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Spatio-temporal variability of soil respiration in a spruce-dominated headwater catchment in western Germany

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Abstract

CO₂ production and transport from forest floors is an important component of the carbon cycle and is closely related to the global atmosphere CO₂ concentration. If we are to understand the feedback between soil processes and atmospheric CO₂, we need to know more about the spatio-temporal variability of this soil respiration under different environmental conditions. In this study, long-term measurements were conducted in a spruce-dominated forest ecosystem in western Germany. Multivariate analysis-based similarities between different measurements sites led to the detection of site clusters along two CO₂ emission axes: (1) mainly controlled by soil temperature and moisture condition, and (2) mainly controlled by root biomass and the forest floor litter. The combined effects of soil temperature and soil moisture were used as a time-dependent rating factor affecting the optimal CO₂ production and transport at cluster level. High/moderate/weak time-dependent rating factors were associated with the different clusters. The process-based most distant clusters were identified using specified pattern characteristics: the reaction rates in the soil layers, the activation energy for bio-chemical reactions, the water sorption and desorption constant, the root biomass factor, the litter layer factor and the organic matter factor. A HYDRUS-1D model system was inversely used to compute soil hydraulic parameters from soil moisture measurements. Heat transport parameters were adjusted based on observed soil temperatures. The results were used to adjust CO₂ production and transport characteristics such as the molecular diffusion coefficient of carbon dioxide in air and water and the CO₂ production by soil microorganisms and plant roots under optimal conditions for each cluster. Although the uncertainty associated with the HYDRUS-1-D simulations is higher, the results were consistent with both the multivariate clustering and the time-dependent rating of site production/transport.

Finally, four clusters with significantly different environmental conditions (i.e., permanent high soil moisture condition, accumulated litter amount, high variability in soil moisture content, dominant temperature-dependence) were found relevant in explaining the

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spatio-temporal variability of CO₂ efflux and providing reference specific characteristic values for the investigated area.

1 Introduction

Understanding the feedback between terrestrial ecosystems and the atmosphere is one of the key issues for predicting the evolution of atmospheric CO₂ concentration and global climatic change (Longdoz et al., 2000). Accordingly more studies are required on the role of soil processes if we are to improve our understanding of the flux rate functions and the stability and resilience of soil processes that contribute to large-scale surface fluxes of water, heat and greenhouse gases (Fang and Moncrieff, 1999).

The release of CO₂ from the soil surface is the result of a number of complex processes, including CO₂ production, gas transport and interactions between physical and biological factors within the soil (Moncrieff and Fang, 1999). Production of CO₂ in soil is the result of microbial and root respiration, which are functions of the type and distribution of organic matter and roots in soil and are mainly governed by soil temperature and water content (Jassal et al., 2005). The effects of soil temperature and soil moisture on CO₂ effluxes are non-linear and complex. A change in soil moisture has a greater impact when the temperatures are high while a change in temperatures has a greater impact when the soil is humid (Howard and Howard, 1979; Joffre et al., 2003). Many previous studies (Hashimoto et al., 2009; Shi et al., 2006; Niinistö et al., 2011; Fiener et al., 2011) have based CO₂ efflux estimation purely on soil temperature (using e.g. Arrhenius law) because soil moisture is found not to be a limiting factor in most of the studied regions. However, soil CO₂ diffusivity changes with air-filled porosity, which in turn is affected by soil bulk density and soil water content (Jassal et al., 2005). This finding implies a potential link between changes in soil CO₂ diffusivity and the water sorption and desorption velocity that characterizes a specific location. While analyzing pesticide degradation by microorganisms, Richter et al. (1996) suggested estimating the degradation rate in the soil layers by combining the Arrhenius law for temperature

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dependency with Walker's empirical formula (Walker and Allen, 1984) for soil moisture dependency. This combination of laws could then be used as a rating factor of soil CO₂ efflux in regions where dependence on soil moisture is high.

Only a small number of studies have based direct estimation of CO₂ efflux on soil moisture content. For example, Xu and Qi (2001) applied soil moisture thresholds depending on specific-site conditions to inter-seasonal CO₂ efflux measurements to determine periods of high/weak temperature dependence and periods of positive/negative contributing effects of soil moisture. They used a nonlinear regression model including soil temperature and moisture and found explanations for 76 % and 95 % of the variation in soil CO₂ efflux for soil volumetric moistures < 19 % and > 19 %, respectively. However, although the results were good, they were forced to conclude that soil temperature and moisture are good predictors of the temporal variation of CO₂ efflux but poor predictors of the spatial variations of soil CO₂ efflux.

