Modelling time-integrated fluxes of CO_2 and CH_4 in peatlands: A review

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SUMMARY

There is widespread interest in estimating annual carbon dioxide (CO_2) and methane (CH_4) budgets for peatlands using data collected from flux chambers. Flux-chamber measurements are a snapshot of the conditions on a particular site and may not adequately represent fluxes between measurements. However, these measurements can be used in simple models to estimate time-integrated fluxes of CO_2 and CH_4. This paper reviews modelling approaches used for estimating such time-integrated fluxes and provides what we hope is a 'one-stop-shop' for new researchers, such as PhD students, considering using such models. The review is written for those with a non-mathematical background.

KEY WORDS: flux chambers, models, peatland-atmosphere greenhouse gas exchanges, time integration

INTRODUCTION

Peatlands are important global carbon (C) stores (e.g. Yu 2011), and there is widespread interest among peatland scientists in estimating peatland-atmosphere fluxes of the C gases carbon dioxide (CO_2) and methane (CH_4), and in budgeting for these gases on an annual timescale (see, e.g., Olson *et al*. (2013) and Meng *et al*. (2016) who edited a special issue on the topic in the journal *Environmental Research Letters*). Such budgeting is relatively straightforward when fluxes are estimated using flux tower methods, such as eddy covariance, because measurements are made continuously throughout a year (e.g. Levy & Gray 2015). Flux tower methods tend to apply to reasonably large spatial scales, typically linear scales of several tens of metres or more. While useful for estimating whole-peatland C budgets, these methods are less useful for revealing controls on C budgets at smaller spatial scales. For example, there is interest in how different peatland microhabitats, such as pools, hollows, lawns, and hummocks/ridges (Belyea & Clymo 2001, Laine *et al*. 2006), compare in terms of CO_2 and CH_4 uptake and release and what controls smaller-scale variability in C fluxes (Laine *et al*. 2006). At these smaller scales, flux chambers are usually used to measure fluxes (see Alm *et al*. (2007) and Denmead (2008) for details). Flux chamber measurements are typically made weekly or fortnightly, although higher frequencies are sometimes used (Waddington & Roulet 1996, Dinsmore *et al*. 2010; Baird *et al*. 2010; Moore *et al*. 2011; Dooling *et al*. 2018). Flux-chamber measurements represent a snapshot of the conditions on a particular site. Net CO_2 exchanges, for example, vary over time with solar irradiance and other environmental variables (e.g. soil temperature and water table). Therefore, a chamber measurement of CO_2 flux at a particular time of day will typically be a poor reflection of net CO_2 exchange at other times on that day or of the period until the next chamber measurement. To estimate fluxes and net exchanges for the hours and days between measurements, it is necessary to use models that relate net CO_2 exchange (net ecosystem exchange – *NEE* – see next section), or its components, to solar irradiance and environmental variables, such as soil temperature, water-table position, and vegetation composition and vigour. It is also necessary for these other supporting variables to be measured at a high frequency throughout the year, so that the flux model can also be applied across the year to provide an annual estimate of CO_2 exchanges.

This paper arose through a realisation that there is no 'go-to' review in which different flux models are described and explained and their relative merits discussed. From discussions with first-year PhD students, we also became aware that a review that assumed only a basic mathematical background (up to basic calculus) on the part of the reader would be very welcome. Therefore, in the review that follows, it has been assumed that readers have a maths

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background typical of that of a competent 16-year old, with familiarity of basic mathematical operations and concepts including exponentiation and logarithms. We have further assumed that readers have been taught introductory statistics at university, including regression and model fitting. In writing the paper, we were aware of the dangers of trying to consider all, or most, of the papers in which C flux models have been applied to peatlands. Although there is merit in undertaking a systematic review of peatland C-flux studies, we were keen to keep the original purpose of the paper in sight. Thus, we have not tried to provide a comprehensive list of papers in which particular models have been used; rather, our aim has been to describe and discuss the main models in use and to cite *examples* of studies that have used these models. We hope authors of papers that we have not cited forgive us.

MODELLING CO_2 EXCHANGE

Net ecosystem exchange (*NEE*)

Net ecosystem exchange (*NEE*) – defined as the net CO_2 exchange between a peatland and the atmosphere – can be divided into two components: gross photosynthesis, P_G (M L^{-2} T^{-1} or mass of CO_2 per unit area per unit time)[1], and ecosystem respiration, R_T (dimensions and units as for P_G). *NEE* is given by

$$NEE = P_G + R_T \quad [1]$$

so that

$$P_G = NEE - R_T \quad [2]$$

In Equations [1] and [2], P_G is negative (indicating uptake by the peatland) and R_T positive (indicating release from the peatland). Therefore, *NEE* will be negative (net uptake) when the absolute magnitude of P_G exceeds that of R_T. P_G is defined as the rate of total CO_2 uptake during light conditions by photosynthesising organisms and is sometimes called the 'real' or 'true' photosynthesis (Mohr & Schopfer 1995). R_T is the sum of all respiration taking place in the system and comprises decomposition processes in the soil (heterotrophic respiration) and root, shoot, and leaf respiration (autotrophic respiration). If a flux chamber contains all of the vegetation canopy, R_T may be estimated using data from a dark test (one where the flux chamber is shrouded and all *I* excluded), while *NEE* is measured in a light chamber test. Different authors use different terms to describe the same thing and it is worth being aware that P_G is also denoted *GP* or called gross primary production/productivity (*GPP*), while R_T is also often denoted using R_{eco}, *ER* and E_R.

Modelling gross photosynthesis (P_G)

In most papers, *NEE* is modelled by considering P_G and R_T separately. P_G is almost always described using a model of the following form:

$$P_G = \frac{Q \times I}{k + I} \quad [3]$$

or

$$P_G = \frac{Q \times I}{k + I} \times X_1 \times X_2 \times \ldots \times X_n \quad [4]$$

The quotient on the right-hand side of Equation [3] produces a rectangular hyperbola as shown in Figure 1 and is of the same form as the well-known Michaelis-Menten curve used to describe enzyme kinetics (Johnson & Goody 2011). In Equation [3], *Q* may be thought of as an asymptotic limit[2] of P_G, *I* is irradiance (W m^{-2} – dimensions of M T^{-3})[3], and *k* is the so-called half saturation constant (units as for irradiance) and affects the shape of the relationship between P_G and *I* (the rate at which the curve approaches its asymptote). *Q* is also commonly referred to as GP_{max} (theoretical maximum gross photosynthesis). Equation [3] has been extended by many authors by adding factors to the right of the quotient (i.e. X_1, X_2, … , X_n) (Equation [4]). These factors are environmental variables, such as the cover of different plant types (see **EXAMPLE MODEL APPLICATIONS** below), water-table depth, and air or soil temperature. The introduction of these means that *Q* alone, no longer defines the asymptotic limit of P_G.

