



# Annual CO<sub>2</sub> Budget Estimation From Chamber-Based Flux Measurements on Intensively Drained Peat Meadows: Effect of Gap-Filling Strategies

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### Specialty section:

This article was submitted to  
Soil Processes,  
a section of the journal  
Frontiers in Environmental Science

**Received:** 28 October 2021

**Accepted:** 04 March 2022

**Published:** 02 May 2022

### Citation:

Liu W, Fritz C, Weideveld STJ,  
Aben RCH, van den Berg M and  
Velthuis M (2022) Annual CO<sub>2</sub> Budget  
Estimation From Chamber-Based Flux  
Measurements on Intensively Drained  
Peat Meadows: Effect of Gap-  
Filling Strategies.  
Front. Environ. Sci. 10:803746.  
doi: 10.3389/fenvs.2022.803746

Estimating annual CO<sub>2</sub> budgets on drained peatlands is important in understanding the significance of CO<sub>2</sub> emissions from peatland degradation and evaluating the effectiveness of mitigation techniques. The closed-chamber technique is widely used in combination with gap-filling of CO<sub>2</sub> fluxes by parameter fitting empirical models of ecosystem respiration (R<sub>eco</sub>) and gross primary production (GPP). However, numerous gap-filling strategies are available which are suitable for different circumstances and can result in large variances in annual budget estimates. Therefore, a need for guidance on the selection of gap-filling methodology and its influence on the results exists. Here, we propose a framework of gap-filling methods with four Tiers following increasing model complexity at structural and temporal levels. Tier one is a simple parameter fitting of basic empirical models on an annual basis. Tier two adds structural complexity by including extra environmental factors such as grass height, groundwater level and drought condition. Tier three introduces temporal complexity by separation of annual datasets into seasons. Tier four is a campaign-specific parameter fitting approach, representing highest temporal complexity. The methods were demonstrated on two chamber-based CO<sub>2</sub> flux datasets, one of which was previously published. Performance of the empirical models were compared in terms of error statistics. Annual budget estimates were indirectly validated with carbon export values. In conclusion, different gap-filling methodologies gave similar annual estimates but different intra-annual CO<sub>2</sub> fluxes, which did not affect the detection of the treatment effects. The campaign-wise gap-filling at Tier four gave the best model performances, while Tier three seasonal gap-filling produced satisfactory results throughout, even under data scarcity. Given the need for more complete carbon balances in drained peatlands, our four-Tier framework can serve as a methodological guidance to the handling of chamber-measured CO<sub>2</sub> fluxes, which is fundamental in understanding emissions from degraded peatlands and its mitigation. The performance of models on intra-annual data should be validated in future research with continuous measured CO<sub>2</sub> flux data.

**Keywords:** closed-chamber methods, drained peatland, carbon dioxide, CO<sub>2</sub> flux modeling, data interpolation

## 1 INTRODUCTION

Covering only 3% of the global land surface, peatland contains over 600 Gt of carbon, which is nearly 30% of all global soil carbon (Parish et al., 2008; Yu et al., 2010). However, centuries of peatland drainage for agriculture and forestry have changed large peatland areas from carbon sinks into sources. At present, around 10% of global peatland is degraded due to drainage or exploitation (Joosten, 2010). Drained peatlands are estimated to annually emit 1.91 Gt CO<sub>2</sub>-equivalents without further exploitation (Leifeld and Menichetti, 2018). This comprises an estimated 12–41% of the greenhouse gas (GHG) emission budget for keeping global warming below +1.5 to +2°C (Leifeld et al., 2019). Given the importance of emissions from degraded peatlands, numerous studies have focused on the measurement of the net ecosystem exchange (NEE), and, subsequently, estimation of the annual CO<sub>2</sub> budgets. These studies helped understanding the magnitude of emissions among different peatland systems (Campbell et al., 2014; Tiemeyer et al., 2016), influences of environmental factors (Järveoja et al., 2016; Hoyt et al., 2019), effects of land use and management (Beetz et al., 2013; Günther et al., 2015; Renou-Wilson et al., 2016), and peatland's contribution to large-scale CO<sub>2</sub> emission inventories (Wilson et al., 2016a; Tiemeyer et al., 2020). Annual CO<sub>2</sub> budgets provide straightforward information that could be easily adopted in policy- or decision-making regarding peatland degradation.

Closed-chamber methods represent an inexpensive and easy-to-use technique that is suitable for use on a wide range of ecosystems (Heng, 2021). At larger scale, however, estimation of annual CO<sub>2</sub> budgets is heavily dependent on spatial and temporal interpolation, i.e., gap-filling of chamber measurement data. The most frequently-used gap-filling methodologies include parameter fitting of empirical models, such as the simple temperature and PAR (photosynthetically active radiation) dependent functions of ecosystem respiration ( $R_{\text{eco}}$ ) and gross primary production (GPP), respectively. The most frequently used relations are the Arrhenius-type  $R_{\text{eco}}$  relation (Lloyd and Taylor, 1994) and rectangular hyperbolic light response equation of GPP (Michaelis and Menten, 1913).

A wide variety of models with different complexity can be applied for better interpretation of the processes. In model structure, various environmental factors can be incorporated to improve model performance. For example, hydrological regimes (e.g., soil moisture content, groundwater level) regulates  $R_{\text{eco}}$  by establishing aerobic and anaerobic zones within the soil profile (Juszczak et al., 2013). Plant composition, biomass and phenology can reflect the temporal variations on the contributions from microbial heterotrophic and plant autotrophic respiration to  $R_{\text{eco}}$  (Järveoja et al., 2020) and the photosynthesis capacity of the plants to GPP (Peichl et al., 2018). An extensive summary of commonly used model structures and environmental factors are presented in **Supplementary Table S1**. Parameter fitting of these models are applied with time scales from campaign-specific (e.g., Beetz et al., 2013) to seasonal (Waddington and Roulet, 2000) or annual (Wilson et al., 2016b), adding a temporal dimension of the model's complexity.

Such diversity of gap-filling methodology creates variations in the annual CO<sub>2</sub> budget estimation, which may lead to uncertainties on the ability of the methodology to reach budget estimates closest to the real CO<sub>2</sub> fluxes. Such uncertainties affect upscaling of the CO<sub>2</sub> emission and conclusions in field trials and comparative studies (Hoffmann et al., 2015). Huth et al. (2017) found strongly diverse CO<sub>2</sub> budgets (−7.3 to 15.6 t ha<sup>−1</sup>) across gap-filling options with different pooling methods of measured data (temporal complexity). Karki et al. (2019) calculated widely variable NEE estimates, ranging from −9.35 to −2.08 t ha<sup>−1</sup> yr<sup>−1</sup> on one plot, when combining eight  $R_{\text{eco}}$  and eight GPP models (structural complexity). Previous studies attempted to mitigate such uncertainties by standardizing the data acquisition and processing approaches. Hoffmann et al. (2015) proposed a standardized automatic data processing algorithm for campaign-specific modeling. Huth et al. (2017) provided options of the timing of the flux measurements, strategies of data pooling and methods of flux partitioning. However, the methodological diversity of gap-filling and the subsequent uncertainties still complicates the application and interpretation of chamber-based flux data.

Manual closed chamber measurements require human resources to carry out the measurements. Which makes that the current state of the method may be limited due to practical issues, such as accessibility of the sites, equipment deficiency, and/or unexpected influence from management or weather events (e.g., in Weideveld et al., 2021), resulting in flux datasets with potentially low measurement frequency, prolonged data gaps, and/or large variations. The standard campaign-specific method may not be possible under such circumstances, requiring additional procedures in the gap-filling data processing and modeling.