By assuming that the influence of soil moisture and temperature was negligible, Fang et al. (1998) have followed ideas developed by Sokal and Rohlf (1995) where root and microbial respiration are considered as predictor variables when characterizing the spatial variability of CO₂ efflux in a forest ecosystem in a Florida slash pine plantation. They developed a simple model to specify the spatial variation in CO₂ efflux by further assuming that (1) live and dead biomass dominate the distribution of CO₂ efflux on the forest floor and (2) microbial respiration in the mineral soil is inversely related to the amount of organic matter. Satisfactory results were obtained with the percentages of the variation in CO₂ efflux accounted for by the variation in a predictor variable and associated variations in other variables. Thus 86 %, 64 % and 36 % of the variation was accounted for in the microbial respiration in the mineral soil, fine root respiration and the microbial respiration in the surface layer, respectively. These results suggest that such an approach may be extended by incorporating a time-dependent rating factor to account for regions where soil moisture is a limiting factor.

Accounting simultaneously for effects of bio-chemical reactions at a specific location and for time-dependent factors such as soil moisture and temperature is only possi-

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ble with a relatively small number of process-based models (e.g. SOILCO₂, PATCIS, HYDRUS-1D) (Šimůnek and Suarez, 1993a, b; Fang and Moncrieff, 1999; Šimůnek et al., 2005). In these models, CO₂ production in the soil layers is related to the amount and quality of organic matter and to the live and dead root distribution through the soil layers. CO₂ transport in the soil is linked to gas diffusion, liquid dispersion, gas convection and vertical water movement. The uncertainties associated with these models' results can be significantly reduced by inversely computing the model parameters from field measurements while minimizing the residual sum of squares. However, even if the models are able to predict CO₂ dynamics relatively accurately, the large numbers of parameters to be calibrated, the poor data availability and the costs of experimental measurements mean that they are still weak models. Furthermore, the complexity of the models hampers the understanding of the processes and variables included in the model (Pumpanen et al., 2003).

This study involved measurements sites with both similar and significantly different topographic conditions. This procedure was chosen because it was assumed that different topographic conditions may result in different soil parameters with different moisture dynamics but may not necessarily show comparable root biomass contents or litter depths, for instance. If this assumption proves to be viable, it indicates that a high level of complexity may exist and affect the specification of CO₂ variability within the study area. Multivariate analyses such as multiple factor analyses and normality tests based on quantile distribution may potentially provide linkages between environmental properties and CO₂ efflux and account for similarities and dissimilarities between the investigated measurement sites.

The objectives of this study are to analyze the spatio-temporal variability of CO₂ efflux from the studied forest floor. These objectives are met by applying multivariate data analysis techniques to develop a simple nonlinear model describing a time-dependent rating of specific-site CO₂ production and transport and comparing results with the output of the process-based HYDRUS-1D model system. The aim is to understand the spatio-temporal variability of CO₂-efflux patterns and their determining factors.

2 Materials and methods

2.1 Site description

The study was carried out in the Wüstebach catchment (38 ha in size, Fig. 1) located in the low mountain area of the Eifel National Park (50°30' N, 6°19' E, WGS84), Germany. It is a spruce-dominated headwater catchment, a tributary of the Erkersruhr River in western Germany. The catchment has a warm temperate oceanic climate with a mean annual temperature of 7 °C, a yearly mean sunshine from 1500 to 1600 h and a mean annual precipitation usually ranging from 1100 to 1200 mm (Sciuto and Diekkrüger, 2010). The altitude increases from 595 m in the north to 628 m in the south, while the mean slope is 3.6 % with a maximum of 10.4 % (Bogena et al., 2010; Rosenbaum et al., 2012). The bedrock consists of Devonian shales with sporadic sandstone inclusions and is covered by a 1 to 3 m thick periglacial solifluction layer in which mainly Cambisols in the western part and stagnic Cambisols in the eastern part of the site have developed (Rosenbaum et al., 2012). Gleysols, Stagnosols or Histosols are present in the groundwater influenced floodplains alongside the Wüstebach stream, (Dwersteg, 2012). The catchment is densely forested by Norway spruce (*Picea abies*), a species characterized by a shallow root system; the plant coverage is about 90 % (Sciuto and Diekkrüger, 2010).