Equation [3] has been widely used in peatland

[1] All physical quantities can be expressed in terms of their fundamental dimensions, where M is mass, L is length, T is time, Θ is absolute temperature, and N is amount (countable units). These symbols should always be presented in normal case, not italics, and not bold. Each dimension may have different *units*. L, for example, may be given in m or cm.

[2] An asymptote is the straight line to which some functions approach but never reach. For example, the exponential function $y = e^{-a \times x}$ (or $y = 1/(e^{a \times x})$), where *e* is base of the natural logarithm (or Euler's (pronounced 'oil-er') number) (2.71828...) and *a* is a constant, has as its asymptote $y = 0$; i.e., as *x* increases, the value of the function gets closer to, but never reaches, 0.

[3] Irradiance may also be expressed as a photon flux density (PFD), with units of mol m^{-2} s^{-1} and dimensions of N L^{-2} T^{-1}. PPFD is the photosynthetic photon flux density and is equivalent to PAR (photosynthetically active radiation).

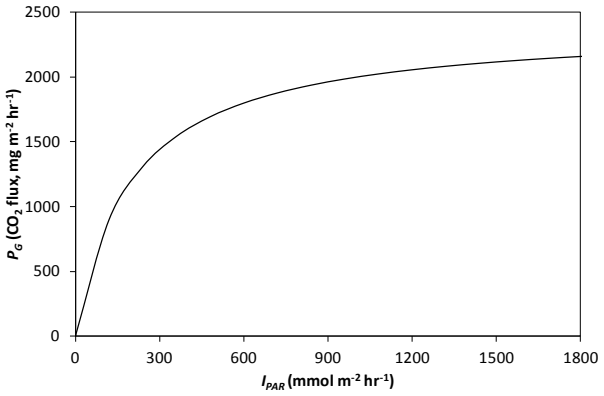

Figure 1. Example response of gross photosynthesis (P_G) to changes in solar irradiance. The curve shown is based loosely on data (July to August) reported in Tuittila *et al*. (1999) for an *Eriophorum vaginatum* L. tussock in a restored bog in southern Finland (their Figure 4a). I_{PAR} is photosynthetically active irradiance (see Equation [5]). Note that for the purposes of plotting, P_G has been given as positive values.

studies and is a two-parameter model – the parameters being Q and k – and can be fitted to data using a form of non-linear regression (e.g. Tuittila *et al*. 1999, Samaritani *et al*. 2011). Model error may be estimated as the sum of the squared differences between the modelled and observed P_G values (see **EXAMPLE MODEL APPLICATIONS** below). This sum may be minimised by altering the values of Q and k using a numerical optimisation tool such as Solver, which is available as a Microsoft Excel add on. Non-linear regression can be carried out in most statistical packages, including R (e.g. the 'nls.multstart' R package written by Padfield & Matheson (2018)).

Equation [3] comes in a range of guises. A version that is widely used among North American and European research groups working on a range of peatlands and organic (tundra) soils (e.g. Whiting *et al*. 1992, Whiting 1994, Waddington & Roulet 1996, Bellisario *et al*. 1998, Bubier *et al*. 1999, Drösler 2005, Veenendaal *et al*. 2007, Elsgaard *et al*. 2012, Beetz *et al*. 2013, Hoffmann *et al*. 2015, Vanselow-Algan *et al*. 2015) is

$$P_G = \frac{Q \times a \times I_{PAR}}{(a \times I_{PAR}) + Q} \qquad [5]$$

where I_{PAR} is photosynthetically-active radiation and a is the initial slope between P_G and I_{PAR}. Equation [5] is missing the environmental factors (X_1, X_2, … , X_n) to the right of the quotient seen in Equation [4], and the quotient itself looks superficially somewhat different from that in Equation [3]. However, the right-hand side of [5] yields the quotient in [3] if the numerator and denominator are divided by a, to give

$$\frac{Q \times I_{PAR}}{I_{PAR} + \frac{Q}{a}} \equiv \frac{Q \times I_{PAR}}{k + I_{PAR}}, \text{ where } k = \frac{Q}{a}.$$

The origin of the rectangular hyperbola as a model for P_G for a vegetation canopy is unclear. Whiting *et al*. (1992) may have been the first to use it in the form given here, but Whiting (1994) suggests the model is based on Hilbert *et al*. (1987). Ultimately, the model is derived from the empirical, non-rectangular hyperbola model of leaf photosynthesis (e.g. Thornley 1998); it is a special case and simplification of that model.

Many plants and vegetation types conform reasonably well to the relationship given in Equation [3] (or its equivalent – Equation [5]). However, the equation may not always be appropriate. Photo-inhibition has been observed in Sphagna and may cause the relationship between P_G and irradiance to vary over time and to depart from a rectangular hyperbola. For example, Murray *et al*. (1993) investigated photo-inhibition in Sphagna in both field and laboratory experiments; *Sphagnum* plants exposed to high-light conditions, even for short periods of time (48 hours), showed reduced photosynthetic capacity for periods of at least two weeks thereafter. Hájek *et al*. (2009) also studied photo-inhibition in a range of Sphagna growing under different circumstances and found that photo-inhibition could explain the lower photosynthetic capacity of Sphagna growing in full-light (open mire) compared to the shade under shrubs and trees. Hájek *et al*. (2009) assumed that Equation [3] (or Equation [5]) is appropriate for describing P_G *vs I*, but did not consider temporal changes in the relationship in the same way as Murray *et al*. (1993). It is possible that, for sites that have a high cover of *Sphagnum*, Equation [3] (Equation [5]) will not apply in a simple manner over the course of a growing season. It is possible too that the parameters in Equation [3] (Equation [5]) may change for other plant types, such as *Eriophorum* spp. depending on the growth phase through the summer. Bellisario *et al*. (1998), for example, found that a (Equation [5]) generally declined during the growing season at their sites, which ranged from a low-shrub rich fen to permafrost collapse bog. To account for seasonal changes in a and Q, recent studies have applied Equation [5] on a campaign basis where multiple chamber measurements have been carried out on each day. For