The above-mentioned methodological challenges regarding diversity of the methods, uncertainties, and data deficiency confounds the handling of chamber-measured flux data, as well as the subsequent data analysis of comparative studies or field trails. A streamlined framework for the gap-filling strategy is timely needed that contributes to the current methodological standards. The main objectives of this study are: 1) present a systematic framework of gap-filling methodologies following a gradient of structural and temporal model complexity; 2) demonstrate and compare the statistical performances of the gap-filling methods using multiple datasets; 3) investigate the potential influence of gap-filling method selection on the detection of treatment effects in a field trial.

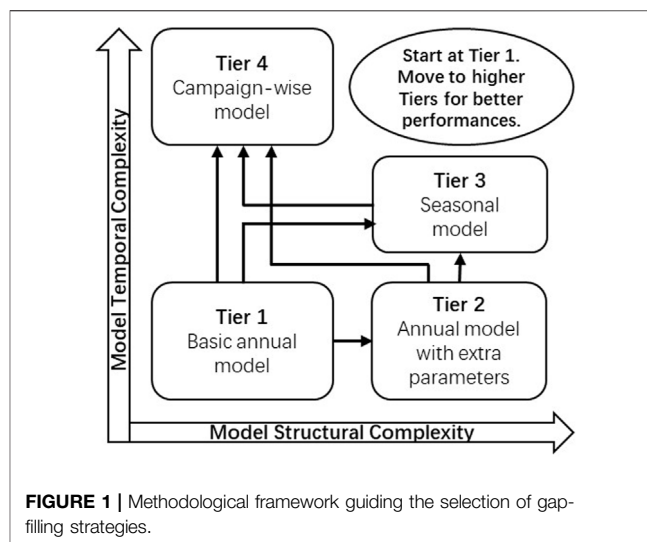
## 2 MATERIALS AND METHODS

### 2.1 CO<sub>2</sub> Flux Dataset

Selected gap-filling methodologies were tested on an existing chamber-based CO<sub>2</sub> flux dataset from the province of Friesland, the Netherlands, published in Weideveld et al. (2021). CO<sub>2</sub> exchanges were monitored from January 2017 till December 2018 at four farms. All farm locations have large fields with deep drainage (ditch water levels from 60 to 90 cm below surface)

and intensive fertilization ( $>230 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ). The peat soils have a thickness of 0.8–2.0 m, some of which are covered with a carbon-rich clay layer of 20–40 cm. The grasslands are dominated by *Lolium perenne*. Each farm was set up with a control site containing traditional drainage and infiltration ditches, and a treatment site containing sub-soil irrigation (SSI) drains. The SSI system functions by installing permeable drainage/irrigation pipes at around 10 cm below ditch water level. It was proposed to elevate groundwater level in the dry summer season to reduce CO<sub>2</sub> emissions, while fulfilling a drainage function when the groundwater level is above the ditch water level (van den Akker et al., 2010; Querner et al., 2012 as cited in; Weideveld et al., 2021).

CO<sub>2</sub> fluxes were measured on all four farms twice a month during the growing season (April–September) and once a month during the rest of the year. On each site, three 15 cm-deep soil collars for flux measurements with chambers ( $80 \times 80 \times 50 \text{ cm}$ ) were installed as replicates. An opaque (dark) chamber was used to measure ecosystem respiration ( $R_{\text{eco}}$ ) and a transparent (light) chamber for the measurement of net ecosystem exchange (NEE). Gross primary production (GPP) was directly derived from NEE using measured daytime  $R_{\text{eco}}$ , which could avoid propagating  $R_{\text{eco}}$  modeling errors into GPP models (Huth et al., 2017), while light and dark measurements were performed in sequence to minimize errors due to deviations in temperature over time. During each campaign, per field flux measurements were performed from sunrise to noon, or from noon to sunset. Depending on the duration of sunlight, an average of nine light and 10 dark measurements during winter, and 18 light and 20 dark measurements were achieved. An average of 383 measured CO<sub>2</sub> fluxes were collected per site and year (Weideveld et al., 2021; **Supplementary Table S2**). Grass height and groundwater table (GWT) were measured at the start of every field campaign. Photosynthetically active radiation (PAR) and soil temperature at 5 and 10 cm depth were measured during the campaigns. PAR, soil temperature and air temperature were also continuously recorded every 5 min during and between field campaigns. The recorded data was allocated into hourly averages to simplify the computation in the following gap-filling extrapolation. According to Hoffmann et al. (2015), the use of hourly average PAR and temperature could induce systematic bias in the gap-filled annual budget estimates. The positively skewed distribution pattern of the GPP functions could result in an overestimation of over  $1 \text{ t CO}_2 \text{ ha}^{-1} \text{ yr}^{-1}$  in the GPP estimates (Hoffmann et al., 2015). Meanwhile, bias in the  $R_{\text{eco}}$  estimates in our case was presumably small since soil temperature as the driving environmental factor for the  $R_{\text{eco}}$  functions changes slower than air temperature. Grass yield inside soil collars was harvested eight times in 2017 and five times in 2018. Total carbon was measured in dry plant material ( $\text{t C ha}^{-1} \text{ yr}^{-1}$ ) to determine C-export via harvest. Slurry manure was applied four times per year at rates of  $119\text{--}181 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  with a C/N ratio of  $16.3 \pm 1.3$  (mean $\pm$ SD) to simulate C-import via farm management. Export and import of carbon were converted from carbon content to CO<sub>2</sub> for calculating the CO<sub>2</sub> balance. More details on the experimental design, flux measurements and data treatment are available in Weideveld et al. (2021).



In the previous analysis in Weideveld et al. (2021), a campaign-wise gap-filling strategy was applied and no effect from the SSI technique was detected. In 2018, the experimental farms suffered from an extreme drought. Parameter fitting of the data therefore faced difficulties and led to uncertainties in the CO<sub>2</sub> budget estimates, which was presumably due to drought effect that could not be explained by the measured environmental factors such as soil moisture and GWT. This extensive dataset combining multiple years and locations with the unexpected drought events provided opportunities to test the performances of gap-filling strategies and exemplify their differences.

## 2.2 Gap-Filling Methodological Tiers

A framework of four Tiers of gap-filling methodologies was constructed (Figure 1). A Tier represents a level of methodological complexity, which has been used in the IPCC GHG inventory reporting methods (IPCC, 2019). Tier 1 is the basic method applying the original form of the empirical models without extra independent variables on annual datasets. Higher Tiers are more demanding in terms of model complexity and data requirements. Within each Tier, the most commonly used empirical models of  $R_{\text{eco}}$  and GPP were selected from **Supplementary Table S1**. Parameter fitting was performed using non-linear least square (NLS) models with the R package *lme4* (Bates et al., 2015). Model complexity was determined by two aspects: model structure and temporal scale. Structural complexity was increased by adding extra parameters to the basic empirical models. Temporal complexity was increased by shortening modeling periods by separating the dataset according to seasonality or applying campaign-specific models. For both  $R_{\text{eco}}$  and GPP, multiple model structures were tested at each Tier. Significance of the parameters was determined by the  $p$ -value and  $t$ -statistic of the parameter estimate from the NLS model. Models that performed poorly (non-converging regressions, insignificant/abnormal parameter values, etc.) were discarded while the best