2.2 Measurements

Soil respiration is often measured as a flux of carbon dioxide from the soil surface i.e. as soil CO₂ efflux, which approximately equals soil respiration at annual scale but is influenced by transport conditions over shorter time steps (Raich and Schlesinger, 1992; Niinistö et al., 2011). There are several factors associated with CO₂ production and transport. Carbon dioxide in the soil is produced by the oxidation of soil organic matter during litter decomposition by heterotrophic microorganisms and the respiration by plant roots (Jenkinson et al., 1991; Hui and Luo, 2004; Pandey et al., 2010; Jassal et al.,

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2005). In some soils, however not in the studied catchment area, CO₂ is also generated by the action of rainwater on calcareous substrates. Respiration is a suite of metabolic reactions regulated by two major abiotic factors, temperature and moisture, with soil temperature usually having an overriding influence in forest ecosystems (Schlesinger, 1977; Niinistö et al., 2011; Jassal et al., 2005). Soil CO₂ transport to the atmosphere is controlled by the rate of CO₂ production in the soil, the CO₂ concentration gradient between the soil and the atmosphere, soil physical properties, and environmental conditions (diffusion through air-filled pores and cracks in the soil) (Raich and Schlesinger, 1992; Hui and Luo, 2004).

10 In this study, soil CO₂ efflux was measured on a weekly basis using a closed dynamic chamber system (LI 8100, Licor Biosciences Ltd). The CO₂ diffusion from the soil was estimated by placing the chamber on PVC collars (Ø 20 cm) and measuring the increase of CO₂ within the chamber. The insertion depth of the collars was 5–8 cm into the forest floor. Along with soil CO₂ efflux, the soil temperature and soil moisture were measured weekly and a soil survey analysis was conducted, including soil bulk density, root biomass, organic matter content and grain size distribution. Soil temperature was measured with a Testo 100 (Testo AG, Germany) temperature device at the depths of 5 and 11 cm. Soil moisture was measured with a TDR soil moisture probe (Trime-FM soil moisture probe, IMKO, Germany) over an interval of 15 cm (including soil litter). Since 2006, 80 points at two different transects across the Wüstebach river and at a grid setup in the southern part of the catchment was monitored (Dwersteg, 2012). In this particular study, significant differences of various factors such as the topography, soil type and proximity to the river are accounted for by considering ten of the investigation sites (Fig. 1).

25 As reported by Dwersteg (2012), each measurement point was sampled for bulk density in 10 cm depth and bulk density of the litter layer using metal cylinders (Ø 8 cm), and detailed soil profiles for bulk density were generated for each soil type (in total 8 profiles) using soil core sampling. The organic matter content and root biomass were determined through six soil profiles representing six different soil types. The organic

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matter content in the soil or litter was determined using a Carbon/Nitrogen/Sulphur analyzer (Leco CNS-2000). Soil bulk density was determined by retrieving undisturbed cores of known volume to subsequently oven-dry the samples at 105 °C until a constant weight was reached. Samples for determining root biomass were rinsed and sieved to
 5 detach roots from soil mineral particles. The washed root mass was then determined by classifying into diameter classes and weighing after being oven-dried at 70 °C for 48 h. The grain size distribution was analyzed according to Köhn (ISO 11277) and by using a particle analyzer (Analysette 22, Fritsch, Germany). Soil information for the model
 10 was taken from a soil map (1 : 5000; Fig. 1) produced by the Geologischer Dienst NRW and from literature (AG Bodenkunde, 2005).

2.3 Time-dependent rating of specific-site CO₂ efflux

The combined effects of soil temperature and soil moisture were used as a time-dependent rating factor affecting a site-specific optimal CO₂ production and transport. This method is a generalized estimation approach to characterize CO₂ efflux within the
 15 catchment. In the method, observed soil temperature, soil moisture, soil parameters and soil CO₂ efflux are used to automatically solve a generalized equation where only site-specific CO₂ production and transport parameters are unknown. The classical law of Arrhenius, the empirical formula of Walker and Allen (1984) and a formula characterizing a specific-site CO₂ efflux developed by Fang et al. (1998) are combined to
 20 account for the temporal pattern of soil CO₂ efflux. An Excel solver engine was used to find optimal parameter values based on the Generalized Reduced Gradient Nonlinear approach.