example, Beetz *et al.* (2013) conducted up to 72 light chamber tests and 42 dark chamber tests per measurement day across three locations, allowing a P_G model to be developed for each day. From this group of models, parameters were linearly interpolated between measurement campaigns and fluxes calculated on an hourly basis from continuous environmental data (see **INTRODUCTION**). Although it would be desirable to conduct multiple measurements per chamber location per day, the logistical demands of doing so are considerable and Equation [5] (Equation [3]) is usually applied to datasets comprising data from chamber tests taken over several seasons or even several years. Despite the problem of possible changes in parameter values across a year, there does not seem to be an obvious simple alternative to Equation [3] (Equation [5]) when the approach adopted by Beetz *et al*. (2013) is not feasible. Therefore, we suggest using the equation as a first 'port of call' and then assessing its suitability (see **EXAMPLE MODEL APPLICATIONS** below). In addition, a number of research groups have introduced a factor to the model that captures phenological changes in vegetation over the season and this is discussed below.

Bubier *et al*. (1999) note that the relationship between P_G and I may change during a season and suggest it can be accounted for by adding a phenological or seasonality factor to the rectangular hyperbola model (i.e. one of the X factors in Equation [4]). The factor is given by T_m/T_s where the numerator is the seven-day running mean of the soil temperature at a depth of 5 cm, while the denominator is the seasonal average soil temperature at the same depth. Bubier *et al*. (1999) suggest this expression can take values only from 0 to 1, although this seems to be incorrect, because the seven-day running mean must sometimes exceed the seasonal average to give values greater than 1. However, it's clear that the value of the expression will rise and fall through the season representing the increase and subsequent decrease in photosynthetic activity as new leaves form, as the plants reach maximal green leaf area, and as the leaves senesce towards the end of summer. A similar approach has been adopted by Alm *et al*. (1997) and Tuittila *et al*. (1999) who used a factor called the effective temperature sum index or *ETI*. *ETI* is the ratio of the cumulative temperature sum to the number of temperature sum days. Mathematically, the *ETI* is given by

$$ETI_j = \left(\sum_{i=1}^{j} \overline{T}_{air,i} \right) \Big/ j \qquad [6]$$

where j is the day of interest (counted from the first day when the five-day moving average air temperature exceeds a threshold temperature), $\overline{T}_{air}$ is daily-average air temperature (°C) and i is day number. Tuittila *et al*. (1999) note that a threshold temperature has to be reached before the *ETI* is calculated, and estimated *ETI* only for that part of the year (for a site in southern Finland) when the five-day moving average air temperature was over 5 °C. The assumption of such a threshold is that plants senesce or become dormant below it and do not photosynthesise.

As an alternative to the temperature-based approach of Bubier *et al*. (1999) and Tuittila *et al*. (1999), vegetation metrics can be introduced as a factor in a modified form of Equation [3] (Equation [5]) to account for seasonality in the relationship between P_G and I. For example, the foliar (above-ground) biomass of vascular plants (f_b) was used by Burrows *et al.* (2005), as follows:

$$P_G = \frac{b \times f_b \times a \times I_{PAR}}{(a \times I_{PAR}) + (b \times f_b)} \qquad [7]$$

where b is a parameter and $b \times f_b$ is substituted for Q (Equation [5]). Somewhat similarly, Görres *et al.* (2014) used a ratio vegetation index (*RVI*) to provide a measure of actively-growing green biomass and included it in the same way f_b is included in Equation [7]. The inclusion of *RVI* in the P_G model generally improved the model fit, compared with using only the light response model (Equation [5]). However, annual estimates were not significantly altered with the inclusion of *RVI* due to the high uncertainties of the models (Görres *et al.* 2014). Wilson *et al*. (2007) used a version of Equation [4] that included vascular green area (VGA) as a factor. Based on measurements from a range of vascular plant species found on peatlands, they represented the seasonal variation of VGA in Equation [4] and found that the equation gave substantially better predictions of P_G than the basic model (Equation [3]) alone. An alternative approach is to develop separate relationships between P_G and I or I_{PAR} for the 'pre-green', 'green', and 'post-green' periods of the season. An example of this simpler approach is Waddington *et al*. (2010) who used the non-rectangular hyperbola model (see discussion after Equation [5] above).

There is increasing interest in measuring CO_2 and CH_4 fluxes in drained peatlands used for agriculture, such as the East Anglian Fens in the UK (Peacock *et al*. 2019). In these systems, the concept of P_G needs modification because P_G may not be added to the peatland as plant litter but instead removed as a crop and then consumed, with the CO_2 that was taken up

by the crop returning rapidly to the atmosphere. However, P_G in terms of root and below-ground tissue production may be important in the peatland C balance. In addition, crop cycles (e.g. for crops such as lettuce) may be so short (< 4–6 weeks) that it is not possible to develop robust models for the seasonal integration of P_G. Recent studies on peatlands used for cropland have overcome this problem by (a) taking multiple measurements per chamber location per day to capture the full range of I_{PAR} and temperature, and (b) modelling P_G on a measurement-day basis (e.g. Elsgaard *et al.* 2012, Beyer *et al.* 2015). Nevertheless, such work can be very time-consuming and expensive, as discussed above (this section), and it may be better to use root in-growth tubes/bags or mini-rhizotrons as alternative methods for estimating below-ground production (e.g. Finér & Laine 2010, Iversen *et al*. 2012).

Finally, it is worth noting that a time-efficient approach to developing relationships between P_G and I or I_{PAR} is to take multiple chamber measurements within a short period of time using calibrated shrouds. These are placed over the chamber to reduce I or I_{PAR} in set steps (e.g. Whiting, 1994). For example, within 30–60 minutes it is possible to obtain estimates of P_G from ambient I or I_{PAR} down to light levels that represent dawn or dusk (as noted above, a chamber test where all light is excluded – a dark chamber test – provides an estimate of R_T – see **Net ecosystem exchange (*NEE*)**). However, soil and air temperatures will tend to be similar or the same for the different values of I or I_{PAR} experienced during the steps, potentially making it difficult to fit Equation [4] to the data. In other words, it is still useful to collect P_G data for a range of environmental conditions and not just a range of values of I or I_{PAR} on one or a few occasions.

