnover rates (woody pools) represents a significant fraction of the total C in mature ecosystems. In contrast to C pools that turnover more rapidly, woody C pools require longer periods to achieve new ‘equilibrium’ conditions after natural or human induced disturbances. The direct and indirect effects of management regimes, historical land-use changes and/or natural disturbances have significant implications on ecosystem C sink/source magnitudes at decadal time scales (Barford et al., 2001; Nabuurs, 2004). These perturbations impact the ecosystem C flow between vegetation, litter and soil pools. The prescription of such dynamics can significantly improve ecosystem models (Thornton et al., 2002). In this regard, the slow dynamics of woody C pools may be expected to influence model performance and parameter estimation as has been shown for soil C pools.

We aim to examine if ecosystem sink or source conditions could be partially or fully explained by nonequilibrium states in slow turnover vegetation C pools (wood) and in soil C pools. We hypothesize that errors in net ecosystem fluxes estimation induced by steady-state conditions cannot be circumvented by solely relaxing woody pools because other pools (soil and litter) with similar turnover rates are likely to significantly affect estimates of carbon fluxes. The importance of wood and/or soil C pools magnitudes for NEP estimates emerges from the model-data agreement of different model structures. We further ask whether the assimilation of carbon fluxes from eddy covariance and biometric measurements improves our ability to identify limitations stemming from model structure.

Differing initial states, parameterizations or model structures can yield similar model performance results: representing equifinality (e.g., Franks et al., 1997; Medlyn et al., 2005). Model vulnerability to equifinality, among other factors, can be associated with the gap between parameterized processes and observational constraints (e.g., Beven, 1989); as well as with limited variability in inputs and observations (e.g., Franks et al., 1997). Thus, the emergence of issues related to equifinality may compromise confidence in prognostic simulations: process misrepresentation may be unimportant at short time scales albeit significant at longer time scales (Crout et al., 2009; Fox et al., 2009). Here, we address these issues by evaluating different model structures and integrating C flux data representative of different temporal scales, in an attempt to identify and resolve equifinality issues.

For this study we modify the Carnegie–Ames–Stanford Approach (CASA) model (Potter et al., 1993) to enable the prescription of direct and indirect effects of C wood pools on net ecosystem production (NEP). We further implement a systematic experimental design to test the significance of the vegetation woody C pools on nonsteady-state conditions in model parameter optimization.

**Materials and methods**

**Eddy covariance sites data**

The current study focuses on a set of eddy covariance sites in the Carboeurope – IP network of eddy covariance flux mea-
urement towers (http://www.carboeurope.org). The sites were selected as representative of Mediterranean climate classes or ecosystems present in the Iberian Peninsula (Table 1). Further, the selected sites met minimum data availability requirements for: (1) remotely sensed leaf area index and fraction of photosynthetically active radiation absorbed by vegetation and (2) in situ daily measurements of climate variables (temperature, precipitation and solar radiation) and ecosystem C fluxes. The CO₂ fluxes were first corrected for within-canopy CO₂ storage and then controlled for insufficient turbulence (u* filtered) and outliers (‘spikes’) (Papale et al., 2006). Daily flux integrals were only used for the analysis when more than 80% of the half-hourly data were either original or gap-filled with high confidence (Category A in Reichstein et al., 2005).

The collection of selected sites (Table 1) represents a range of different disturbance backgrounds, management practices and climate regimes. ES-ES1 became a natural area in 1986 and no fire events or human disturbances have been recorded since the 1970s. FR-Hes is a young Beech stand (~34-year-old) (Granier et al., 2008). In FR-LBr, forest management practices include selective thinning (1991 and 1996, 20% of stems removed) (Loustau et al., 1999). The latest disturbances recorded in FR-Pue consist of a clear cut circa 60 years ago (Joffre et al., 1996). In 1992, IT-Non transited from an agricultural to a forested area. IT-PT1 is a managed poplar plantation site with rotation of 9–12 years, last planted in 1993 and harvested in 2005; here, the residues and stumps are removed after each logging (Ferré et al., 2005; Migliavacca et al., 2009). IT-Ren is located on an unevenly aged coniferous forest (Montagnani et al., 2009) with mean tree age of ~85 years and the harvest cycles represent a 10% removal of above-ground biomass. IT-Ro1 and IT-Ro2 are two coppice management sites with very different times since coppicing: 2 and 11 years, respectively (Rey et al., 2002). PT-Mi1 consists of a Quercus suber L. and Quercus ilex L. stand (~90 years) strongly influenced by drought regimes (Jarvis et al., 2007; Pereira et al., 2007).

The set of sites includes deciduous broadleaf (DBF), evergreen needle leaf (ENF), mixed deciduous/evergreen (MF) and evergreen broadleaf (EBF) forests, as well as an EBF scattered tree canopy (savannah-type) with understory (EBG). Although this study includes limited plant functional types and climate regimes, the site collection characteristics represents a manageable set for testing our hypothesis on the different model structures assumptions.

**Changes in the CASA model**

The CASA model is a production efficiency model that estimates NEP as the difference between NPP and Rₘ (Potter et al., 1993; Field et al., 1995; Randerson et al., 1996; Friedlingstein et al., 1999). We modified CASA to estimate NPP as the difference between gross primary production (GPP) and Rₘ (CASAm) to fully explore the dependence of the ecosystem fluxes to the vegetation carbon pools. The model adjustments link Rₘ, hence NPP, to plant biomass in contrast to standard CASA (for details, see Appendix S1).