According to Fang et al. (1998), a specific-site CO₂ efflux from the soil surface at a certain time t and in a forest environment can be expressed as a sum of root and
 25 microbial respiration:

$$F^* = R_r + R_{ml} + R_{ms} \quad (1)$$

where F^* is the CO_2 efflux from the soil surface and R_r , R_{ml} , and R_{ms} are root respiration, microbial respiration in litter and humus layers and microbial respiration in the mineral soil, respectively. F^* is finally expressed as:

$$F^* = a + bB\phi + cMl - d \ln(Ms) / \phi P \quad (2)$$

where B is the biomass of live fine roots in the soil, ϕP is the soil total porosity, Ml is the present amount of litter and humus of forest floor, M_s is the amount of organic matter in the mineral soil at time t and a , b , c and d are parameters to be determined in agreement to the observations. \ln is the logarithmic function with base e . It is assumed that soil parameters do not change within the short time of the investigations.

Richter et al. (1996) mentioned that under field conditions soil temperature (T) and soil humidity (θ) act simultaneously as a kinetic parameter K (Eq. 3) affecting the degradation rate of pesticide through soil layers. The approach used in this work assumed the same effect but as a rating factor on the optimal CO_2 production/transport at a specific location. Thus CO_2 efflux at a specific location over time, F (Eq. 4), can be expressed as the product of F^* (Fang et al., 1998) by K (Richter et al., 1996).

$$K(\theta, T) = K(\theta)K(T) = A\theta^\alpha k_0 e^{-\frac{\Delta E}{RT}} \quad (3)$$

where $K(\theta)$ is the empirical formula of Walker and Allen (1984), $K(T)$ is the classical law of Arrhenius, k_0 is the reaction rate at reference temperature T_0 [T^{-1}], ΔE is the activation energy [J mol^{-1}], α is the velocity constant for sorption and desorption [T^{-1}], A is the humidity response parameter set equal to 1 in the following steps as in Richter et al. (1996).

$$F = F^*K(\theta, T) = (a + bB\phi + cMl - d \ln(Ms) / \phi P)\theta^\alpha k_0 e^{-\frac{\Delta E}{RT}} \quad (4)$$

where a , b , c , d , k_0 , ΔE and α are parameters to be determined in agreement to the measurements (soil temperature, soil moisture, CO_2 efflux and soil parameters).

In this study, the soil total porosity and the amount of litter present on the forest floor are replaced by the bulk density and the litter depth respectively, thus accounting for effects hidden in the parameters b , c and d .

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2.4 HYDRUS-1D parameterization

HYDRUS-1D (Šimůnek et al., 2005) is an one-dimensional process-based model used in this study to simulate daily soil CO₂ efflux. HYDRUS-1D incorporates simulation components such as water flow, heat transport and the movement of solutes considering first-order decay reactions in variably-saturated soils. HYDRUS-D uses the Richards equation (Eq. 5) for simulating variably-saturated flow and the Fickian-based advection-dispersion equations for heat and solute transport. The water flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[K \left(\frac{\partial h}{\partial x} + \cos \beta \right) \right] - S \quad (5)$$

where h is the water pressure head [L], θ is the volumetric water content [$L^3 L^{-3}$], t is the time [T], x is the spatial coordinate [L] (positive upward), S is the sink term [$L^3 L^{-3} T^{-1}$], β is the angle between the flow direction and the vertical axis (i.e., $\beta = 0^\circ$ for vertical flow, 90° for horizontal flow, and $0^\circ < \beta < 90^\circ$ for inclined flow), and K is the unsaturated hydraulic conductivity function [$L T^{-1}$]. The sink term, S , is defined as the volume of water removed from a unit volume of soil per unit time due to plant water uptake as described by Feddes et al. (1978).

HYDRUS-1D assumes that the individual CO₂ production processes are additive and performs the calculation as the superposition of individual processes that reduce production from the optimal value (Šimůnek and Suarez, 1993a). Thus, the production of CO₂ is considered as the sum of the production by soil microorganisms and by plant roots. HYDRUS-1D also assumes that the CO₂ transport in the unsaturated zone can occur in both the liquid and gas phases. Furthermore it is assumed that the CO₂ concentration in the soil is governed by two transport processes: convective and diffusive transport in both gas and aqueous phases and CO₂ production and/or removal (Patwardhan et al., 1988).

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In this study, the atmospheric boundary condition at the surface layer (i.e., daily potential evaporation and transpiration fluxes, daily rainfall, and daily air temperature) is used for the upper water flow boundary condition. This condition permits water to build up on the surface. The height of the surface water layer increases due to precipitation and is reduced because of infiltration and evaporation. The lower water flow boundary condition is set to constant pressure head. The upper heat transport boundary condition is set to temperature boundary condition, and the lower heat transport boundary condition is set to zero gradient. The snow melting constant, the amount of snow that will melt during one day for each °C, is set to 0.43 cm while the sublimation constant used to reduce the potential evaporation from an existing snow layer is set to 0.4.