Modelling ecosystem respiration (R_T)

When considered separately, R_T is often modelled using multiple regression where R_T or its logarithm is expressed as a function of environmental and vegetation-related variables (plant abundance and growth stage). An example is the following equation from Tuittila *et al*. (1999):

$$\ln(R_T) = a + (b_1 \times EV) + (b_2 \times T_{soil,5}) + (b_3 \times WT) + (b_4 \times ETI) + (b_5 \times EV \times WT) \quad [8]$$

where *ln* denotes the natural logarithm, *EV* is the cover of *E. vaginatum*, $T_{soil,5}$ is soil temperature at 5 cm below the ground surface (°C), *WT* is water level[4] (assigned negative values by Tuittila *et al*. (1999) when below the surface, meaning that b_3 must also be negative for R_T to increase as water tables deepen) (cm), *ETI* is the effective temperature sum index (see Equation [6] above), and a and $b_{1\text{-}5}$ are regression parameters. Equation [8] also includes an interaction term involving *EV* and *WT*. Tuittila *et al*. (1999) studied a regenerating cutover bog on which *E. vaginatum* had re-established. Samaritani *et al*. (2011) used a similar modelling approach to Tuittila *et al*. (1999). However, although they worked on a similar type of site to Tuittila *et al*. (1999), they included only water level, soil temperature at a depth of 30 cm ($T_{soil,30}$) and air temperature (T_{air}) as explanatory variables. The adjusted r^2 of the R_T models was variable across both studies and ranged between 0.45 and 0.84. In other studies, all on peatland or tundra sites, a variety of R_T models have been used and these are considered below.

Bubier *et al*. (1999) modelled R_T using a version of Equation [8] in which the second, fourth, fifth and sixth terms were omitted, i.e.:

$$ln(R_T) = a + (b \times T_{soil,5}) \quad [9]$$

They found that $T_{soil,5}$ was co-linear with water level and that the latter did not add any additional explanation (in the statistical sense) to the model. Equation [9] is the simple exponential formula. If we let both sides of the equation be exponents of e, the base of the natural logarithm (see footnote 2), we have:

$$R_T = e^{a+(b \times T_{soil,5})} \equiv e^a \times e^{(b \times T_{soil,5})} \equiv c \times e^{g \times T} \quad [10]$$

The version of the equation to the far right is simply a generic form of the exponential equation with two parameters – c and g – which in this instance are, respectively, equal to e^a and b. In this equation, when T = 0 °C, the value of $e^{g \times T}$ is 1, so that $R_T = c$. Hence, c is simply R_T when T = 0 °C. g (or b) controls the exponential gradient and, therefore, the rate at which R_T increases with T.

Many biological and chemical processes are assumed to be described well by a Q_{10} value, which describes how much the rate of the process increases with a 10 °C increase in temperature. Thus, a Q_{10} of 2 means there is a doubling in rate of a process with every 10 °C rise in temperature. Q_{10} may be defined mathematically as:

[4] This term applies to a free surface above, at, or below the ground surface. Strictly, the term 'water table' which is implied by *WT* applies only to the free-surface *within* a porous medium.

$$\alpha_T = \alpha_{T_b} \times Q_{10}^{(T-T_b)/10} \quad [11]$$

where α_T is the rate of a process at temperature T, and α_{T_b} is the rate at the reference temperature T_b. Q_{10} is widely used in peatland science (e.g. Whiting 1994, Silvola *et al*. 1996, Bragazza *et al*. 2016) but Equation [11] is identical to the simple exponential equation. This can be demonstrated as follows. If T_b is assumed to be 0 °C, we may write

$$Q_{10}^{T/10} = e^{g \times T}$$

$$ln\left(Q_{10}^{T/10}\right) = g \times T$$

$$ln\left(Q_{10}^{1/10}\right) = g$$

$$ln\left(Q_{10}\right) = 10 \times g$$

$$Q_{10} = e^{10 \times g}$$

If we substitute this definition of Q_{10} into Equation [11], we end up with Equation [10]:

$$\alpha_T = \alpha_{T_b} \times \left(e^{10 \times g}\right)^{T/10} \equiv \alpha_{T_b} \times e^{g \times T}$$

Because R_T in Equations [8] and [9] has been log-transformed, the equation in each case is a linear equation that can be fitted to data using ordinary least-squares regression. After the equation has been fitted and values of the parameters estimated, the equation can be used to estimate $ln(R_T)$, given any values of the explanatory variable (*T*, *EV*, *WT* etc). However, these $ln(R_T)$ values have to be converted back to the original units when estimating time-integrated CO_2 fluxes for an area of peatland. A problem with doing this transformation is that it biases the estimates of R_T because the optimal values of the regression parameters (a, b_1 etc) have been fitted to the *ln*-transformed values of R_T. This bias is known as 'detransformation bias' or 're-transformation bias' and has long been known as a problem in biology, geography, and statistics. A good discussion of the problem in the context of sediment-discharge rating curves in streams (using log-log regressions) may be found in Ferguson (1986). The magnitude of the bias depends on the scatter in the data. Ferguson (1986) noted errors of as much as 50 % were possible, but it is likely biases will be much smaller for the estimation of R_T. The bias can be dealt with in a number of ways as discussed by Duan (1983) and Miller (1984). A simple alternative to bias correction of a linear regression model is to undertake numerical non-linear regression on the untransformed data using error minimisation algorithms such as Solver (see discussion of Equation [3] above). In other words, the original or non-linear form of the equation (e.g. Equation [10] instead of Equation [9]) is fitted directly to the data.