### Table 1 Characteristics of the different sites used in this study

<table>
<thead>
<tr>
<th>Site name</th>
<th>Site code</th>
<th>PFT</th>
<th>Latitude</th>
<th>Longitude</th>
<th>Temperature (°C)</th>
<th>Solar radiation (W m⁻²)</th>
<th>Carbon Sequestration Rate (g C m⁻² yr⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>El Saber ES-ES1</td>
<td>ENF</td>
<td>Evergreen needle-leaf forest (ENF)</td>
<td>39.34</td>
<td>-0.32</td>
<td>17.35</td>
<td>167.46</td>
<td>439.81</td>
</tr>
<tr>
<td>Hesse FR-Hes</td>
<td>DBF</td>
<td>Deciduous broadleaf forest (DBF)</td>
<td>48.67</td>
<td>-0.32</td>
<td>10.96</td>
<td>439.81</td>
<td>490.33</td>
</tr>
<tr>
<td>Le Bray FR-LBr</td>
<td>ENF</td>
<td>Evergreen needle-leaf forest (ENF)</td>
<td>44.72</td>
<td>-0.77</td>
<td>13.79</td>
<td>180.15</td>
<td>349.81</td>
</tr>
<tr>
<td>Puechabon FR-Pue</td>
<td>EBF</td>
<td>Evergreen broadleaf forest (EBF)</td>
<td>43.74</td>
<td>-0.77</td>
<td>13.56</td>
<td>213.15</td>
<td>349.81</td>
</tr>
<tr>
<td>Nonantola IT-Non</td>
<td>MF</td>
<td>Mixed forest (MF)</td>
<td>44.69</td>
<td>-0.77</td>
<td>13.56</td>
<td>213.15</td>
<td>349.81</td>
</tr>
<tr>
<td>Parco Ticino IT-PT1</td>
<td>DBF</td>
<td>Deciduous broadleaf forest (DBF)</td>
<td>45.20</td>
<td>-0.77</td>
<td>13.56</td>
<td>706.25</td>
<td>349.81</td>
</tr>
<tr>
<td>Renon IT-Ren</td>
<td>ENF</td>
<td>Evergreen needle-leaf forest (ENF)</td>
<td>46.59</td>
<td>-0.77</td>
<td>13.56</td>
<td>706.25</td>
<td>122.80</td>
</tr>
<tr>
<td>Roccarespam</td>
<td>EBG</td>
<td>Mixed Forest (EBG)</td>
<td>42.41</td>
<td>-0.77</td>
<td>13.56</td>
<td>122.80</td>
<td>122.80</td>
</tr>
</tbody>
</table>

Available vegetation pools information from the Luyssaert et al. (2007) database is indicated: above-ground biomass (AGB); wood NPP (NPP W); and wood biomass (C W).
The experimental design consists in evaluating different modeling setups that are defined by specific parameter vectors optimized individually for each of the selected sites. The optimization relies on the comparison of model outputs with observational data (see section ‘Integration of vegetation pools in the model optimization’ for details). The selected compilation of different parameter vectors for optimization aims to evaluate the relevance of the slow turnover vegetation pools on the ecosystem (non)steady-state assumption. Figure 1 shows a schematic representation of the model and the different scalars used; while a synthesis of all parameter vectors in the experimental design can be found in Table 2. This factorial experimental design relies on the optimization of the following parameter vectors representing different model structures:

1. The parameter optimization under equilibrium conditions is executed after the model is spun until steady state without further adjustments to the ecosystem C pools. This approach is considered an optimization under fixed initial conditions and is identified by \( \theta_0 \). Although poorer model-data agreement and higher parameter uncertainties occur under fixed conditions (Carvalhais et al., 2008) we make use of \( \theta_0 \) to confirm that flux simulations in CASAC\(_c\) are more sensitive than CASA to the vegetation pools.

2. The relaxation of the steady-state assumption is performed in \( \theta^\text{emp}_y \), where nonequilibrium conditions are allowed solely on soil level C pools of slow turnover rates and microbial pools (Carvalhais et al., 2008). \( \theta^\text{emp}_y \) represents an empirical approach for the steady-state problem and in the current experiment is considered a benchmark for evaluation of the role of slow turnover vegetation pools in explaining fluxes under nonsteady-state conditions.

Additionally, we introduce a new set of ‘\( \eta \)-type’ scalars – \( \eta_W \), \( \eta_{WL} \) and \( \eta_{WD} \) – that adjust wood related C pools at the end of the spin-up (Fig. 1). These can affect empirically only the woody (\( \eta_W \)) or the woody and litter pools (\( \eta_{WL} \)); or allow for a dynamic recovery after a disturbance (\( \eta_{WD} \)) (Fig. 1). This set of wood related scalars are identified as \( \eta_{\text{wood}} \) parameters from here on. Each \( \eta_{\text{wood}} \) parameter represents the prescription of an empirical or more mechanistic approach, depending on its structural application and on the parameter vector used (Table 2), namely:

3. By following an empirical approach analogous to \( \theta^\text{emp}_y \) but now scaling the vegetation pools – here \( \theta^\text{emp}_V \). In \( \theta^\text{emp}_V \) we include a new \( \eta_{\text{wood}} \) parameter – \( \eta_W \) – that scales the vegetation woody pools empirically after equilibrium is reached. This setup aims at assessing the sensitivity of CASA vs. CASAC\(_c\) to changes in vegetation pools. CASAC\(_c\) should be significantly more sensitive to \( \eta_W \) than CASA since the estimates of NEP fluxes in CASAC\(_c\) are expected to be more responsive to vegetation pools (through \( R_a \)) than in CASA. Consequently, the differences in the model performance of CASA between \( \theta_0 \) and \( \theta^\text{emp}_V \) should be modest compared with the differences in CASAC\(_c\).

4. The first approach to relax both vegetation and soil pools from equilibrium is strictly empirical. Here, in \( \theta^\text{emp}_S \), we optimize \( \eta_{WL} \) – this \( \eta_{\text{wood}} \) parameter scales the vegetation woody and slow litter pools equally after the spin-up. This simultaneous and equal scaling implies proportionality between woody and slow litter pools disequilibrium. Additionally, nonequilibrium conditions in soil pools are prescribed by \( \eta' \) that relaxes the steady state in the microbial and slow soil pools (Fig. 1). The role of \( \theta^\text{emp}_S \) is then to assess the impacts of nonsteady-state conditions in vegetation and litter pools and in soil pools using a purely empirical approach.

5. Additionally, we implement a semimechanistic setup that allows the vegetation pools to recover from prescribed disturbances – \( \theta^\text{mix}_y \). In \( \theta^\text{mix}_V \), we introduce a new \( \eta_{\text{wood}} \) parameter – \( \eta_{\text{mix}} \) – that prescribes a complete tree cut after spin-up completion (\( P_1 \)) and allows a dynamic recovery during a second initialization routine (\( P_2 \), Fig. 2). At \( P_1 \) the wood carbon pool (\( C_W \)) which was in equilibrium (\( C_{W,eq} \)) is removed (set to zero) while leaves and roots are killed, but not removed from the system. This procedure is not the same for all sites since the specific site history entails dynamics that are
mechanistically different from such general prescription. Hence: (1) in ES-ES1 we do not remove the killed trees from the system but we remove the surface pools, due to its fire history; (2) in IT-PT1 we remove all the vegetation and surface litter pools from the system, since the clear cut activities remove all surface litter; and (3) since IT-Ro1 and IT-Ro2 are coppice sites the roots are not killed. The model is then spun-up during a second spin-up phase (P2) which lasts until C_W = C_W,ne (Fig. 2), upon which nonequilibrium C_W(C_W,ne) is estimated as:

\[ C_{W,ne} = C_{W,eq} \eta_{WD} \]  

being \( \eta_{WD} \) parameterized during the optimization. During both spin up phases – P1 and P2 – the model simulations were performed with a mean year of drivers for the observation years (Table 1). In the general dynamic prescription the coarse woody debris is affected indirectly, through the complete reduction of C inputs from the wood pool after P1 that dynamically increase during P2 (Fig. 2d). The coarse root litter pool experiences an immediate increase of C inputs after P1 and a decrease in early P2, followed by a dynamic increase analogously to the coarse woody debris pool (Fig. 2c). In the specific cases, the dynamics are: (1) for ES-ES1 the slow litter pools experience an immediate increase of C inputs after P1 and a decrease in early P2, followed by dynamic increases as vegetation recovers and inputs carbon to the litter pools (Fig. 2c); (2) in IT-PT1 all surface litter pools restart a spin up from zero, growing from vegetation inputs during P2 (Fig. 2b); and (3) for IT-Ro1 and IT-Ro2 the only difference to the general case is that the coarse root litter dynamics are not changed (the coarse woody debris follow Fig. 2d). Further, \( \eta' \) is also included in the parameter vector, empirically relaxing the slow and microbial soil pools. Overall, \( \theta_{V}^{\text{syn}} \) aims to reproduce the impacts of past vegetation disturbances following a semi-mechanistic approach: through the dynamic prescription of \( \eta_{WD} \) and the heuristic approach of \( \eta' \).

6. In \( \theta_{V}^{\text{syn}} \), nonequilibrium conditions are solely prescribed through \( \eta_{WD} \), which is integrated in the parameter vector exactly as in the \( \theta_{V}^{\text{mix}} \) setup. Here, the occurrence of

<table>
<thead>
<tr>
<th>Parameter vector</th>
<th>( \eta )</th>
<th>( \eta' )</th>
<th>( \eta_{WL} )</th>
<th>( \eta_{WD} )</th>
<th>( \eta_{W} )</th>
<th>General assumptions of the optimization setup</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_{0} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Fixed steady state</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{emp}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Empirical relaxation of steady state on decomposition pools</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{mix}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Empirical relaxation of vegetation and some soil pools</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{emp}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Dynamic recovery of vegetation and empirical relaxation some soil pools</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{emp}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Dynamic recovery of vegetation.</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{emp}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Dynamic recovery of vegetation adjusting turnover rates (( k_{WD} ))</td>
</tr>
<tr>
<td>( \theta_{V}^{\text{emp}} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Empirical relaxation of vegetation pools</td>
</tr>
</tbody>
</table>

Each \( \theta \) stands for a parameter set; \( \theta_{0} \) represents the fix steady-state approach. \( \theta_{V}^{\text{emp}} \) identifies the base parameter set: the subscript letter ‘S’ indicates that we are prescribing nonequilibrium dynamics in soil pools, and the superscript designates the approach followed, in this case an empirical approach (emp). The subscript ‘V’ identifies experiments in which the steady state is also challenged in the 'S' indicates that we are prescribing nonequilibrium dynamics in soil pools, and the superscript designates the approach followed, in this case an empirical approach (emp). The subscript ‘V’ identifies experiments in which the steady state is also challenged in the

![Fig. 2](image-url)
nonsteady-state conditions in nonvegetation pools results only from changes in the dynamics of C inputs from vegetation pools. It is the intent of $\theta^{\text{phys}}_k$ to test whether the prescription of a dynamic disturbance recovery in a mechanically consistent manner is comparable to the model performance of semimechanistic and fully empirical approaches.

7. The $\theta^{\text{phys}}_k$ experiment builds on the $\theta^{\text{phys}}_k$ setup by adding a parameter that adjusts the wood and coarse root turnover rates ($k_{\text{WR}}$). The prescribed dynamics and implications are identical to $\theta^{\text{phys}}_k$. However, by adjusting the turnover rates of the slow vegetation pools we seek to correct potential inconsistencies in model dynamics during the second phase of the spin-up (P$_2$, Fig. 2). Despite the heuristic character of $k_{\text{WR}}$, this setup allows assessment as to whether the potential falsification of $\theta^{\text{phys}}_k$ might be due to its fixed turnover rate.

Throughout the collection of parameter vectors we constantly include maximum energy to mass conversion rates ($\varepsilon^*$ and $\varepsilon_p$) and parameters that control the response curves of light use efficiency and $R_\text{SI}$ to climate and environmental drivers: optimum temperature for photosynthesis ($T_{\text{opt}}$); sensitivity of photosynthesis to water stress ($B_{\text{ws}}$); increase in soil biological activity for a 10°C increase in temperature ($Q_10$); and $R_\text{SI}$ sensitivity to water availability ($A_{\text{ws}}$) (Appendix S2, for further details see Carvalhais et al., 2008).

Integration of vegetation pools in the model optimization

The model parameters in each setup are optimized through the minimization of the residual sum of squares between modelled daily NEP estimates and daily integrals of eddy covariance measurements of CO$_2$ fluxes (g C m$^{-2}$ day$^{-1}$) (Aubinet et al., 2000). The optimization is performed individually for each parameter vector and for each ecosystem site (Table 1), using the Levenberg–Marquardt algorithm (Levenberg, 1944; Marquardt, 1963). The integration of information related to wood biomass (C$_W$, g C m$^{-2}$), aboveground biomass (AGB, g C m$^{-2}$) and wood NPP (NPP$_W$ – carbon accumulation in the wood pool – g C m$^{-2}$ yr$^{-1}$) in the cost function is performed where such data is available (Table 1 and Appendix S3).

The observational data of vegetation pools was extracted from the Luyssaert et al. (2007) database in sites where available, including observations of AGB, NPP$_W$ and C$_W$ for four sites used (Table 1).

Statistical analysis

The model performance was evaluated independently per optimization by selected statistical indicators according to Janssen & Heuberger (1995): normalized average error (NAE); variance ratio (VR); modelling efficiency (MEP) and correlation coefficient, ($r^2$). The model performance in estimating vegetation C pools was based on the normalized mean absolute error (NMAE) (Appendix S4).