2.5 Inverse simulation approach

Hydraulic parameters behind the CO₂ simulations were estimated and optimized from the soil moisture measurements using an inverse modeling approach included in HYDRUS-1D. An objective function φ (Eq. 6) minimized during the parameter estimation process is described by Simunek et al. (1998). The first term represents deviations between the measured and calculated space-time variables (water contents at different locations and/or time in the flow domain). The second term represents differences between independently measured and predicted soil hydraulic properties (e.g., retention, hydraulic conductivity). The last term represents a penalty function for deviations between prior knowledge of the soil hydraulic parameters and their final estimates.

$$\begin{aligned} \varphi(b, q, p) = & \sum_{j=1}^{m_q} v_j \sum_{i=1}^{n_{qj}} w_{i,j} \left[q_j^*(x, t_i) - q_j(x, t_i, b) \right]^2 \\ & + \sum_{j=1}^{m_p} v_j \sum_{i=1}^{n_{pj}} w_{i,j} \left[p_j^*(\varepsilon_i) - p_j(\varepsilon, b) \right]^2 + \sum_{j=1}^{n_b} v_j \left[b_j^* - b_j \right]^2 \end{aligned} \quad (6)$$

where, m_q m_p are the number of different sets of measurements, n_{qj} and n_{pj} are the number of measurements in a particular measurement set, $q_j^*(x, t_i)$ and $p_j^*(\varepsilon_i)$ represent specific measurements at time t_i for the j th measurement set at location x ,

$q_j(x, t_i, b)$ and $p_j(\varepsilon_i, b)$ are the corresponding model predictions for the vector of optimized parameters b (e.g., θ_r, θ_s, a, n , and K_s , van Genuchten parameters), v_j and $w_{j,i}$ are weights associated with a particular measurement set or point, respectively.

2.6 Uncertainty approach

5 A new processing and executing routine was developed (using a FORTRAN environment) for the HYDRUS-1D model allowing the user to run hundreds of simulations at once based on a very large parameter matrix that can be obtained by e.g. Latin Hypercube sampling (McKay et al., 1979). The quality measure of the model performance (fitting to the measurements) is evaluated by the coefficient of determination R^2 , the model efficiency (ME) of Nash and Sutcliffe (1970) and the index of agreement of Willmott (1981). The coefficient of determination R^2 describes the linear dependency
10 of Willmott (1981). The coefficient of determination R^2 describes the linear dependency between measured and simulated values within the range of 0 to 1. The ME describes the degree of accordancy between observed and simulated values and varies between $-\infty$ to 1. The index of agreement ranging between 0 and 1 is fairly strongly influenced
15 by the mean value (simulated or observed variable) and evaluates the performance of the temporal characteristics of the simulated curves. A value of 1 indicates a complete agreement between measured and simulated values.

The initial model parameter sets considered in the uncertainty analysis are: (1) optimized parameter sets (a, b, c, d, α, k_0 and ΔE) obtained by applying the Excel solver engine with the Generalized Reduced Gradient Nonlinear approach, (2) inversely computed hydraulic parameters using the HYDRUS-1D model and based on measured soil moisture, and (3) adjusted heat parameters, optimal CO_2 production and transport parameters using HYDRUS-1D and based on measured temperature and CO_2 efflux. To quantify the prediction uncertainties, an uncertainty of $\pm 1\%$ was assumed
20 for each parameter, thus generating parameter ranges for the Latin Hypercube sampling. The uncertainties in the predictions are quantified by the percentage of measurements bracketed by the 95% prediction uncertainty band (P-factor) (Abbaspour et al., 2004). The 95% uncertainty prediction is calculated at the 2.5% and 97.5%
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levels of cumulative distribution of an output variable obtained through e.g. Latin Hypercube sampling, excluding 5 % of the very bad simulations (due to very bad parameter combination). The ratio of average distance between 2.5 and 97.5 percentiles of the cumulative distribution of the simulated variable and the standard deviation of the corresponding measured variable (R-factor) provided insights into the thickness of the uncertainty band (Abbaspour et al., 2004).