In a study of soil respiration (not ecosystem respiration), Lloyd & Taylor (1994) noted that the exponential or Q_{10} approach can lead to biased fits to data, and proposed instead the following model, which, although still essentially empirical, has a sounder theoretical basis than Equation [10] (or [11]):

$$R_{soil} = R_{soil,10} \times e^{E_0 \times \left(\frac{1}{283.15 - T_0} - \frac{1}{T - T_0}\right)} \quad [12]$$

where $R_{soil,10}$ is soil respiration at a reference temperature of 283.15 K (10 °C), E_0 is an 'activation' parameter (K), T_0 is the temperature constant (K; Lloyd & Taylor (1994) set this to 227.13 K) and T is the soil temperature (K). Equation [12] can be fitted to data using non-linear optimisation methods (e.g. Solver – see discussion after Equation [3]). Soil respiration consists of heterotrophic and root respiration. It differs from R_T in that it does not include respiration from the above-ground parts of plants. Despite being developed for R_{soil}, Equation [12] has been widely used to model R_T in European peatland studies (e.g. Drösler 2005, Veenendaal *et al.* 2007, Elsgaard *et al.* 2012, Beetz *et al.* 2013, Leiber-Sauheitl *et al.* 2014, Beyer *et al.* 2015, Eickenscheidt *et al.* 2015, Hoffmann *et al.* 2015). Although the equation appears to perform well for R_T, the inclusion of either water-table level or volumetric moisture content may further improve model fits on managed organic soils where wet-dry cycles can have a significant effect on respiration rates (Renou-Wilson *et al.* 2014).

In a study of tundra soils, Shaver *et al*. (2013) adopted a variant of the exponential or Q_{10} model for simulating R_T. They used a model with a mix of multiplicative and additive terms as follows:

$$R_T = \left(c \times e^{g \times T_{air}} \times LAI\right) + d \quad [13]$$

where c (denoted R_0 by Shaver *et al*. 2013) is modified non-linearly by air temperature T_{air} (°C) (as in Equation [10]) and linearly by leaf area index (*LAI*). d (denoted R_x by Shaver *et al*. 2013) is a constant respiration source that is independent of other factors. Shaver *et al*. (2013) note that the

inclusion of *d* improves the model fit to data and prevents R_T becoming zero when *LAI* is zero.

Waddington & Roulet (1996) modelled R_T using linear relationships with either air temperature or peat temperature (i.e. R_T was not logged as in Equation [8]), with their choice between the two alternatives depending on model fit to data. They measured peat temperatures at depths of 2, 20, 40, 80 and 150 cm but do not say which of these was used in the peat temperature version of the R_T model. Bellisario *et al*. (1998) modelled R_T as a simple linear function of *WT* and/or air temperature (T_{air}), while Strack & Zuback (2013) modelled R_T as a linear function of *WT* and $T_{soil,5}$. With the exception of Strack & Zuback (2013) (r^2 = 0.29), none of the above authors provide any detail on the goodness of fit of their R_T models.

The very simplest approach is to assume that R_T is a constant. Such an assumption was made by Bubier *et al*. (1998) who fitted their *NEE* data directly to the following model:

$$NEE = R_T - \frac{Q \times \alpha \times I_{PAR}}{(\alpha \times I_{PAR}) + Q} \quad [14]$$

In Equation [14], R_T is the intercept on the *y* axis (when I_{PAR} is zero). Bubier *et al*. (1998) developed different parameterisations of Equation [14] for the early, mid, and latter part of the growing season for each peatland site they looked at, and used the fitted values of *Q* and R_T to compare sites (a similar approach to Waddington *et al*. (2010) – see the discussion after Equation [7]). However, even within each part of the growing season one might expect R_T to vary over time as factors, such as T_{soil}, vary. Whiting *et al*. (1992) also fitted Equation [14] directly to their *NEE* data, but applied the fitted model to periods of 24 hours to investigate the diurnal response of *NEE* to I_{PAR}. Under such circumstances it is probably reasonable to treat R_T as a constant.

MODELLING CH_4 EXCHANGES

In contrast to CO_2, many of the studies that have estimated the time-integrated flux of CH_4 have used linear interpolation rather than models (e.g. Waddington & Roulet 1996, Roulet *et al*. 2007, Beetz *et al*. 2013, Leiber-Sauheitl *et al*. 2014, Renou-Wilson *et al*. 2014, Beyer & Höper 2015, Eickenscheidt *et al*. 2015, Vanselow-Algan *et al*. 2015). The integrated flux (F_g; e.g. mg m^{-2}) of CH_4 between a pair of flux measurements at times 1 and 2 (t_1, t_2) may be estimated using:

$$F_{g,1-2} = \frac{1}{2}(f_{g,1} + f_{g,2})(t_2 - t_1) \quad [15]$$

where f_g is the instantaneous flux (e.g. mg m^{-2} day^{-1}). The F_g values for each time pair may then be summed to give an annual total. If the intervals between measurements are identical across the year, the simple average of the flux measurements multiplied by the time period (i.e. 365 days) over which measurements were taken will give the total.

Studies that use an interpolation-based approach to calculate annual CH_4 emissions tend to measure at a high temporal frequency (such as biweekly). Nevertheless, day-to-day variability is often evident in CH_4 flux data, and will not necessarily be properly represented by interpolation (Green & Baird 2017). In addition, it may not be practicable to conduct field measurements at a high frequency, and a modelling approach may be preferred. The key processes affecting CH_4 emissions from a peatland are CH_4 production (archaeal methanogenesis), CH_4 consumption (bacterial methanotrophy), and CH_4 transport (via diffusion through the soil, via ebullition, and through the tissue of vascular plants) (Baird *et al*. 2009). These processes have been represented in a range of mechanistic wetland CH_4 models, such as that developed by Walter *et al*. (1996) (also Walter *et al*. 2001). However, such models are generally quite complicated, and, because of their demanding data requirements (for model setup and calibration), they are not generally suitable for use in estimating annual CH_4 fluxes. Therefore, where authors have not used interpolation to estimate annual fluxes, they have instead mostly developed relatively simple statistical models. For example, for a range of Canadian peatlands, Bubier *et al*. (1993) and Bubier (1995) found relatively strong relationships between the log of the seasonal mean CH_4 flux ($ln(\overline{f_{CH_4}})$) and the seasonal mean water-table depth:

$$ln(\overline{f_{CH_4}}) = a + (b \times WT) \quad [16]$$

where *a* and *b* are parameters. Unlike the third term in brackets in Equation [8], where R_T increases as the water table deepens (*WT* becomes more negative – see explanation of Equation [8]), CH_4 flux increases as the water table becomes more shallow (*WT* becomes less negative) (and *b* in Equation [16] takes positive values unlike b_3 in Equation [8]). In addition, as shown for Equation [9] (see also Equation [10]), Equation [16] is an exponential equation. In contrast to Bubier *et al*. (1993) and Bubier (1995), Bubier *et al*. (1995) found that, although water-table position was important, $ln(\overline{f_{CH_4}})$ was best explained by mean seasonal peat temperature at the average position of the water table. Although relationships may be found

 DOI: 10.19189/MaP.2019.DW.395

between the seasonal average CH_4 flux and variables such as *WT* and T_{soil}, models of $\overline{f_{CH_4}}$ are prone to the same problem as interpolation: i.e., particularly high fluxes on one or two occasions may distort the average and, therefore, the seasonal or annual flux estimate.