The comparisons between model performance statistics and optimized parameter values were supported by the sign test (Sprent & Smeeton, 2001). We tested the null hypothesis that the median of the difference vector between two variables was zero, for a 5% significance level. The sign test avoids: (i) the normal distribution assumption; and (ii) distribution symmetry; in our case, relevant advantages over the $t$-test and the Wilcoxon’s signed-rank test (Sprent & Smeeton, 2001; Yang et al., 2004).

Further, the experimental design includes parameter vectors with different number of parameters. In some cases, the improvements in model performance could also be originated from the addition of extra free parameters to the parameter vector. To account for the influences of the different sets of free parameters represented by the various model structures we computed the Akaike information criterion (AIC) (Akaike, 1974) for each optimization:

$$\text{AIC} = n \log(\hat{\sigma}^2) + 2P,$$

where $n$ is the number of observations, $\hat{\sigma}^2$ is the mean sum of squares and $P$ is the number of free parameters in the model (Burnham & Anderson, 2004). The computation of AIC relies on arbitrary constants [Eqn (2)] and its values can range from negative to positive through several orders of magnitude. For ease of interpretation we adopt the AIC scaling ($\Delta_0$) suggested by (Burnham & Anderson, 2004):

$$\Delta_0 = \text{AIC}_\theta - \text{AIC}_{\text{min}},$$

where $\Delta_0$ is the AIC scaling for a certain experiment $\theta$ for a given site, while $\text{AIC}_\theta$ is its respective AIC value and $\text{AIC}_{\text{min}}$ is the minimum AIC of all the experiments for that site. The parsimonious model is the one with the smaller AIC score and in this case is going to be the model that yields a $\Delta_0 = 0$.

Also, following the current experimental design, different factors (site, model version, parameter vector and cost function type) could have contributed to the variability in both model performance and optimized parameters. The identification of the main determinants of variance of a variable was supported by $n$-way analysis of variance (ANOVA), 95% confidence degree (Hogg & Ledolter, 1987).

Results and discussion

Structural changes in the CASA model

The adjustments in the CASA model (CASA$_G$, see Appendix S1) yield significant increases in the sensitivity of ecosystem fluxes to vegetation pools as intended. Yet, the differences in model performance for NEP between CASA and CASA$_G$ are not significant (Table 3), nor are the differences in the optimized parameter – except between $\varepsilon^*$ and $\varepsilon_p$, as expected. The inter-site variation in the carbon use efficiency (CUE = NPP/GPP) calculated by CASA$_G$ is well within values reported by other studies (DeLucia et al., 2007; Litton et al., 2007) (see supporting information). Further, the overall NPP GPP relationship follows a significant linear pattern (Fig. S4), with a slope closer to global values for optimizations considering multiple constraints approaches (for details, see supporting information). These results support the utilization of CASA$_G$ for the...
current experiment; hence, further analyses refer to CASA_C, except where indicated otherwise.

Model optimization under steady-state conditions

Overall, the model ability to simulate net ecosystem fluxes varies significantly among sites, although there is a clear effect of the optimization setup in model performance (corresponding to variant parameter vectors in Table 2) (Fig. S5). The fixed steady-state approaches ($\theta_{ss}$) show poorer model performance than relaxed steady-state approaches (Fig. 3). Further, the AIC results show invariably the highest values (poorest results) for $\theta_{ss}$, emphasizing the role of considering relaxed approaches in inverse optimization exercises.

The differences found in the parameter optimization results (Fig. 4, Table 4) are also consistent with previous results (Carvalhais et al., 2008): higher $B_{wo}$ (22% increase in $\theta_{wo}$ on average), associated with lower $Q_{10}$ values. The decreases in the sensitivity of light use efficiency to water availability (higher $B_{wo}$) yielded higher estimates of NPP under water limiting conditions while the decreases in $R_{11}$ responses to temperature (lower $Q_{10}$) reduced $R_{11}$ estimates. This behavior was previously shown to force C sink simulations under fixed steady-state approaches by forcing higher differences between NPP and $R_{11}$ (Carvalhais et al., 2008): the biases in parameters governing the sensitivity to climate drivers tend to compensate for an initial condition problem.

Impacts of solely prescribing wood in nonequilibrium conditions

Here we evaluate the impacts of prescribing nonequilibrium conditions solely in woody C pools on the model optimization results by adding $\eta$ parameters to the parameter vectors. The integration of $\eta$ parameters is done for both dynamic (in $\theta_{V_k}^{\text{dyn}}$ and $\theta_{V_k}^{\text{emp}}$ parameter vectors) and the empirical (in $\theta_{V_k}^{\text{emp}}$) approaches. In all cases, prescribing nonequilibrium conditions solely in the wood pools yields inferior model performance compared to approaches where only the soil pools have been adjusted ($\theta_{V_k}^{\text{emp}}$): mean losses in MEF of 15% ($P<0.11$) and significant deterioration ($P<0.003$) in NAE estimates (~126%). These results are consistent with the AIC results that are systematically higher for $\theta_{V_k}^{\text{emp}}$ than for $\theta_{V_k}^{\text{emp}}$ (Table 5).

In general, decreasing model performance is also observed for the dynamic approaches, $\theta_{V_k}^{\text{dyn}}$ and $\theta_{V_k}^{\text{emp}}$, where the vegetation pools are cut and allowed to recover following Eqn (1). For each experiment, we observe a mean loss in MEF of 6% when compared with $\theta_{V_k}^{\text{emp}}$. These differences are not significant ($P<0.35$). The differences in NAE (Fig. 3) show a significant deterioration ($P<0.03$) from $\theta_{V_k}^{\text{emp}}$ to $\theta_{V_k}^{\text{dyn}}$ (~95%) and between $\theta_{V_k}^{\text{emp}}$ and $\theta_{V_k}^{\text{dyn}}$ (~105%, although $P<0.11$). The regulation of turnover rates (subscript k) only modestly improves model performance and the differences between both experiments are not statistically significant. Furthermore, AIC is seldom significantly lower for $\theta_{V_k}^{\text{dyn}}$ compared with $\theta_{V_k}^{\text{emp}}$ (Table 5) reflecting very low information gain and that the slight improvements in $\theta_{V_k}^{\text{emp}}$ are at the expense of model parsimony.