3 Results and discussion

3.1 Multivariate dependence of CO₂ efflux

The measurements ($n = 984$ observations) analyzed in this work are from ten sites characterized by significantly different slope values ranging from 3.6 % to 10.4 %. In some cases, the sites are very close to the river bed, e.g. sites WA6 and WA7 (cf. Fig. 1). Here, lateral flow may differently influence specific-site soil moistures and thus greatly affect the CO₂ efflux from soil. Table 1 shows descriptive statistics of all measured variables at the different sites. The soil parameters are presented as mean values for the entire soil profiles. This table shows that the litter depth and the density of root biomass displayed the highest coefficients of variation and may be relevant factors for characterizing a specific-site behavior. Nevertheless, this result should also be analyzed with caution since randomly distributed observations are obtained for the density of root biomass and not for the litter depth (Table 1). Thus, all investigated soil parameters are randomly distributed except the litter depth, which may be highly influenced by local scale factors such as wind or transport through preferential surface flow.

Figure 2 shows CO₂ efflux rates for the investigated sites with their dependences on soil temperature and soil moisture for seasonal means over the period 2011 to 2012. The circle sizes indicate the rate of CO₂ efflux at a given site. The transition from spring to summer is expressed by an average increase of soil temperature of about 5 °C and an average decrease in soil moisture of about 5 %. A global view on the flux pattern

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at relatively fix temperature ranges (seasonal means) shows that emmision rates decrease with increasing soil moisture, which reveals diffusion as a limiting factor. A clear dependence of the CO₂ pattern on soil temperature (transition from spring to summer) is not necessarily shown even if the humidity condition are similar, which is likely for the sites WA6 and WA7 as they are close to the river bed (permanently wet). In addition, CO₂ emmission rate may increase (e.g., WA1) or decrease (e.g., WB3) with increasing temperature and decreasing soil moisture. With a clearly changed moisture condition from spring to summer, the CO₂ efflux rate may also remain similar (e.g., M8). Thus, CO₂ efflux rate remained, for instance, almost unchanged at the site M8 while soil moisture decreased and soil temperature increased, a condition that, in principle, should simply lead to an increase of the flux (Shibistova et al., 2002). This result led us to conclude that in such an ecosystem, CO₂ efflux from soil may not be highly affected by temporal factors, but it may be affected by spatial factors. The other sites M1, WA10, WA11, WA15 and WB4 may be classified anywhere between or within the cases mentioned above. It is important to remember that the measurement sites involved in this study may have differences and similarities (strongly linked to environmental properties) that cannot be clearly shown from a description based only on soil temperature and soil moisture measurements.

Figure 3 shows a scattergram of observed quantiles vs. estimated quantiles for a normal distribution with the same mean and variance as the observed CO₂ efflux. The results show that seasonal averages of CO₂ efflux at the measurement sites are randomly distributed with maximum values for the site M1 and minimum values for the site WA6.

In summary, the site WA6 is charaterized by very low CO₂ efflux due to permanent moisture conditions while both the high emission rate of the site M1 and the relatively constant emission rate of M8 still have to be clarified. Particular behaviors of the other sites, if existing, remain unclear.

Combining information from Figs. 2 and 4, it can be seen that:

1. a seasonal (spring) mean soil CO₂ efflux ranging from 1.2 to 3 μmol m⁻² s⁻¹ was associated with a large range of seasonal mean volumetric soil moisture ranging from 12 % to 33 %, while the mean soil temperature remain relatively close to 8 °C;
2. a seasonal (summer) mean soil CO₂ efflux ranging from 1.7 to 4.5 μmol m⁻² s⁻¹ was associated with a large range of seasonal mean volumetric soil moisture ranging from 8 % to 30 % while the mean soil temperature remains relatively close to 12 °C.

Both environmental factors and seasonal means of observed variables (e.g., CO₂ efflux, soil moisture and soil temperature) from 2011 to 2012 were combined as multivariate data for a multiple factor analysis. The results show in Fig. 4 two main axes (factors F1 and F2) controlling about 70 % of the total observed variance. CO₂ significantly contributed to both axes at about 20 % but at a higher rate for the axis F1. The factor F1 is mainly controlled by soil moisture and soil temperature, with a predominant influence of temperature in spring and a predominant influence of soil moisture in summer. CO₂ efflux is positively correlated with soil temperature and negatively correlated with soil moisture. The factor F2 is mainly controlled by the litter depth and the root biomass, and this result seems to be consistent with the information previously drawn from Table 1. CO₂ efflux is positively correlated with the root biomass and negatively correlated with the litter depth. Similarities between the sites are shown in the same axis system on the right side of the graphics (multivariate clustering). The arrows of the axes indicate emission gradients with M1 (cluster C1, Table 2) pointed out as the most important emission site. M1 is mainly dependent on soil temperature and should benefit from the transition from spring to summer, but this benefit is not clearly shown in Fig. 2, maybe due to adverse effects from soil moisture. The very low emission rate at the site WA6 is a result of the permanent moisture distribution along the underlying soil profile. The relatively constant and low emission rate at the site M8 results mainly from the litter depth. The figures show that if the litter is a factor indirectly and positively influencing the CO₂ efflux through microorganism respiration, it could be at the same