For instantaneous CH_4 fluxes (f_{CH_4}) from a Dutch drained agricultural peatland, Schrier-Uijl *et al*. (2010) also found that temperature was the primary explanatory variable. However, instead of log-transforming f_{CH_4} and using linear regression to fit their model to data (as per Bubier *et al*. (1995)), they used non-linear regression to fit the exponential equation:

$$f_{CH_4} = c \times e^{g \times T} \quad [17]$$

Equation [17] is the same as Equation [10], although the parameter values (*c* and *g*) will differ. The problems of fitting models in which the flux is log-transformed are discussed above (see **Modelling ecosystem respiration (R_T)**). For a semi-natural peaty grassland, again in the Netherlands, Hendriks *et al.* (2007) also found a significant exponential relationship between f_{CH_4} and temperature; nevertheless, they found that model uncertainty was very high, and used linear interpolation as well as the exponential model to estimate annual fluxes.

Like Bubier *et al*. (1995), Laine *et al*. (2007) found that both temperature and water-table position were significant explanatory variables, and applied the following model:

$$f_{CH_4} = \left(q + \left(r \times WT\right)\right) \times e^{s \times T_{soil}} \quad [18]$$

where *q*, *r*, and *s* are parameters, *WT* has the same definition as in Equations [8] and [16], and T_{soil} is soil temperature. Although they measured temperature at a range of depths, Laine *et al*. (2007) used the temperature from a depth of 20 cm in Equation [18]. They fitted Equation [18] using non-linear regression separately to each of 21 flux chamber locations (i.e. 21 separate models were created). In all cases, T_{soil} was significant and in a majority of cases *WT* was too; however, in eight of the 21 flux chamber locations *WT* did not add explanatory power to the model.

As long ago as 1993, Moore & Roulet noted that, while many studies show relationships between CH_4 emissions, temperature, and water-table position, many do not. They investigated why simple relationships between f_{CH_4} and water-table position do not always occur. In a laboratory experiment on peat cores in which water tables were first lowered and then raised, they found hysteresis in the relationship between CH_4 flux and water-table depth. CH_4 fluxes initially increased as the water table was lowered (became deeper), before later decreasing, and were much lower as the water table was raised to the surface after a period of 15 days when it had been held at a low stand of 50 cm below the peatland surface. Moore & Roulet (1993) attributed the initial rise in CH_4 emissions as water tables were lowered to (a) the release of CH_4 stored in the peat profile, and (b) diffusion through the air spaces in partially-saturated peat above the water table being much more rapid than diffusion through the peat below the water table (see also Moore & Dalva (1993)).

Some laboratory studies suggest very strong relationships between f_{CH_4} and temperature and water-table position (e.g. Daulat & Clymo 1998). However, these studies often relate to 'ideal' conditions in which fluxes are allowed to settle after a new temperature or water-table level has been set, and do not reflect the complications of the real system, as partly recreated by Moore & Roulet (1993). As well as the potential for non-linearity and hysteresis in the relationship between f_{CH_4} and *WT*, it is important to appreciate that methanogenesis and methanotrophy respond differently to temperature[5]. These two processes occur at different, and often varying, depths in the peat profile, and the temperatures at these different depths may be quite distinct from each other and show different patterns over time. It is, therefore, perhaps more noteworthy when relationships exist between f_{CH_4} and temperature recorded at a single fixed depth than when they do not.

The complications noted above mean that the researcher is left with a dilemma. Simple statistical models vary in their ability to describe CH_4 fluxes, and sometimes fail, while the detailed mechanistic models are too complicated for routine use. Perhaps the best approach is to use a statistical model that takes some account of the separate controls on CH_4 production, consumption, and transport in the peat profile (Granberg *et al*. 1997). For example, rather than use temperatures from a single, fixed depth, it may make more sense to have two temperature variables, one from the zone of methanogenesis and

[5] In a review of the literature Granberg *et al.* (1997) note that Q_{10} values for the relationship between methanogenesis and temperature range from 3.0 to 16.0, while for methanotrophy the range is between 1.4 and 2.1.

 DOI: 10.19189/MaP.2019.DW.395

one from the zone of methanotrophy (Granberg *et al*. 1997), and to recognise that these zones may vary in depth through the year. Likewise, rather than using a single measure of water-table position, it may be better to incorporate variables that describe the behaviour of the water table prior to a f_{CH_4} reading, thus accounting for some of the effects observed by Moore & Roulet (1993). Nevertheless, adopting this more detailed statistical approach requires taking more field measurements, and a researcher may decide that it is simply better to use interpolation with higher-frequency sampling than a modelling approach. Further information on the choice between models and interpolation may be found in Green & Baird (2017).

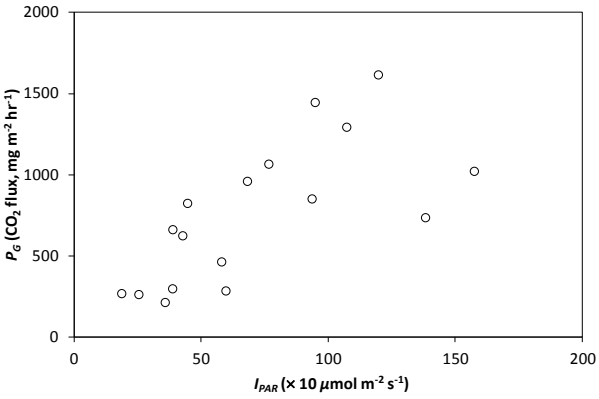

Figure 2. Variation in gross photosynthesis (P_G) with photosynthetically active radiation for one of the collars at the North Wales blanket peatland site. Note that for the purposes of plotting, P_G has been given as positive values.