In general, the sole prescription of nonequilibrium conditions in wood pools leads to changes in optimized parameters compared with approaches where the soil pools have been adjusted, $\theta_{V_k}^{\text{emp}}$ (Fig. 4, Table 4). There is a general pattern of increases in $\eta$ and for the sensitivity of light use efficiency to water availability ($B_{wo}$); these differences are systematic but not always significant.
Also the estimates of optimum temperature for photosynthesis (\(T_{\text{opt}}\)) are systematically significantly lower than in \(\theta_{\text{emp}}^S\) (\(P<0.003\)). The compensation biases previously observed in CASA are mostly noted in \(\theta_{\text{emp}}^S\) and \(Q_{10}\), forcing an ecosystem sink by reducing the impacts of water availability in NPP and temperature in \(\theta_{\text{emp}}^S\) (Carvalhais et al., 2008). The implementation of the \(R_A\) submodel in CASA G adds complexity to the potential responses: higher GPP estimates for \(\theta_{\text{emp}}^S\) and \(\theta_{\text{emp}}^V\) through lower sensitivity of light use efficiency to water availability (higher \(B_{\text{we}}\) or higher \(\varepsilon_{\text{e}}^*\)) also increases \(R_A\) (through maintenance respiration) reducing the trend of compensation effects on \(Q_{10}\). These prescribed changes in the model reduce the compensation effects in parameters.

Overall, experimental setups that adjust only the wood pools to nonsteady-state conditions show a decrease in model performance, although the deterioration of MEF is not significant under prescriptions of dynamic recovery (\(\theta_{\text{emp}}^S\) and \(\theta_{\text{emp}}^V\)). The similarity between the model performances of \(\theta_{\text{emp}}^S\) and \(\theta_{\text{emp}}^V\) suggests that the additional adjustments to the turnover times of woody pools remain insufficient to address the impacts of the steady-state assumption. In this regard, improvements in the recovery dynamics may be realized by investigating slow surface litter dynamics (e.g., comparing C transfers from vegetation to soil pools or by optimization of turnover rates). Further, although modest, the changes in model parameters show a compensation pattern. These results suggest that the sole

Table 4 Mean normalized differences (%) of both optimized parameter estimates and parameters uncertainties (values in parenthesis) between \(\theta_{\text{emp}}^S\) and the other parameter vectors (having \(\theta_{\text{emp}}^S\) as the reference)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(\theta_0)</th>
<th>(\theta_{\text{emp}}^S)</th>
<th>(\theta_{\text{mix}}^S)</th>
<th>(\theta_{\text{emp}}^V)</th>
<th>(\theta_{\text{emp}}^V)</th>
<th>(\theta_{\text{emp}}^V)</th>
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</thead>
<tbody>
<tr>
<td>(e_{\theta}^*)</td>
<td>6.82 (8.68)</td>
<td>5.12 (−4.45)</td>
<td>12.63 (−1.19)</td>
<td>12.55 (6.23)</td>
<td>13.59 (1.14)</td>
<td>1.72 (0.94)</td>
</tr>
<tr>
<td>(T_{\text{opt}})</td>
<td>−5.08 (5.42)</td>
<td>−4.49 (−0.44)</td>
<td>−7.99 (6.05)</td>
<td>−8.27 (16.40)</td>
<td>−8.13 (−13.82)</td>
<td>−5.18 (7.79)</td>
</tr>
<tr>
<td>(B_{\text{we}})</td>
<td>22.08 (6.2)</td>
<td>−0.44 (−3.25)</td>
<td>10.73 (−2.34)</td>
<td>11.33 (14.88)</td>
<td>13.69 (−0.72)</td>
<td>12.40 (8.58)</td>
</tr>
<tr>
<td>(Q_{10})</td>
<td>9.01 (−24.04)</td>
<td>−0.64 (−10.30)</td>
<td>2.63 (−18.77)</td>
<td>4.61 (−23.15)</td>
<td>8.00 (−32.86)</td>
<td>−3.40 (−34.94)</td>
</tr>
<tr>
<td>(A_{\text{ws}})</td>
<td>−16.51 (−49.12)</td>
<td>−5.99 (−26.21)</td>
<td>−4.71 (−42.63)</td>
<td>−8.71 (−48.81)</td>
<td>−6.78 (−50.70)</td>
<td>−9.78 (−44.57)</td>
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</table>

Bold values indicate significant differences.
Table 5 Differences between the Akaike information criterion (AIC) and the minimum AIC (AIC_{min}) for each experiment for each site

<table>
<thead>
<tr>
<th>Site</th>
<th>$\theta_{S}^{emp}$</th>
<th>$\theta_{D}$</th>
<th>$\theta_{S}^{emp}$</th>
<th>$\theta_{S}^{mix}$</th>
<th>$\theta_{dyn}$</th>
<th>$\theta_{D}^{emp}$</th>
<th>$\theta_{D}^{dyn}$</th>
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</thead>
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<td>ES-ES1</td>
<td>0.0</td>
<td>709.9</td>
<td>13.0</td>
<td>164.1</td>
<td>412.8</td>
<td>159.2</td>
<td>621.4</td>
</tr>
<tr>
<td>FR-Hes</td>
<td>188.6</td>
<td>523.3</td>
<td>0.0</td>
<td>94.9</td>
<td>251.6</td>
<td>260.6</td>
<td>237.6</td>
</tr>
<tr>
<td>FR-LBr</td>
<td>0.4</td>
<td>277.9</td>
<td>0.0</td>
<td>15.1</td>
<td>129.2</td>
<td>76.4</td>
<td>219.1</td>
</tr>
<tr>
<td>FR-Pue</td>
<td>130.5</td>
<td>434.0</td>
<td>0.0</td>
<td>16.7</td>
<td>237.7</td>
<td>242.4</td>
<td>271.1</td>
</tr>
<tr>
<td>IT-Non</td>
<td>0.0</td>
<td>376.5</td>
<td>55.6</td>
<td>174.4</td>
<td>320.5</td>
<td>324.1</td>
<td>319.0</td>
</tr>
<tr>
<td>IT-PT1</td>
<td>492.1</td>
<td>778.1</td>
<td>103.2</td>
<td>0.0</td>
<td>142.7</td>
<td>140.6</td>
<td>537.9</td>
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<td>0.0</td>
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<td>621.5</td>
<td>731.2</td>
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<td>0.0</td>
<td>55.8</td>
<td>53.2</td>
<td>48.2</td>
</tr>
<tr>
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<td>173.2</td>
<td>581.8</td>
<td>0.0</td>
<td>55.2</td>
<td>143.4</td>
<td>158.7</td>
<td>175.7</td>
</tr>
<tr>
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<td>39.3</td>
<td>16.5</td>
<td>0.0</td>
<td>31.1</td>
<td>30.1</td>
<td>24.7</td>
</tr>
</tbody>
</table>

Underlined values represent the highest (worst) AIC values while bold values identify the lowest (best) AIC (AIC = \text{AIC}_{\text{min}}).