**TABLE 1** | Equations of the empirical models selected for the gap-filling framework.

	<b>R<sub>eco</sub></b>	<b>GPP</b>
Tier 1–BASIC	<b>ARR</b> : $R_{ref} \times e^{E_0 \times (\frac{1}{T_{ref}-T_0} - \frac{1}{T-T_0})}$ (1) <b>Exp</b> : $A \times e^{bT}$ (2)	<b>MM</b> : $\frac{GPP_{max} \times \alpha \times PAR}{GPP_{max} + \alpha \times PAR}$ (3) <b>SMT</b> : $\frac{GPP_{max} \times \alpha \times PAR}{\sqrt{GPP_{max}^2 + (\alpha \times PAR)^2}}$ (4) <b>MIT</b> : $GPP_{max} \times (1 - e^{-\frac{\alpha \times PAR}{GPP_{max}}})$ (5)
Tier 2–PARA	<b>ARR – D</b> : $R_{ref} \times e^{E_0 \times (\frac{1}{T_{ref}-T_0} - \frac{1}{T-T_0})} + a \times DI$ (6)	<b>MM – G</b> : $\frac{GPP_{max} \times GH \times \alpha \times PAR}{(GPP_{max} \times GH) + \alpha \times PAR}$ (7) <b>MM – GT</b> : $\frac{GPP_{max} \times GH \times \alpha \times PAR}{(GPP_{max} \times GH) + \alpha \times PAR} \times Ft$ (8) <b>MM – GTD</b> : $\frac{GPP_{max} \times GH \times \alpha \times PAR}{(GPP_{max} \times GH) + \alpha \times PAR} \times Ft + a \times DI$ (9)
Tier 3–SS	<b>Non-drought: Eq. 1</b> <b>Drought: Eq. 6</b> (Linear $a \times T + b \times DI + c$ ) (10) <sup>a</sup>	<b>Non-drought: Eq. 8</b> <b>Drought: Eq. 9</b>
Tier 4–CW	<b>Eq. 1</b>	<b>Eq. 3</b>

**Abbreviations:** BASIC, basic annual models; PARA, annual models with extra parameters; SS, seasonal gap-filling; CW, campaign-wise gap-filling; ARR, Lloyd-Taylor modified Arrhenius model; EXP, Van't Hoff exponential model; MM, Michaelis-Menten/SMT, Smith's/MIT, Mitscherlich's light response curve; -D, with drought index; -G, with grass height; -T, with temperature function (Ft).

<sup>a</sup>A linear model was used for the drought season in 2017, where ARR-D did not result in acceptable performance.

performing model combinations (see **Section 2.3**) were selected to be used in the next Tiers and for further statistical analysis.

### 2.2.1 Tier One: Basic Annual Models

From **Supplementary Table S1**, the most widely-used empirical models were selected as the basic annual models. For  $R_{eco}$ , temperature-dependent functions including the Lloyd-Taylor modified Arrhenius (**Table 1, Eq. 1**) and Van't Hoff exponential (**Table 1, Eq. 2**) models were selected. Air temperature, soil temperature at 5 and 10 cm depth were tested in the parameter fitting. Soil temperature at 5 cm depth consistently provided better performances in different models and was therefore selected to be used in other Tiers. For GPP, rectangular hyperbolic functions including the Michaelis-Menten's (**Table 1, Eq. 3**), Smith's (**Table 1, Eq. 4**) and Mitscherlich's (**Table 1, Eq. 5**) light response curves were selected. For the parameter fitting, flux measurement data was pooled over the entire year. The Lloyd-Taylor modified Arrhenius and Michaelis-Menten's hyperbolic functions were selected to be used in the higher Tiers.

### 2.2.2 Tier Two: Annual Models With Extra Parameters

#### 2.2.2.1 Inclusion of Extra Environmental Factors

Extra environmental factors were introduced into the Tier one models for an increased model structural complexity. Multiple mathematical forms of the environmental factors were tested and compared for the best model performance (**Supplementary Table S1B**). Grass height was used as a vegetation index since it is correlated to a wide range of vegetation indexes, such as Normalized Difference Vegetation Index (NDVI), Leaf Area Index (LAI) and Difference Vegetation Index (DVI) (Payero et al., 2004), although rarely used directly. The GPP model with grass height modified  $GPP_{max}$  (Karki et al., 2019, **Table 1, Eq. 7**) was selected for further calculations.  $R_{eco}$  models with grass height were not included due to frequently

insignificant parameter fitting, indicating a weak correlation. A temperature function (**Supplementary Table S1B**) was introduced to the GPP function with grass height (Karki et al., 2019, **Table 1, Eq. 8**) to account for the influence of low temperature during winter and spring (Yamori et al., 2014). Groundwater table, although frequently used in other studies (see references in **Supplementary Table S1B**), was discarded from the models due to its generally poor model performance in this study. Soil moisture was not tested due to lack of continuous measurements.

#### 2.2.2.2 Introducing a Drought Index

In order to describe the contrasting climate conditions in the studied years, a drought index was defined based on drought events (any period with more than three consecutive days without precipitation, Jassey and Signarbieux, 2019) and the cumulative atmospheric water flux (precipitation minus evapotranspiration, P-ET, Stagge et al., 2015). The daily precipitation and evapotranspiration data were collected from the nearest official KNMI weather station (weather station Leeuwarden, 18–30 km distance from research sites, Weideveld et al., 2021). The accumulated P-ET was reset to zero at the beginning of both years. Pulses of water from small precipitation events can stimulate the carbon flux (Munson et al., 2010; Shen et al., 2015). Munson et al. (2010) found on a semiarid grassland that water is less limiting to carbon fluxes after rain events above 5 mm. No such study was found for peat meadows. Therefore, we reset the accumulated P-ET also after rain events above 5 mm, assuming a reduced drought effect. The drought index was then calculated as absolute values of the accumulated P-ET that remained negative with resets after rain events (**Supplementary Figure S1**). The drought index was then tested in different forms and included as a residual term in both the  $R_{eco}$  and GPP models (**Table 1, Eqs 6, 9**) as only this form resulted in significant model parameters.

**TABLE 2 |** Summary of the analysis of variance (ANOVA) for the mixed-effects models fitted on the gap-filled NEE for each gap-filling strategy. Year, treatment and their interaction are independent variables, and farm location is included as a random effect.

Model combination	Independent variable	Sum of squares	F-F <sub>1, 16</sub>	p value
Tier 1—BASIC	Year	4.50	0.06	0.8150
	Treatment	11.79	0.15	0.7053
	Year × Treatment	162.57	2.04	0.1721
Tier 2—PARA	Year	466.00	6.07	0.0255 (*)
	Treatment	41.51	0.54	0.4730
	Year × Treatment	168.68	2.20	0.1578
Tier 3—SS	Year	1,013.59	14.85	0.0014 (**)
	Treatment	0.28	0.00	0.9496
	Year × Treatment	176.82	2.59	0.1270
Tier 4—CW	Year	182.93	1.86	0.1913
	Treatment	0.39	0.00	0.9505
	Year × Treatment	40.64	0.41	0.5292

BASIC, annual basic model; PARA, model with extra parameters; SS, seasonal; CW, Campaign-wise. Significance is indicated in brackets behind the p-value, with \*p < 0.05, \*\*p < 0.01.