EXAMPLE MODEL APPLICATIONS

The models reviewed in the previous sections may be applied to single chamber locations or to data from multiple chambers. If there are sufficient data for model fitting, the former is attractive because a C budget can be treated as a point measurement in space and as a 'data unit' (datum). This way of estimating C-fluxes has the advantage that they can be treated statistically in the same way as spatial observations of random variables.

The 'per chamber' approach to flux modelling was used on a project funded by the UK Government's Department for Environment, Food, and Rural Affairs, on which three of us (AJB, SMG, and GPD) worked (Defra SP102: https://tinyurl.com/ybh9lm65, last accessed 27.5.2019). This project investigated the effect of ditch blocking on soil-atmosphere exchanges of CO_2 and CH_4 on a blanket peatland in North Wales. More details of the study may be found in Green & Baird (2017) and Green *et al*. (2018). Below we show three example models obtained for three locations in which flux chambers were used to measure P_G, R_T and CH_4 flux. In each example, the vegetation comprised a mix of *Calluna vulgaris* (L.) Hull, *Eriophorum* spp., and *Sphagnum* spp.

Example models

P_G data from one of the chamber locations at the site are shown in Figure 2. The P_G data were derived by subtracting dark chamber test results (which give R_T) from light chamber test results (which give *NEE* – see Equation [2]). The data set was collected over a period of three years (2012–2014 inclusive). As well as measurements of P_G, the following data were collected: the abundance of *Calluna*, *Eriophorum* spp., and *Sphagnum* in the chamber 'footprint' (see Green *et al*. 2018), air temperature (T_{air}), soil temperature ($T_{soil,10}$), I and I_{PAR} (see Equations [3]/[4]/[5] and Figure 1), and water-table depth (expressed as positive below the surface). P_G did not show a strong relationship with I_{PAR} (Figure 2), and there was little suggestion of the expected simple rectangular hyperbola (Equation [3]/[4]). However, inclusion of environmental variables, as in Equation [4], did produce a satisfactory model. The model that was ultimately chosen included T_{air} and *ETI* as factors (Equation [4]), with the other variables making little difference to model performance. T_{air} and *ETI* were fitted by minimising the squared difference between modelled and measured P_G values using the Solver optimisation tool in Excel. Instead of using a threshold for *ETI* (see discussion after Equation [6]), we calculated it for all temperatures (all times of year). We did this principally because the climate of the site is hyper-oceanic; i.e., although the site can have low winter temperatures, it also has periods during the winter months when temperatures are sufficiently high for some plant growth to occur. The correspondence between the measured and modelled P_G values is shown in Figure 3, where measured values are plotted on the *y* axis and modelled values on the *x*. This might seem the wrong way round, but is, in fact, correct, as is explained in the next subsection (**Judging flux model performance**). Ways in which the correspondence between modelled and measured values may be evaluated are also briefly reviewed in the same subsection, including the specific case of P_G in Figure 3.

Figures 4–7 show data and models for R_T and CH_4 flux from two other collars at the North Wales blanket peatland site. R_T showed a strong linear relationship with soil temperature at a depth of 10 cm,

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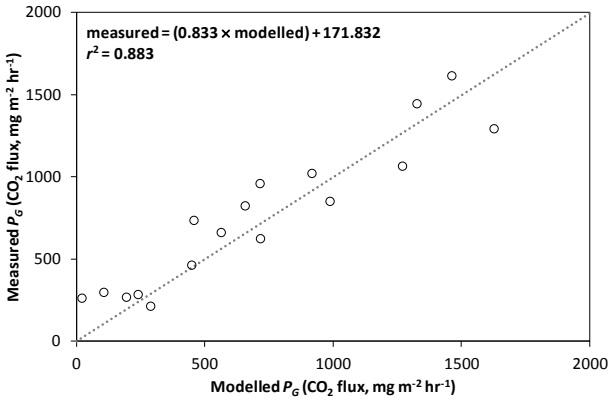

Figure 3. Measured *vs* modelled gross photosynthesis (P_G) for one of the collars at the North Wales blanket peatland site. The dotted line is the 1:1 line. Note that for the purposes of plotting, P_G has been given as positive values.

with R_T dropping to zero for values of $T_{soil,10}$ between 4 and 5 °C. However, testing with a range of independent variables produced a better R_T model that contained $T_{soil,10}$, sedge abundance, air temperature, and *ETI* (as for the P_G model applied across the year), with measured *vs* modelled shown in Figure 5. This example shows that it is important to consider whether a model can be improved even if an apparently satisfactory relationship has already been found (see **Judging flux model performance**).

The data on CH_4 flux in Figure 6 show considerable scatter, with no clear linear or non-linear relationship with soil temperature. Both linear and non-linear models were applied to the CH_4 flux dataset and the model that proved most useful was a multiple linear regression model in which sedge abundance, *ETI*, $T_{soil,10}$, water-table depth, and T_{air} were predictors. The performance of the model may

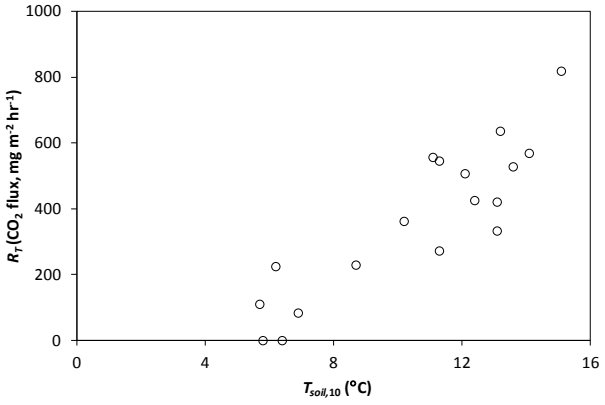

Figure 4. Variation in ecosystem respiration (R_T) with soil temperature at a depth of 10 cm for one of the collars at the North Wales blanket peatland site.