The changes in model performance between $\theta_{S}^{emp}$ and $\theta_{S}^{mix}$ are the less significant; results show an average difference of 2.4% for NAE, while MEF loosens around 1.8%. Consequently, the trade-off between model complexity and performance is not so clear in this case (Table 5). Further, the optimized parameters in $\theta_{S}^{emp}$ and $\theta_{S}^{mix}$ are not statistically different from one another (except in optimum temperature, $T_{opt}$); yet, the changes in the sensitivity of $\epsilon_{g}$ to water availability, $B_{w}$, show a systematic distribution towards lower sensitivity under $\theta_{S}^{mix}$ setups. This pattern is consistent comparing fix and solely wood relaxed (empirical and dynamic) approaches. Soil ($R_{H}$)-related parameters are the least affected in any relaxed steady-state approach optimization and generally parameters uncertainties tend to decrease comparatively to $\theta_{S}^{emp}$ (Fig. S6, Table 4).

Overall, the prescription of a semi-empirical approach ($\theta_{S}^{mix}$) falls short of performing as well as a strictly empirical method ($\theta_{S}^{emp}$), which is more flexible. In $\theta_{S}^{mix}$, the C transfers between vegetation and soil pools during the dynamic recovery period are bounded to model structure and parameterization; and the transfers of carbon from live vegetation to dead litter pools after $P_{L}$, associated with low decomposition rates in slow litter pools, can increase substrate availability for $R_{H}$. The similar results between $\theta_{S}^{dyn}$ and $\theta_{D}^{dyn}$ suggest that optimizing live wood dynamics do not significantly change model performance. The results suggest investigating model controls on the dynamics of C transfers from vegetation to soil pools and/or surface litter pools turnover rates. Further, we observe that model performances of $\theta_{S}^{emp}$ and $\theta_{S}^{mix}$ were similar despite the differences in model structure and parameterization. The distinction between parameterization and/or model structure schemes becomes difficult to disentangle, posing an equifinality problem between $\eta$ (in $\theta_{S}^{emp}$) and $\eta_{WD} + \eta'$ (in $\theta_{S}^{mix}$). One important result is however, that if the aim is to avoid biased parameters caused by the erroneous steady-state assumption, an empirical correction of pool sizes is a sufficient strategy.

Integrating biometric constraints in the optimization

For the studied sites with biometric information the inclusion of data on vegetation pools yields a high sensitivity of the cost-function to $\eta_{wood}$ parameters, and hence a much better constraint on this parameter compared with the single NEP flux constraint (Fig. 5). Consequently, we observed significant reductions of uncertainties in parameters that affect wood and soil carbon pools directly. Furthermore, for single constraint
approaches we observe the occurrence of edge-hitting $\eta_{WL}$ (optimal value of $\eta_{WL}$ equal to 0.05), contrary to multiple constraints approaches (Fig. 5). These results suggest that the role of the different $\eta$-type scalars in the optimization (both reducing ecosystem respiration through $R_A$ and/or $R_H$) is not distinguished by assimilating net ecosystem fluxes alone, forming an ill-posed problem. On the contrary, the integration of biometric data in the cost function avoids borderline parameters and reduces uncertainties. Additionally, the results show that biometric data are not broadly inconsistent with eddy flux data within the model structure.

No significant improvements in uncertainties are observed for parameters governing the responses of GPP and $R_H$ to temperature and water availability (not shown), indicating that these are mostly constrained by the eddy covariance data from daily to seasonal time scales (Braswell et al., 2005).

Introducing biometric constraints in the cost function generally decreases the model performance in simulating NEP fluxes (Fig. S7). However, it leads to significant improvements in the estimation of vegetation C pools that for certain optimization setups correspond to minor changes in flux MEF, suggesting an overall improvement in ecosystem C simulations (Fig. 6). Similar trade-offs in matching observational data are observed in other multiple constraints approaches (Sacks et al., 2006; Moore et al., 2008). Such results suggest a compromise between the minimization of the mismatches in C fluxes and pools, which is subject to model structure limitations and that is also governed by the way the cost function is constructed [Eqns (C1) and (C2)]. Further, these results also show that a better model performance for one type of data (e.g., eddy covariance) does not imply that the whole system is described in a superior way by the model. In this perspective, the assimilation of biometric data may enable further differentiation between model structures.

**Identifying and interpreting equifinality**

The comparison between the model performance of different model structures optimized against C fluxes and pools and sole flux-based optimizations shows

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**Fig. 5** Contour plots for single constraint cost functions (NEP) and for the multiple constraints cost function (NEP, AGB): integrating net ecosystem production fluxes (NEP) and aboveground biomass pools (AGB). Black ‘+’ signs identify the solution pair for single cost functions (black lines contours); whereas black ‘x’ identify solutions for multiple constraints approaches (gray lines contours). The results for each cost function (in natural logarithm) were calculated by varying $\varepsilon_g$ and $\eta_{WL}$ while other model parameters were kept constant.

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significant differences (Fig. 7). In the model optimizations based on single constraints we observe that the model performances for fluxes are fairly close to the one to one line for the different model structures (Fig. 7a). Results show that in these cases the flux data themselves are not able to discriminate between different model representations, implying that equifinality occurs (e.g., Franks et al., 1997; Beven & Freer, 2001; Beven, 2006). These results suggest that different model structures can be compensated by different optimization solutions when assimilating and evaluating net ecosystem fluxes (Medlyn et al., 2005; Mahecha et al., 2009).

The addition of a constraint on vegetation C pools yields a clearer discrimination between the different model representations which allows the identification of limitations and advantages of different model structures (Fig. 7b).

The empirical prescription of nonequilibrium conditions in both soils and vegetation pools yields the best results in general. We also observe an overall confirmation for prescribing a dynamic recovery in vegetation when manipulating the wood turnover rates for regrowing forests in $\theta_{VK}^{\text{emp}}$ (where the pools are allowed to recover following the model dynamics and regulating the woody turnover rates). The similarities in model performance between strictly empirical ($\theta_{VK}^{\text{emp}}$) and mechanistic approaches ($\theta_{VK}^{\text{dyn}}$) are consistent with the dynamic recovery of vegetation after establishment for FR-Hes ( ~ 34 years), FR-Pue (~60 years) and IT-Ro1 (clear cut in the winter of 1999–2000). Further, in FR-Pue the performance of $\theta_{VK}^{\text{dyn}}$ is close to $\theta_{SV}^{\text{emp}}$’s, despite the fact that $\theta_{SV}^{\text{mix}}$ performs significantly worse (Fig. 7b).