### 2.2.3 Tier Three: Seasonal Gap-Filling

The annual flux datasets were split into two seasonal subsets, adding a level of temporal complexity. Here, seasonality was defined based on drought conditions, whereas a drought season had a positive drought index, and non-drought seasons had a drought index equal to zero. The best performing Tier one and Tier two models were tested in the parameter fitting of two seasonal data sets. For non-drought periods, an Arrhenius  $R_{eco}$  model was combined with a Michalis-Menten GPP model with grass height and temperature function. For drought periods, both models were applied with addition of a drought index. The drought period covered only 37 days in 2017 (151 days in 2018), which led to insufficient data points for the model fitting. Therefore, linear regressions were applied to the modeled  $R_{eco}$  for the drought period in 2017 (Table 1, Eq. 10); and the parameter of light response function adopted fixed  $GPP_{max}$  and  $\alpha$  from the annually fitted Tier two models.

### 2.2.4 Tier Four: Campaign-Wise Gap-Filling

Campaign-wise gap-filling refers to parameter fitting of flux data measured on an individual measurement date. The modeling and gap-filling procedure is adopted from Weideveld et al. (2021): Per campaign, Arrhenius and Michalis-Menten functions were fitted for  $R_{eco}$  and GPP, respectively. Pooling of data from two or more adjacent campaigns was applied when the range of PAR did not cover a complete light response curve including the light-limited part and after the light saturation point. This occurred in both years during winter from January to March, and occasionally in 2017 during summer from June to September when data was collected on rainy and cloudy days (see campaign-wise parameters in Supplementary Dataset). Gap-filling between two adjacent campaigns are averages of the CO<sub>2</sub> flux estimates from these two campaign-wise models, weighted by the temporal distances of the gap-filled moment to each of the measurements.

## 2.3 Model Performance

Performances of the fitted models were evaluated by comparing measured and modeled values based on a series of model

indicators following Moriasi et al. (2007) as used by Hoffmann et al. (2015). Mean absolute error (MAE), RMSE (root mean square error)—observations standard deviation ratio (RSR), coefficient of determination ( $r^2$ ), modified index of agreement (md), and Nash–Sutcliffe's model efficiency (NSE) were calculated for each model. Goodness of the fit was determined on a set of thresholds rating the indicators (Hoffmann et al., 2015).

## 2.4 Gap-Filling and Validation

Hourly CO<sub>2</sub> fluxes ( $R_{eco}$ , GPP and NEE) were calculated by feeding the environmental variables (hourly average soil temperature at 5 cm depth, air temperature, PAR, and interpolated grass height) to the selected gap-filling models. Grass height was linearly interpolated between measurement campaigns using the R package zoo (Zeileis and Grothendieck, 2005). More accurate interpolation was not possible due to the lack of high frequency measurement or empirical models for grass height. Depending on the growth stage of the plants, linear interpolation may induce overestimation at short grass after harvest due to the plants' recovery and underestimation at relatively long grass when plant growth is reaching the maxima.

Annual  $R_{eco}$ , GPP and NEE budgets were calculated by summing these hourly fluxes. Model errors and extrapolation errors are the most important sources of uncertainty in the gap-filling of annual CO<sub>2</sub> budgets (Beetz et al., 2013). Only model errors were estimated, since extrapolation errors were partly related to, and therefore discussed by, the selection of different extrapolation methods (Weideveld et al., 2021). A Monte Carlo simulation was included in each gap-filling run for model error estimation (Beetz et al., 2013; Leiber-Sauheitl et al., 2014; Hoffmann et al., 2015; Berger et al., 2019; Zhao et al., 2020) using R package nlstools (Baty et al., 2015). Parameter fitting of  $R_{eco}$  and GPP models was bootstrapped with 1,000 iterations. Annual  $R_{eco}$  and GPP budgets were calculated with all the bootstrapped model parameter sets, from which the standard deviation (SD) was calculated to represent the uncertainties of the estimates. Uncertainty of annual NEE budgets was subsequently calculated by combining the SDs of  $R_{eco}$  and GPP following the law of error propagation.

An independent quantitative validation of the annual budget estimates was also needed alongside the proposed model performance and uncertainty assessments, in order to evaluate the accuracy of the gap-filled CO<sub>2</sub> budgets. However, a direct validation was not possible in absence of a known true value of annual CO<sub>2</sub> budgets. Therefore, only an indirect validation was performed using the positive correlations between GPP and plant biomass presented in previous studies (Otieno et al., 2009; Hirota et al., 2010; Weideveld et al., 2021). Derived annual GPP budgets were linearly correlated with C-export per year and method Tier as a quality check of the estimates by examining the significance of the regression.

## 2.5 Applicability Demonstration

Our Tier list framework was developed mainly in consideration of the drought effect during our measured period that caused large variances in the fluxes data. Meanwhile, the ever-growing number of chamber-based flux measurements set up on global peatlands are performed under influence from various conditions other than drought events. For example, differences in equipment, operational techniques, environmental and weather conditions, etc. Our framework and insights on method selection also need to be tested under other types of variations or data gaps. Therefore, the framework was further demonstrated and evaluated on an unpublished CO<sub>2</sub> flux dataset from the fifth farm location over 2018 and 2019. The fifth farm location was close to the other four main locations in Friesland, with similar soil type and management regime. The farm followed the same experimental setup as the other four farms, with a control site and a treatment site installed with SSI. At this location, the SSI treatment was enhanced by installing a pressure well connected to the drainage ditch. Water level inside the well could be raised by a pump to provide increased inflow pressure, therefore keeping the groundwater level stable throughout the year (van den Akker et al., 2019). Measurement procedures were in line with the previous experiments. The measurement frequency, however, was significantly lower than in the other locations, with in total less than ten campaigns: once per month during the growing season (April–September) and twice during the non-growing season (in October and November/December) (Supplementary Table S2). Parameter fitting of gap-filling models followed the four methodological Tiers. Drought index was not used as a parameter here, since the drought effect was not as pronounced as in the four main locations due to extra irrigation in 2018. Grass height was used instead of the drought index in the R<sub>eco</sub> model from the Tier two method. Model performances and the gap-filled annual budgets were evaluated and compared. Budget estimates under data scarcity with large gaps to fill could further test the applicability of our framework on different datasets and evaluate the strengths and limitations of each Tier.

## 2.6 Statistics

The effect of gap-filling methodology on annual budget estimation and detection of treatment effects were investigated. Correlation of model performance ratings against the Tier position of gap-filling methodologies was tested by a simple

linear regression. Linear mixed-effects models were fitted using R package *lme4* (Bates et al., 2015) with gap-filled CO<sub>2</sub> fluxes (R<sub>eco</sub>, GPP and NEE) as dependent variables; year, treatment, their interaction and gap-filling methodology as fixed effects; and farm location as random effect. Type III analysis of variance tables of the linear mixed-effects models were computed with Satterthwaite's method using the *anova* function from the R basic package *stats*. The post-hoc Tukey's HSD test was used with R package *emmeans* (Lenth et al., 2020) to further detect significant differences between gap-filling methodologies. To test whether selection of different gap-filling methodology would generate a treatment effect, linear mixed-effects models were also fitted separately for all gap-filling methodologies with annual NEE as dependent variable, year, treatment, and their interaction as independent variables, and farm location as random effect. All data was processed and analyzed using R version 4.0.2 (R Core Team, 2020).