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time a factor that regulates the emission rate (negative correlation between the litter depth and CO₂ efflux). The site WA11 is mainly controlled by the root biomass. The sites WA10, WA15 and WB4 gathered in Cluster 5 (Fig. 4 and Table 2) are subjected to the simultaneous effects of the both factors F1 and F2.

One may conclude that the clusters C1 and C5 contain sites highly affected by the time-dependence rating factors, clusters C3 and C6 contain sites moderately affected by the time-dependence rating factor and clusters C2 and C4 contain sites weakly affected by the time-dependence rating factor. The clusters C2, C4 and C5 are the most geometrically distant in reference to the Fig. 4 and should lead to significantly different specific-site parameters shown in Eq. (4) (e.g., reaction rate at reference temperature, activation energy, velocity constant for sorption and desorption, cluster constants).

3.2 Site cluster weighting and characterization

Figure 5 shows the estimated and observed soil CO₂ efflux and the quality measure displayed in the bottom table. As mentioned in Sect. 2, the estimations are based on nonlinear time-dependent rating of specific-site models (Eq. 4). The estimation quality remains on average with coefficients of determination ranging from 0.43 to 0.65, model efficiencies from 0.42 to 0.65 and indices of agreement from 0.76 to 0.88. Uncertainty quality measures are relatively high with more than 50% of the measurements captured by the 95% prediction band, ranging from 57% to 76%. The thickness of the 95% uncertainty band, calculated as the ratio of average distance between 2.5 and 97.5 percentiles of the cumulative distribution of the simulated variable and the standard deviation of the corresponding measured variable, ranges between 0.47 and 1.23. The uncertainty analysis is based on optimized parameter sets obtained by applying the Excel solver engine with the Generalized Reduced Gradient Nonlinear approach. Afterwards an uncertainty of ±1% was assumed for each parameter, thus generating parameter ranges that quantified the prediction uncertainty.

The estimated specific-site parameters are shown in Table 3. This table shows the large dissimilarities between the clusters C2, C4 and C5, compared to the others.

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These dissimilarities are visualized better in Fig. 6, which shows the observed vs. estimated normal distribution with associated probabilities for each parameter. These results are consistent with the multiple factor analysis discussed in the Sect. 3.1 and in which the clusters C2, C4 and C5 were found as the most distant (emission rate as well as predominance of factors). This result clearly shows how well seasonal mean information matches the weekly scale information since the multivariate analyses are performed using seasonal averages data while the parameter estimation are based on the weekly scale data.

Combining information drawn from Figs. 4 and 5, it appears that the clusters C1, C2, C4 and C5 may be seen as representative when characterizing the spatio-temporal pattern of CO₂ efflux from the forest floor of the Wüstebach catchment:

1. Cluster C1 was clearly linked to the high temperature-dependent effects as derived from Fig. 4 and does not display any clear characteristic values in Table 3;
2. as previously found, Cluster C2 is weakly affected by the time-dependent rating factor but highly influenced by combined effects of root biomass and litter depth. The effects of the litter depth are predominant and expressed as an inhibiting factor for CO₂ production and transport. This result clearly explains the very high reaction rate at a reference temperature and the very high activation energy observed in Table 3 and Fig. 6. As discussed in Sect. 3.1, if the litter is a factor influencing indirectly and positively the CO₂ efflux through microorganism respiration, it could be at the same time a factor that regulates the emission rate depending on how important and dense it is (resulting in a negative correlation between the litter depth and CO₂ efflux). As already mentioned, different depth of litter may lead, for instance, to different velocities of heat transport or air diffusion from or into the soil layers. The problem raised here is then related to the quality of the forest floor litter and the organic matter, which may be affected by wind action, preferential runoff transport or deposition from different species as already pointed out by Longdoz et al. (2000);