Fitting the vegetation pools in $\theta_{SV}^{\text{mix}}$ when these show higher magnitudes in observations than model estimates at equilibrium is mostly driven by increasing $\varepsilon_{e}^{\text{mix}}$, since the accumulation of carbon in vegetation pools follows first-order dynamics and no turnover rates are optimized (Table 6). Consequently, higher estimates of $\varepsilon_{e}^{\text{mix}}$ also increase root and leaf pools, indirectly boosting the fast litter pools which have higher turnover rates (Fig. 58). These changes indirectly amplify $R_{A}$ and $R_{11}$ by increasing substrate availability and causing the optimized value of $Q_{10}$ to increase for $\theta_{SV}^{\text{mix}}$ (Table 6). In the dynamic recovery $\theta_{VK}^{\text{dyn}}$ the optimization of the wood turnover rates allows for an extra means to match the observed vegetation pools: the turnover rate is inversely proportional to the pool’s magnitude at equilibrium. In this case, estimated $k_{WR}$ is low (~10% of the initial value) in order to compensate for higher pools at equilibrium. This model structure allows for lower $\varepsilon_{e}^{\text{mix}}$ which reduces the estimates of leaf and root pools at equilibrium and indirectly also reduces the magnitude of the fast litter pools. These results show that the prescription of consistent fast and slow C fluxes in a mechanistic approach are only possible when wood mortality is relatively low since the last disturbance. This may indicate insufficient integration of historical dynamics which were relevant for the current state of the ecosystem and/or the erroneous parameterization of other processes (e.g., litter decomposition rates).

The inability of certain model structures to match both the observed carbon fluxes and pools is significantly site dependent. In general, the best results emerge from strictly empirical approaches ($\theta_{SV}^{\text{emp}}$)
although the prescription of site-specific recovery dynamics also yields comparable modelling efficiencies (Fig. 7). These results suggest the value of empirical approaches as benchmarks against which more mechanistic approaches can be compared. The consideration of multiple constraints highlights the limitations of forcing equilibrium solely on soil (Fig. 8a) or on vegetation pools (Fig. 8b). The prescription of a recovery from a disturbance on vegetation (Fig. 8c) shows similar results to the empirical relaxation on both types of pools (Fig. 8d). These results highlight a multiple constraints approach ability to exclude model representations such as \( \theta_{\text{emp}}^{\text{s}} \) and \( \theta_{\text{wood}}^{\text{emp}} \) setups based on significant reductions in MEF. The results also show a strong similarity in model efficiency between the empirical relaxation of vegetation and soil pools \( (\theta_{\text{emp}}^{\text{SV}}, \theta_{\text{mix}}^{\text{SV}}, \theta_{\text{dyn}}^{\text{V}}) \) and the \( \theta_{\text{dyn}}^{\text{Vk}} \) setup. These results emphasize the indirect role of the vegetation recovery mechanisms on nonsteady-state conditions of ecosystems (Nabuurs, 2004). In this case, the reduction of carbon inputs in the ecosystem caused by the removal of the vegetation pool in the past is translated in nonequilibrium conditions in both vegetation and soil level pools.

If inconsistencies between different types of observational data exist – in this case pools and fluxes – these may hamper multiple constraints approaches. The presence of incompatible measurements of fluxes and pools can bias parameters and/or can erroneously falsify or corroborate model structures. In this regard, the consideration of basic rules for data consistency checks is key (e.g., Luyssaert et al., 2007, 2009). In addition, we recognize an increasing importance in addressing issues of data representation: (1) comparable geographic coverage of flux and biometric data and (2) correspondence between ecosystems modelled and observed C pools. Further, information on uncertainty of different data sources provides information about how constraining the measurements are, and can be indicative of how mutually exclusive (or not) are different sets of observations.

**Overall discussion**

The consideration of multiple constraints in model-data integration approaches permits a more comprehensive evaluation of model structures. From our experimental design, we observed that the sole consideration of woody pools out of equilibrium significantly reduces our model performance. Overall, an empirical approach that submits both wood and soil pools to independent scalars, relaxing the steady-state conditions, shows better model performances in CASAG. The prescription of dynamic driven setups to nonequilibrium conditions imposes past disturbance on vegetation according to site history. The modelling performances of such setups improve over fixed steady-state approaches, since direct and indirect effects of vegetation disturbances generate nonsteady-state conditions in the whole ecosystem (Nabuurs, 2004). However, model performances with dynamic prescriptions of nonsteady state woody pools are still statistically inferior to setups that also explicitly scale soil pools \( (\theta_{\text{emp}}^{\text{SV}}, \theta_{\text{mix}}^{\text{SV}}) \). The reason for this need...
of additional adjustments in the soil pools may stem from disturbances before the last biomass removal (which is quasi simulated in the dynamic approaches). Obviously, the relaxation of the initial conditions in C pools embodies independence from rigid assumptions of model structures, which grants higher flexibility to R and R setups. Our results suggest significant advantages of such approaches for diagnostic purposes.

The inter-annual variability of NEP measurements may also bias the parameterization of η-type scalars and lead to erroneous assumptions about the equilibrium state of the ecosystem. For short NEP time series, positive or negative variations from an equilibrium system may infer sink or source conditions of the site, respectively. Further, positive (or negative) changes in magnitudes of RH fluxes from the start to end of the simulations driven by non simulated processes may lead to higher (lower) estimates of η, initializing the model with higher (lower) C pools estimates which would decrease (increase) throughout the simulation and reduce (increase) RH (Fig. S8). In such cases, other limitations in model structure would be compensated for by imposing nonequilibrium assumptions.

The assimilation of both C fluxes and pools in the model-data integration approach may degrade our ability to correctly simulate NEP fluxes (Williams et al., 2005) but allows the identification of model structures unable to handle both sources of information. Multiple constraints approaches allow the identification of model structures able to conciliate fast fluxes (eddy covariance) with long-term integral of ecosystem respiration data in future studies should help address these problems. Other sources of data such as the integration of routine measurements of annual wood increments at site level, by forest inventories or tree rings measurements, could also contribute to efficient new constraints on annual integrals and inter annual variability of vegetation carbon assimilation.