## 3 RESULTS AND DISCUSSION

### 3.1 Model Performances and Annual Budget Estimates

The model performances under different gap-filling strategies improved significantly ( $p < 0.001$ ) with higher complexity (Figure 2, Supplementary Table S3). However, such improvement did not lead to systematic differences among annual CO<sub>2</sub> budget estimates from the four Tiers (Figure 3). In general, all gap-filling strategies resulted in CO<sub>2</sub> emissions situated in the upper range of emissions from productive grasslands on organic soils (Grønlund et al., 2008; Tiemeyer et al., 2016, 2020). Large variances can be observed between the gap-filled annual budgets (Supplementary Table S4) and daily fluxes (Supplementary Figure S2) resulting from different methods. The basic empirical models from Tier one were not suitable for annual parameter estimates (Figure 2) due to limited explanatory power regarding the environmental and temporal variations. Gap-filled daily fluxes showed mild fluctuations without reflections on rapid changing conditions such as harvest. This resulted in significantly larger annual GPP estimates from the Tier one method in 2017 ( $p < 0.001$ , Figure 3). Influence from environmental changes can be accounted for by higher Tier methodologies with either inclusion of additional variables or season-/campaign-specific modeling. For example, inclusion of grass height and the temperature function in Tier two substantially improved GPP estimates in all aspects, which is in close agreement with other studies stressing the importance of accounting for plant growth and harvest (Eickenscheidt et al., 2015; Huth et al., 2017; Kandel et al., 2013). This, however, could lead to drastic fluctuations and contradicting trends in the daily fluxes (Supplementary Figure S2). The lower soil respiration (Davidson et al., 1998) and photosynthetic CO<sub>2</sub> uptake (Fu et al., 2020; Koebsch et al., 2020) under desiccation stress may have been oversimplified by the drought index proposed in our study, leading to unrealistic peaks and dips of the daily fluxes in Tier two and three. Tier three seasonal gap-filling substantially improved the

model performances by circumventing the lack of good predictors for the drought period that altered important drivers of CO<sub>2</sub> fluxes. However, it is more prone to influences of individual high R<sub>eco</sub> measurements under abrupt environmental changes, such as rain-induced soil respiration pulses (Lee et al., 2004; Ma et al., 2012). Such data “outliers” may have confounded the models when fitted seasonally, leading to less representative temperature-respiration relationships, and may have resulted in the significantly higher R<sub>eco</sub> from Tier three comparing to Tier four in 2017 ( $p < 0.05$ , **Figure 3**). Tier four campaign-wise model fitting further reduced model errors (**Figure 2**). The ability of the Tier four campaign-wise method to reflect environmental changes without complicated parameterization demonstrated its robustness and reliability when applied with sufficient measurement frequency. However, it is subject to over-extrapolation, since a narrow measurement range of temperature from a single campaign could introduce bias when extrapolated outside of that range (Hoffmann et al., 2015; Huth et al., 2017). Pooling of all gap-filling results over locations and treatment sites showed an absence of consistently significant differences (**Figure 3**) in spite of the above-mentioned variances. This implies a strong influence from divergence among years and locations. Gap-filling method selection should therefore be considered case-specifically in light of characteristics of the dataset, such as the time scale and frequency of the measurements and abrupt or abnormal environmental changes.

### 3.2 Sensitivity of Treatment Effect to the Choice of Gap-Filling Method

Despite the seemingly large differences between CO<sub>2</sub> budget estimates of treatment and control plots observed in individual farms (**Supplementary Table S4**), we did not find any significant treatment effect when pooling the data of the four locations (**Table 2**). The differences found in individual locations could be due to random variations in the site-specific biotic and/or abiotic processes between treatment and control plots, such as differences in vegetation growth, microbial activities, and GWT fluctuations. These processes could be highly variable due to the complexity of *in-situ* environmental conditions. Statistical results from the pooled data were less likely to be affected by such random effects. Therefore, testing of treatment effects from field trials requires a combination of multiple locations and a longer timespan (e.g., Maljanen et al., 2007; Elsgaard et al., 2012) to avoid confounding factors from site or year differences. Annual budget estimates from a single location are more consistent in representing the magnitude of CO<sub>2</sub> emissions.

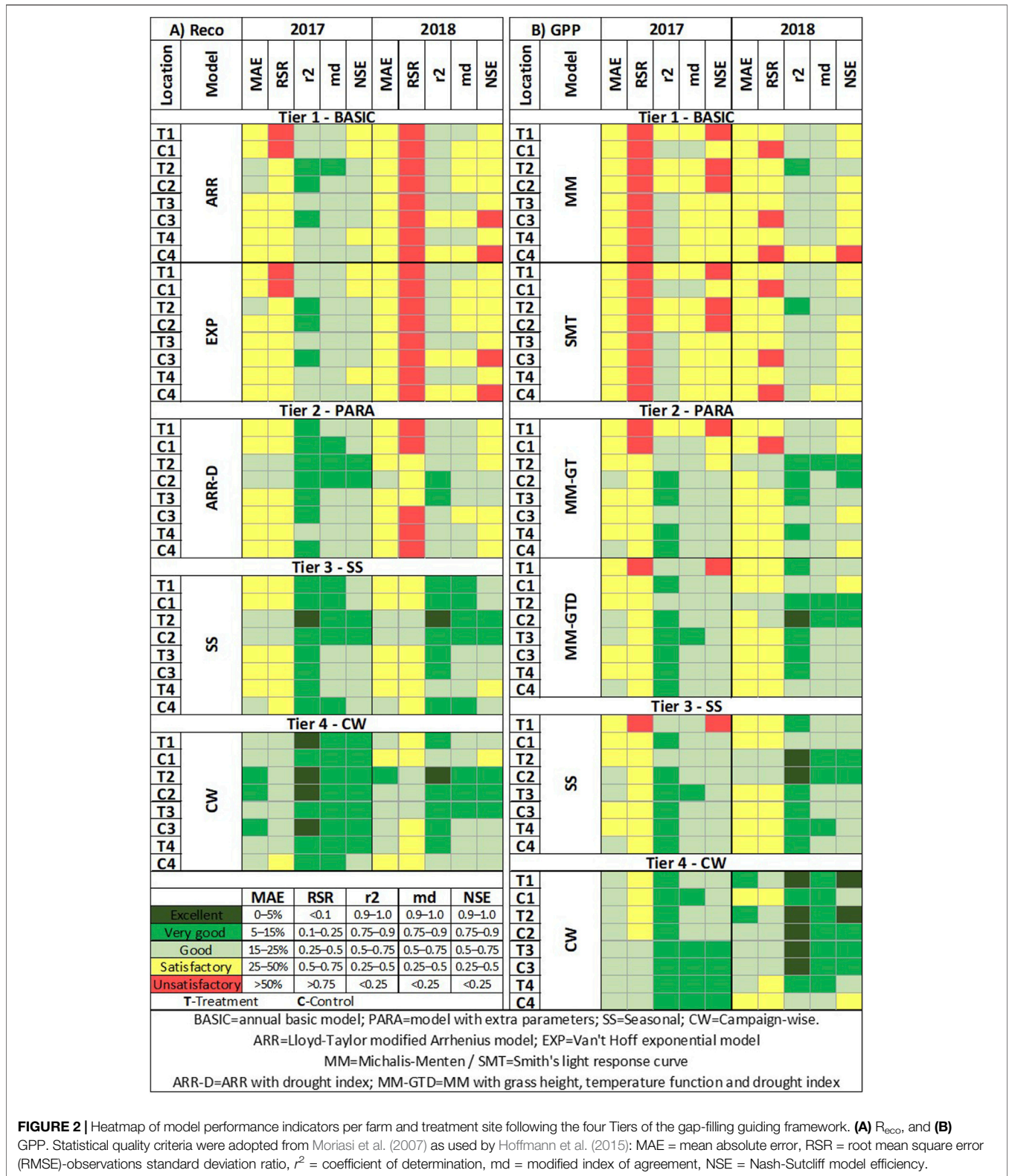
### 3.3 Applicability Demonstration: Gap-Filling Under Data Scarcity