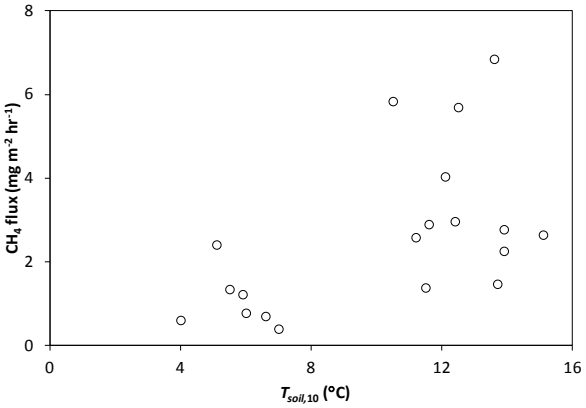

Figure 6. Methane (CH_4) flux *vs* soil temperature at 10 cm depth for one of the collars at the North Wales blanket peatland site.

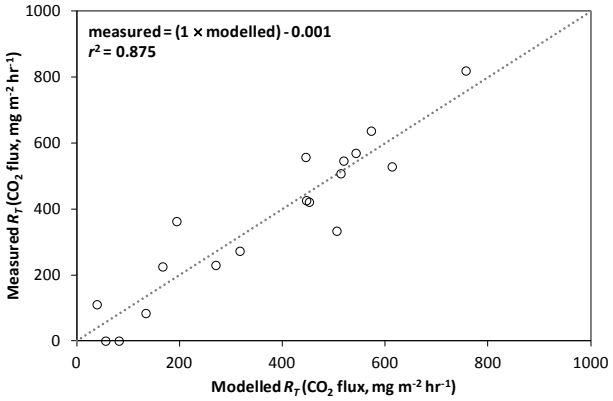

Figure 5. Measured *vs* modelled ecosystem respiration (R_T) for one of the collars at the North Wales blanket peatland site. The dotted line is the 1:1 line.

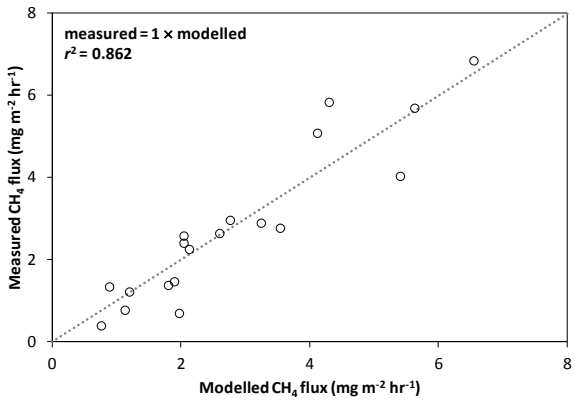

Figure 7. Measured *vs* modelled methane (CH_4) flux for one of the collars at the North Wales blanket peatland site. The dotted line is the 1:1 line.

be assessed visually in Figure 7 (see also **Judging flux model performance**)

Judging flux model performance

For multiple linear regression models, such as that chosen for the R_T and CH_4 flux data in the examples above, it is a simple matter to assess model performance by looking at the r^2 or adjusted r^2, the p values of the slope coefficients, and the residuals (in an unbiased fit they should be scattered around zero). For non-linear models this is not possible; r^2 for such models is effectively meaningless (e.g. Spiess & Neumeyer 2010). Yet it is desirable to compare different flux models regardless of whether they are linear or non-linear. Ultimately, when judging a model's predictions, we wish to see how close the data and predictions are to a 1:1 line. It might seem a simple matter to judge fit to a 1:1 line. For example, an apparently obvious thing to do would be to look at the correlation between modelled values and measured values or to regress modelled against measured and to use the r, r^2 and p of the analysis to evaluate model performance. In another context – that of comparing different measurement instruments or methods – it has been shown that r, r^2 and p can suggest a good model fit when the model is biased but precise; i.e., when the measured *vs* model line departs from the 1:1 line but model-data points cluster closely around the best-fit line. Solutions to this problem include the use of the concordance correlation coefficient, originally proposed by Lin (1989), and a variety of graphical methods developed by Bland & Altmann (1986). This is a large topic and not one that we can do justice to here, so we recommend readers use the cited papers as starting points.

Although r^2 and p values cannot reveal anything about the bias of a model, if used in conjunction with the slope coefficient and the intercept, regression can be a very useful tool in assessing model performance. The question then arises, should one regress modelled on measured or measured on modelled? Intuitively, because a model is developed from the data, we might think of the modelled values being 'dependent' and the measured values being independent, so would regress modelled on measured. Piñeiro *et al*. (2008) show that such intuition is incorrect. R^2 is unaffected by the way in which the regression is done. However, using synthetic data sets based on three functions (linear, quadratic, and logarithmic) and an algebraic argument, Piñeiro *et al*. (2008) show that the slope coefficient gives a biased estimate of the degree to which modelled and measured values lie on the 1:1 line when modelled values are regressed on measured. Conversely, the regression of measured on modelled produces the correct estimators of goodness of fit between the two. This approach was used in the three examples given in Figures 3, 5 and 7. For each model, the r^2 was similar – in the mid 0.8s – but the bias varied. In the R_T and CH_4 models, there was virtually no and no bias respectively, while for the P_G model there was bias due to a modest offset error and a gradient somewhat different from 1.

A final issue to consider is model parsimony. Does a model include independent variables that contribute little to the model's predictions and which, therefore, may be regarded as redundant? If so, can we dispense with the redundant variables and make the model more efficient? The importance of model parsimony depends, in part, on the purpose of the model. When identification of the main controls on a dependent variable is desired, it is important that redundant variables are found and removed from further consideration. In such cases it is useful to be able to make quantitative judgements on variable importance. In traditional multiple linear regression, the adjusted r^2 can be used to identify which variables add explanatory power to the model (Johnson & Omland 2004, Quinn & Keough 2002). For models in general (i.e. across the range of linear and non-linear models that might be used for flux integration) it is common to use the corrected Akaike Information Criterion (AICc) to help select the most efficient model. More information on the criterion and how it can be used for model selection may be found in Akaike (1973, 1974), Bozdogan (1987), Hurvich & Tsai (1989), Johnson & Omland (2004) and Quinn & Keough (2002). Where models are being used, as here, to integrate fluxes over time, it is also desirable to avoid an over-specified model, but it is less important that the most efficient or optimal model is identified; of greater importance is the overall ability of the model to predict fluxes under a range of environmental conditions. To that end we recommend paying more attention to model accuracy than model efficiency.

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