Overall, model structures should be able to be confronted with multiple sources of data relevant to the simulated dynamics. Although the consideration of a more complex model – CASAC vs. CASA – may violate the parsimony principle, it entails the possibility to further assimilate new observational constraints. As expected, the model performances and parameter optimization vary with model structure and cost function constraints at the site level, although not all parameters are equally affected (Sacks et al., 2006). Here, relating different model structures with site history information may corroborate the different simulation dynamics assumed and the mechanisms behind parameter changes. Generally, limitations in simulating dynamic approaches can be addressed with more appropriate or

<table>
<thead>
<tr>
<th>Site</th>
<th>Parameter vector</th>
<th>ε∗ (g C MJ⁻¹ PAR)</th>
<th>T_opt (°C)</th>
<th>Bsec (unitless)</th>
<th>Q10 (unitless)</th>
<th>Asec (unitless)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FR-Hes</td>
<td>θexp</td>
<td>1.42 (0.03)</td>
<td>16.05 (0.31)</td>
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<td>IT-Ro1</td>
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</table>

Values in parentheses represent parameters uncertainties (standard error).
flexible model structures and better prescription of site-specific disturbance dynamics. The apparent limitations in our diagnostic ability may be further addressed by investigating long-term partitioning and transfers of C among the different ecosystem pools from chronosequences.

Conclusions

We demonstrate that nonequilibrium assumptions of the vegetation pools alone are insufficient for simulating NEP fluxes in nonsteady-state ecosystems. Consequently, the relaxation of equilibrium conditions should
ECOSYSTEM C POOLS APART FROM EQUILIBRIUM

be allowed on the full range of pools influencing ecosystem C fluxes. The dynamics that follow the past disturbance of the vegetation pools entail direct and indirect effects on whole ecosystem carbon balance. Yet, the ability of representing these dynamics is significantly site dependent, supporting the empirical relaxation of equilibrium conditions in ecosystem carbon pools.

We establish an assimilation scheme for information of vegetation carbon pool by including biometric data in the optimization cost function. The trade-off between model performance in ecosystem fluxes estimates and vegetation pools estimates highlights model structural limitations. Further, remarked distinctions between different model structures are observed when integrating both sources of information – fluxes and pools – in the cost function, contrasting with similar performance results when constraining the assimilation scheme solely with C fluxes. Our results suggest that multiple constraints in model-data integration approaches provide a means for resolving or reducing equifinality issues. In this regard, further model improvements could be gained from the consideration of separate ecosystem flux components as well as of water and energy fluxes. Further, these results suggest that the assimilation of biomass information from satellite remote sensing could support a more comprehensive characterization of terrestrial ecosystems at larger spatial scales.

Acknowledgements

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References


Supporting Information

Additional Supporting Information may be found in the online version of this article:

Appendix S1. Changes in the CASA model.
Appendix S2. Description of the set of functional parameters included in all parameter vectors.
Appendix S3. Summary of the optimization approach.

Figure S1. Changes between $y_{emp}$ and $y_0$ model efficiency (MEF; left) and normalized average error (NAE; right) by integrating a parameter that only affects the slow turnover vegetation pools after equilibrium ($\eta_{yv}$ in $\theta_y^{\text{emp}}$). The sensitivity to $\eta_{yv}$ is higher in CASAC than in CASA.

Figure S2. Comparison of model performance statistics between CASA C and CASA: a) normalized average error (NAE); and 2) modelling efficiency (MEF). Overall, both versions of the CASA model do not show significant differences in model performance for the analyzed sites and parameter vectors.

Figure S3. Relationship between CASA and CASA C; maximum light use efficiency estimates – $\varepsilon'$ and $\varepsilon'_v$, respectively – (a): regression slope is 0.70 (0.64 to 0.77 confidence bounds – 95%) and intercept 0.17 (0.05 to 0.28 confidence bounds – 95%); $r^2$ of 0.9. Forcing an intercept of zero, slope goes to 0.80 (0.78 to 0.82 confidence bounds – 95%). The CUE for CASA C (b) shows significant inter-site variability and four sites denote a strong variation when integrating $\eta_{ywood}$ parameters in the optimizations, although these results only report to optimizations considering fluxes in the cost function: FR-Hes, FR-Pue, IT-PT1 and IT-Ro2.

Figure S4. Global relationship between NPP and GPP for site level optimizations for: (a) single constraints approaches: the regression slope is 0.61 (0.56 to 0.65 confidence bounds – 95%) and intercept $-1.34$ ($-0.59$ to 0.36 confidence bounds – 95%); $r^2$ of 0.9; and for (b) multiple constraints approaches: the regression slope is 0.53 (0.46 to 0.61 confidence bounds – 95%) and intercept 43.73 ($-65.26$ to 152.7 confidence bounds – 95%); $r^2$ of 0.73.

Figure S5. ANOVA results for the different model performance indicators used. FST: flux site; CMV: CASA model version (CASA or CASA C); PRM: optimized parameter vector; CFT: cost function type. The values correspond to the percentage of variance explained by each factor, or combination of factors, over the total explained variance. Sites with no multiple constraints cost function alternatives were removed here.

Figure S6. Distribution of parameter uncertainties ratios between parameter vectors on x-axis and $\theta_y^{\text{emp}}$. Rectangular boxes are bounded by 25th and 75th percentile (bottom and top, respectively), while the horizontal line inside each rectangle indicates the sample median; vertical individual lines limited by horizontal bars indicate the extent of the remaining data, excluding outliers; plus sign (+) indicates statistical outliers.

Figure S7. Comparison of NEP MEF between multiple constraint cost functions (CFM – considering pools and fluxes) and single constraint cost function (CFv – considering fluxes). Markers identify different parameter vectors and colours the variables included in CFM approaches (light green: NEP and AGB; red: NEP, AGB and NPPW; dark green: NEP, NPPW and blue: NEP and Cv). These patterns are similar in $r^2$ and NAE. Except in IT-Ro1, VR results show occasional improvements under CFM.

Figure S8. Development of vegetation and soil C pools in FR-Pue for three experimental setups: empirically relaxing pools ($\theta_y^{\text{emp}}$S); allowing for a dynamic recovery of vegetation pools and prescribing and empirical distance to equilibrium in soil pools ($\theta_y^{\text{emp}}$V); and simulating non equilibrium conditions solely in vegetation pools, allowing recovery and regulating its turnover rates ($\theta_y^{\text{pl}}$V).

Figure S9. Sensitivity of the below ground soil moisture effect ($W_s$) to the water storage to monthly PET ratio ($B_{gr}$) for different $A_{kos}$ estimates.

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