Parameter fitting and gap-filling for the dataset from the fifth farm location was carried out for demonstration purposes, following the methodological Tier list. The low frequency of the measurement campaigns (<10 per year) in this dataset

insufficiently captured the temporal dynamics in CO<sub>2</sub> fluxes. As a result, Tier four campaign-wise gap-filling, although being the most commonly used standard approach, led to high uncertainties and poor fit of gap-filling model parameters (**Table 3**). Tiers containing models with lower temporal complexity at annual or seasonal levels were proven more applicable, as GPP modeling using Tier one (Michaelis-Menten function) and Tier two (Michaelis-Menten function with grass height) resulted in smaller uncertainties of budget estimates (**Table 3**). However, annual R<sub>eco</sub> modeling methodologies from Tier one and two (Arrhenius function and with drought index) resulted in poor or even unsatisfactory performances (**Table 3**), mainly due to the large variances in the raw flux data. The best model performances were achieved by the Tier three seasonal method (**Table 3**). Meanwhile, gap-filled daily fluxes (**Figure 4**) occasionally showed large fluctuations despite the satisfactory error statistics. For example, R<sub>eco</sub> and GPP fluxes from Tiers one, two and four showed potential overestimations due to low representativeness of the dataset in the winter season. Extreme peaks and dips can be observed in the R<sub>eco</sub> fluxes, especially from the Tier four campaign-wise method, showing strong effects of individual high and low measurements when extrapolated over a prolonged time period (Huth et al., 2017). The extremely low R<sub>eco</sub> fluxes observed in summer 2018 from Tier two method can be imputed to the low explanatory power of the drought index leading to unrealistic outputs from the model. The satisfactory model error statistics achieved by Tier three and four methods (**Table 3**) demonstrated the potential of generating annual budget estimates even from scarce data. However, large uncertainties should be acknowledged given the varying behavior of the models throughout the year (**Figure 4**). It is therefore necessary to test multiple gap-filling methods when the quality and quantity of raw flux data is limited. The resulting annual budget estimates should be interpreted with caution, merely as an indication for the order of magnitude of the emissions.

### 3.4 Validation of the Annual Budget Estimates

Given the lack of known true values of carbon budgets for locations in this study, independent validation of the derived CO<sub>2</sub> exchange was not possible. Nonetheless, an indirect cross-validation of derived annual GPP budgets with C-export via biomass harvest was performed (**Figure 5**). A similar validation for R<sub>eco</sub> was not feasible in our analysis due to lack of comparable environmental datasets. In general, Annual GPP showed strong correlation with C-export when pooling data from all five locations and 3 years from 2017 to 2019 ( $p < 0.001$ ,  $R^2 = 0.42$ ). GPP estimates in 2018 ( $p < 0.001$ ,  $R^2 = 0.52$ ) and 2019 ( $p = 0.007$ ,  $R^2 = 0.69$ ) were roughly in agreement with the general trend. Previous meta-analysis from Tiemeyer et al. (2016) gave average values of GPP and C-export from nutrient-rich deep-drained grassland on organic soils overlapping the range of our estimates (**Figure 5**), also indicating realistic estimation of the GPP values. However, GPP estimates in 2017 showed poor correlation with C-export values ( $p = 0.598$ ,  $R^2 \sim 0$ ) and strong

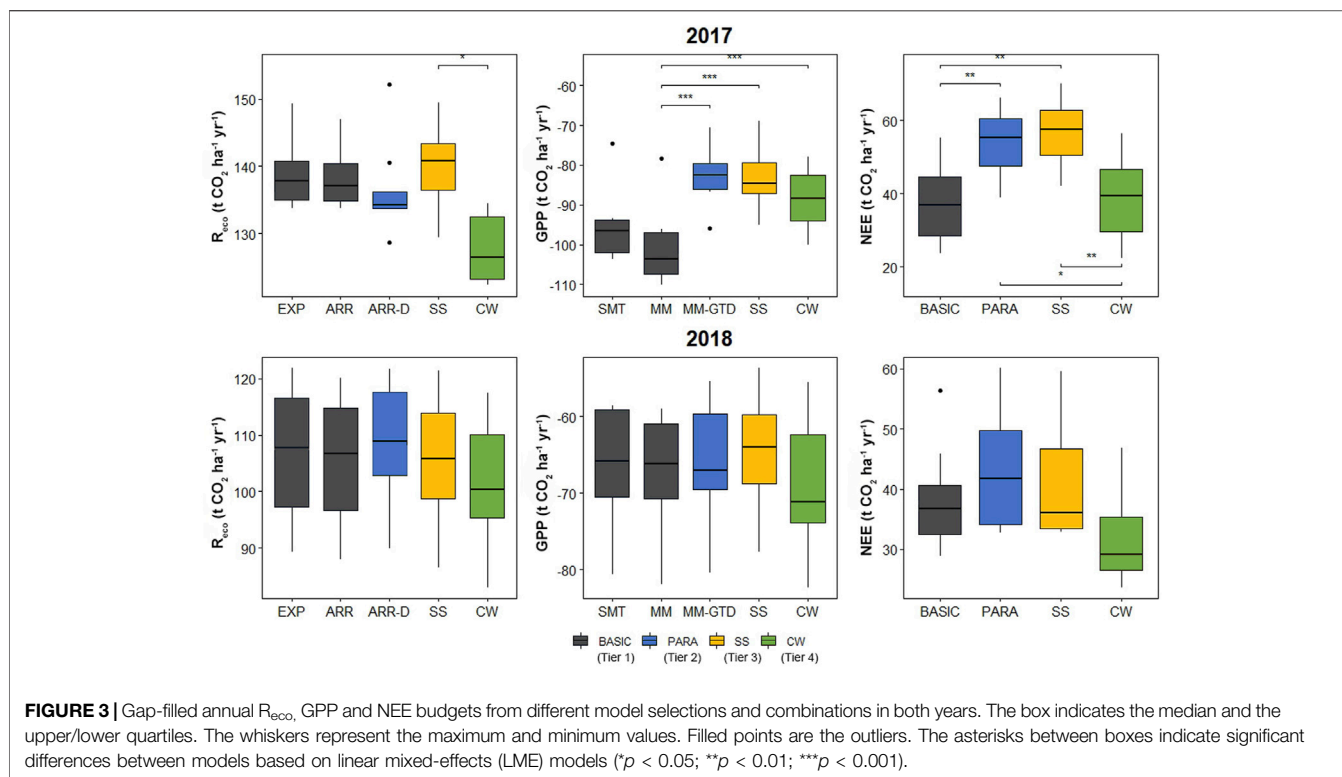


**FIGURE 2 |** Heatmap of model performance indicators per farm and treatment site following the four Tiers of the gap-filling guiding framework. **(A)** Reco, and **(B)** GPP. Statistical quality criteria were adopted from Moriasi et al. (2007) as used by Hoffmann et al. (2015): MAE = mean absolute error, RSR = root mean square error (RMSE)-observations standard deviation ratio, r<sup>2</sup> = coefficient of determination, md = modified index of agreement, NSE = Nash-Sutcliffe model efficiency.

deviation to the general trend, especially with results from the Tier one method. This is in accordance with the significant overestimation of Tier one GPP values identified (Section 3.1,

Figure 3), and is reflected in the Tier one daily fluxes (Supplementary Figure S2) that failed to represent changes of CO<sub>2</sub> exchange due to plant biomass growth and removal.





**FIGURE 3 |** Gap-filled annual  $R_{eco}$ , GPP and NEE budgets from different model selections and combinations in both years. The box indicates the median and the upper/lower quartiles. The whiskers represent the maximum and minimum values. Filled points are the outliers. The asterisks between boxes indicate significant differences between models based on linear mixed-effects (LME) models ( $*p < 0.05$ ;  $**p < 0.01$ ;  $***p < 0.001$ ).

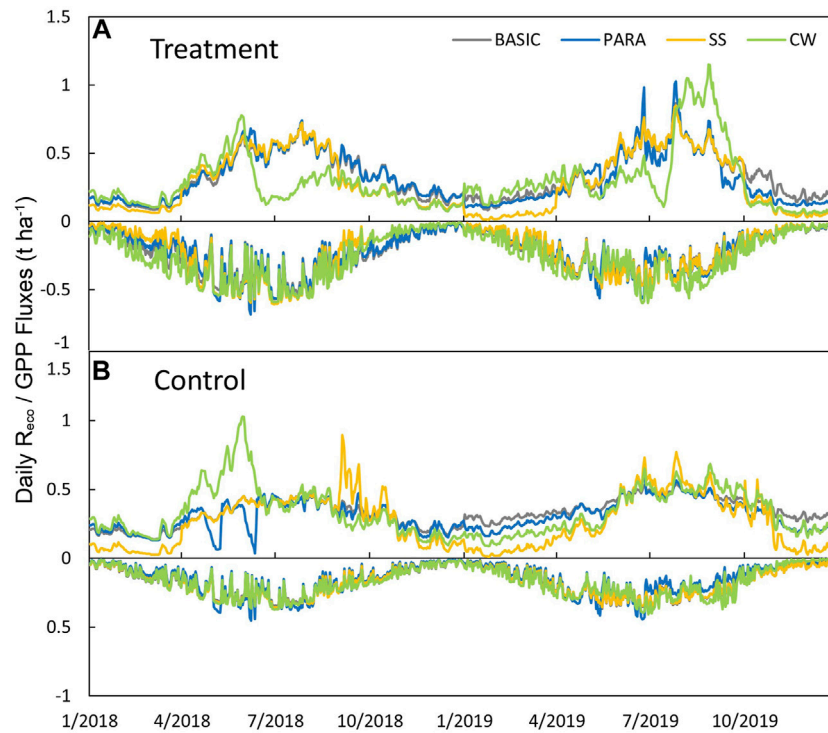
**TABLE 3 |** Annual CO<sub>2</sub> budgets of the fifth farm location as a demonstration of the framework applicability. Data are CO<sub>2</sub> budget estimates in t ha<sup>-1</sup> yr<sup>-1</sup> (±SD). C-export was translated from grass yield in t CO<sub>2</sub>-eq ha<sup>-1</sup> yr<sup>-1</sup>.

	Year	2018		2019	
		SSI	Control	SSI	Control
Reco	Tier 1—BASIC	118.2 (±10.1)	107.2 (±7.4)	124.2 (±6.5)	136.6 (±9.7)
	Tier 2—PARA	121.8 (±10)	103.8 (±6.9)	111.2 (±4.4)	121.1 (±9.6)
	Tier 3—SS	105.9 (±4.8)	96.3 (±4.2)	100.4 (±3.5)	95 (±5.4)
	Tier 4—CW	91 (±13.2)	124.5 (±7.1)	116.8 (±16.3)	118.1 (±20.1)
GPP	Tier 1—BASIC	-80.5 (±4.5)	-61.7 (±3.5)	-77.2 (±2.6)	-63.6 (±2.6)
	Tier 2—PARA	-72.3 (±3.2)	-57.6 (±4.1)	-72.2 (±2)	-53.9 (±2.2)
	Tier 3—SS	-75.4 (±4.6)	-61.1 (±3.3)	-76.3 (±2.4)	-63.7 (±3)
	Tier 4—CW	-78.6 (±17.9)	-62.2 (±35.3)	-89.1 (±13.5)	-62.8 (±11.1)
NEE	Tier 1—BASIC	37.6 (±11.1)	45.5 (±8.2)	47 (±7)	73 (±10.1)
	Tier 2—PARA	49.5 (±10.5)	46.3 (±8.1)	39 (±4.8)	67.2 (±9.8)
	Tier 3—SS	30.5 (±6.7)	35.2 (±5.3)	24.1 (±4.2)	31.2 (±6.2)
	Tier 4—CW	12.4 (±22.2)	62.2 (±36)	27.7 (±21.1)	55.3 (±22.9)
	C-export	16.2	12.1	18.0	10.7

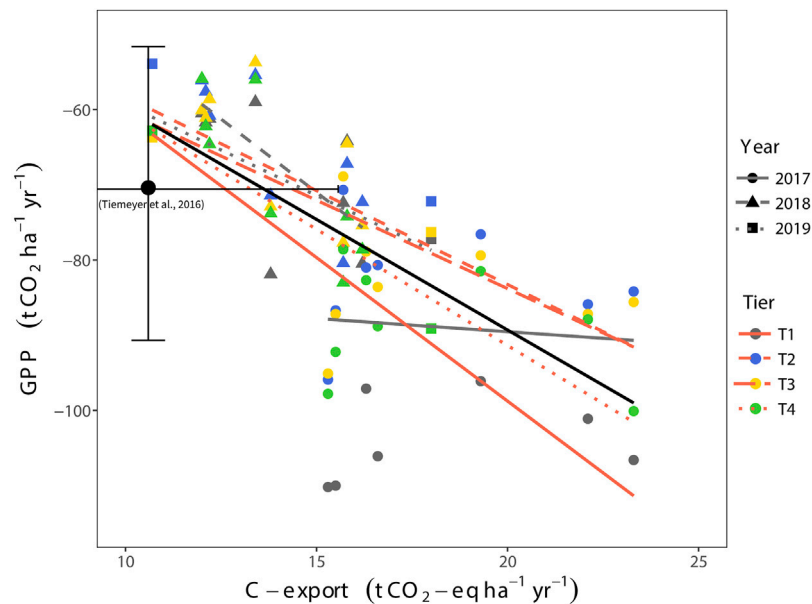
Tier 1—BASIC = annual basic model; Tier 2—PARA = model with extra parameters; Tier 3—SS = seasonal; Tier 4—CW = Campaign-wise. Colour of the cells represents model performances, following legend of **Figure 2** (red—unsatisfactory, yellow—satisfactory, light green—good, dark green—very good), adopted from Moriasi et al. (2007) as used in Hoffmann et al. (2015).

Accuracy of GPP estimates in 2017 should therefore be given low confidence. Within-day timing and frequency of the measurements (Huth et al., 2017; Gana et al., 2018; Järveoja et al., 2020) could also be a cause of this low accuracy. Our midday measurements at a fixed timeframe in 2017 resulted in poor coverage of different PAR ranges. Meanwhile, results from the four Tiers all showed strong correlation with C-export ( $p < 0.01$ ,  $R^2 = 0.38-0.43$ ) when tested separately, including the Tier one

method that also produced GPP values in good agreement with the GPP~C-export correlation in 2018 and 2019 (**Figure 5**). Therefore, the general feasibility of all four method Tiers can be concluded. However, Tiers one and two methods are more prone to bias when analyzing raw flux datasets with poor representativeness for the environmental conditions and management events, leading to potentially large variations in the GPP estimates.



**FIGURE 4** | Gap-filled daily summed CO<sub>2</sub> fluxes ( $R_{\text{eco}}$  and GPP are depicted as the positive and negative values, respectively) from different models at **(A)** treatment and **(B)** control site of the demonstration location 5.



**FIGURE 5** | Indirect validation by comparing derived annual GPP with C-export per method Tier and year. The black solid line is the result of general linear regression of the entire dataset ( $p < 0.001$ ,  $R^2 = 0.42$ ). Grey lines are regression lines per year (2017,  $p = 0.598$ ,  $R^2 = 0$ ; 2018,  $p < 0.001$ ,  $R^2 = 0.52$ ; 2019,  $p = 0.007$ ,  $R^2 = 0.69$ ). Red lines are regression lines per method Tier (Tier one,  $p = 0.002$ ,  $R^2 = 0.42$ ; Tier two,  $p = 0.002$ ,  $R^2 = 0.43$ ; Tier three,  $p = 0.002$ ,  $R^2 = 0.042$ ; Tier four,  $p < 0.001$ ,  $R^2 = 0.38$ ). Black point with error bars represents average values of GPP and C-export from nutrient-rich deep-drained grassland adopted from Tiemeyer et al. (2016).

Better estimates of carbon pools including plant biomass could serve as a valid data source for indirect cross-validation. For example, a process-based growth model for plant biomass could

better correlate with the derived GPP values by avoiding uncertainties introduced by the harvest practice. However, such models are normally parameterized only for mineral soils

and requires extensive growth data for local calibration (e.g., Barrett et al., 2005). Long-term carbon fluxes monitoring can also be cross-validated with soil carbon pool. Hoffmann et al. (2017) validated chamber-derived net ecosystem carbon balance by resampling of soil organic carbon. Net carbon losses could be proxied by monitoring soil subsidence (Couwenberg and Hooijer, 2013), while such estimated emissions are highly uncertain due to the complicated processes involved in soil surface changes including the oscillation of peat soil (Fritz et al., 2008).

It is still challenging to sufficiently validate chamber-based annual budgets estimates given the limitations of the above-mentioned indirect validation approaches. Paired comparison of the discrete manual chamber fluxes with continuous flux measurements from eddy-covariance and automatic chamber techniques could potentially enable independent validation of the gap-filling methods and budget estimates. Lucas-Moffat et al. (2018) presented highly correlated fluxes between manual chamber and eddy-covariance fluxes from a cropland. Meanwhile, Cappoci and Vargas, (2022) discovered up to 60% underestimation of annual CO<sub>2</sub> efflux by manual chamber compared to automatic chamber in a tidal marsh. More continuous measurements with higher resolution in long term are needed for the improvement of the validation and therefore the refinement of the gap-filling methods. An ongoing year-round automatic chamber measurement including farm locations of this study (Erkens, 2020) could provide opportunities for robust cross-validation of the gap-filling approaches in the near future. However, not without acknowledgement of the specific shortcomings in each method. For example, while manual chamber provides low temporal resolution and lack of night-time fluxes; eddy-covariance measurements have a variable footprint and insufficient energy closure; automatic chambers could lead to heating up to the vegetation and upper soil layer, and are subject to disturbance of the precipitation/evapotranspiration process. Therefore, our statistical comparison provides insights for the selection of available gap-filling methods to meet the growing number of chamber measurements as well as the need to derive more annual carbon balances in drained peatlands. Despite the fact that a “best” approach could not be identified.

## 4 CONCLUSION AND IMPLICATION

In this study, we summarized the most commonly-used empirical models of R<sub>eco</sub> and GPP for gap-filling manual chamber-based CO<sub>2</sub> flux into a framework of four Tiers with increasing model complexity. Model performance of the methods from the four Tiers were systematically compared in terms of error statistics. The annual CO<sub>2</sub> exchange was in the same order of magnitude with values from literature on similar ecosystems. Detection of treatment effects requires large number of independent observations (locations) and longer period of time (years) to reduce its sensitivity to random variances. Indirect validation of GPP estimates showed good agreement with the GPP~C-export correlation, except for the year 2017. However, without independent validations using high-resolution long-term continuous flux measurements, the true precision of the methods cannot be discussed but are better suited to determine only the magnitude

of the annual CO<sub>2</sub> budgets. Nonetheless, specific recommendation could be given for each Tier supporting the selection of suitable methods:

1) Tier one annual basic gap-filling is feasible when higher model complexity is not possible due to deficiency of data required for model input or a low number of measurements. However, Tier one models are not likely to provide robust parameter fitting in most cases, because the variance in CO<sub>2</sub> fluxes cannot be sufficiently explained by the limited number of explanatory variables in the models. 2) Tier two methodology introduces higher structural complexity with additional parameterization but remains temporally simple with annual parameter fitting. Robustness of such models depends on the explanatory power of the included variables as well as the representativeness and frequency of the flux measurements. However, the number of variables should be limited to avoid overfitting. 3) Tier three seasonal gap-filling has a moderate overall complexity. It is a potential solution in situations where representativeness of data is an issue, such as with low measurement frequency. The definition of the seasons used to cluster the data is essential when accounting for the unexplained temporal variation in CO<sub>2</sub> fluxes. 4) Tier four campaign-wise gap-filling represents the highest temporal complexity by fitting simple relations per measurement campaign. It is the most commonly used procedure in chamber-based CO<sub>2</sub> fluxes studies, and the most reliable way of gap-filling when data is adequately available. However, the risk of over-extrapolation should be considered in case the range in temperature or PAR is limited in single measurement campaigns.

Besides in the gap-filling of CO<sub>2</sub> fluxes from drained temperate peatlands, similar empirical models of R<sub>eco</sub> and GPP have been applied also on cropland (e.g., Struck et al., 2020), forest (e.g., Zhao et al., 2020), and tropical peatlands (e.g., Hirano et al., 2014; Gana et al., 2018) with consideration of influences of temperature, groundwater table and plant phenology. The Tier system following an increased model structural and temporal complexity proposed in this study is potentially applicable to these other ecosystems. For example, CO<sub>2</sub> and CH<sub>4</sub> fluxes from waterbodies can show clear correlations with temperature and water chemistry indicators, and display seasonal differences (Peacock et al., 2021). All in all, the Tier system can provide opportunities in the modeling of various greenhouse gasses in a multitude of ecosystems, though empirical relationships and independent environmental variables should be considered.

## DATA AVAILABILITY STATEMENT

The raw data, intermediate results, and R scripts that support the findings of this study are openly available on the DANS platform at <https://doi.org/10.17026/dans-xtq-ajzs>.

## AUTHOR CONTRIBUTIONS

WL designed the methodology, performed the formal analysis and drafted the manuscript. CF conceived and supervised the study. WL and SW collected and processed the data. All authors

contributed to the review and editing of the manuscript and approved the final version.

## FUNDING

WL is supported by the China Scholarship Council (201706350201). The work of MV is funded by NWO-Veni grant 202.053. MB and CF received funding through PEATWISE (NWO ALW-GAS No.4). This research was supported by Interreg-NWE Carbon Connects.

## ACKNOWLEDGMENTS

We would like to thank all technical staff, students and volunteers who helped in the field and in the laboratory, as well as the

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- landowners who granted access to the measurement sites. Specifically, we are grateful for the help of Sebastian Krosse, Paul van der Ven, staff from the General Instrumentation and Roy Peters for the chemical analyses. We appreciate Reinder Nouta from Wetterskip Fryslân for insightful discussions on the flux data. We acknowledge Peter Crujisen for his assistance in fieldwork and analyses. We sincerely thank the editor and reviewers for their critical remarks that helped improving the manuscript.

## SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fenvs.2022.803746/full#supplementary-material>

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