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3. Cluster C4 was found to be weakly influenced by both the time-dependent rating factor and a permanent moisture condition. These influences result in a moderate reaction rate at reference temperature and a very specific (negative) value as for the cluster constant (Table 3 and Fig. 6);

5 4. Cluster C5 is highly influenced by the combined effects of the time-dependent rating factor and the root biomass. This result is explained by the extremely high value obtained for the velocity constant for water sorption and desorption and the specific (positive) value obtained for the cluster constant (Table 3 and Fig. 6). This high value of the velocity constant for water sorption and desorption suggests that
10 Cluster C5 is characterized by high temporal changes in the soil air-filled pores and points to the predominant effects of both soil moisture and soil temperature.

Many studies have investigated the litter control on soil respiration. Li et al. (2004) studied the effects of litter exclusion (exclusion of new litterfall over a 7 yr experiment) on soil CO₂ efflux and found out that soil respiration was significantly reduced. Sulzman et al. (2005) studied the contribution of litter to total soil CO₂ efflux in an old growth
15 coniferous forest and found that measured fluxes from plots with doubled needle litter led to an additional flux. Metcalfe et al. (2007) investigated factors controlling spatio-temporal variation in CO₂ efflux from surface litter at four rain forest sites in the eastern Amazon. They found that litter contribution showed no clear seasonal change, though
20 experimental precipitation exclusion was associated with a ten-fold reduction in litter respiration relative to unmodified sites. These findings invite more attention and studies on how litter controls CO₂ efflux.

Table 4 shows a significantly higher correlation between the cluster constant and the other site-specific factors (e.g., root biomass factor, litter layer factor, organic matter
25 factor). This result does not allow independent analysis of the clusters based on the quantile distributions of the estimated factors *b*, *c* and *d*.

3.3 CO₂ production and transport through soil layers

As mentioned in Sect. 2, soil hydraulic parameters were derived from soil moisture measurements using inverse solutions through the HYDRUS-1D model system. The calibrated hydraulic parameters were first combined with soil temperature measurements to adjust heat transport parameters. All these parameters were finally used to simulate soil CO₂ efflux for one site picked from each cluster presented in the previous sub-sections.

Figure 7 shows observations vs. best simulations with the associated uncertainty ranges for the soil CO₂ efflux of the measurement sites picked up from the clusters. The table associated with Fig. 7 provides the quality measure of the simulation for the different sites taken from the clusters. The quality measures are just acceptable. The coefficient of determination (R^2), the model efficiency (ME) and the index of agreement (IA) range from 0.26 to 0.86. The percentage of measurements captured by 95 % prediction uncertainty ranges from 71 % to 88 % while the uncertainty bands are relatively large (from 1.32 to 2.72).

In overall, the uncertainty of the simulations using the HYDRUS-1D model were relatively high compared to those of the estimations presented in Sect. 3.2, where combined effects of soil moisture and soil temperature were directly used as a time-dependent rating factor for specific-site CO₂ production and transport.

Table 5 shows calibrated values for specific-site CO₂ production and transport parameters such as the molecular diffusion coefficient of carbon dioxide in air, the molecular diffusion coefficient of carbon dioxide in water, the optimal CO₂ production by soil microorganisms for the entire soil profile and the optimal CO₂ production by plant roots for the entire soil profile. These values might be seen as characteristic values for both the investigated sites and the underlying clusters. The lowest respiration is observed for Cluster C4 and can be explained by the permanent moisture condition, which inhibits microbial activity. The highest respiration rates are observed at Cluster C3, which may be seen as a predominant effect non-extreme/intermediary and suitable soil moisture

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condition resulting in optimal conditions for microorganism. It should be mentioned that Cluster C3 was identified in Sect. 3.2 as under moderate influence of the time-dependent rating factor (combined effects of soil moisture and soil temperature). The lowest root activities are observed for Cluster C2 (site M8) and Cluster C6 (site WA11) and are consistent with conclusions drawn from Fig. 4 in Sect. 3.1, where attention was drawn to a likely inhibiting effect of the litter depth on the CO₂ production and transport with a direct link to very low air and heat circulation. This result helps to understand why the activation energy found in Sect. 3.2 (Table 3) is very high. The highest CO₂ production from root biomass (Table 5) is shown for Cluster C1 (site M1) and Cluster C5. This result is also consistent with the efflux gradient shown in Fig. 4 (Sect. 3.1).

The information shown in Fig. 8 is in line with that from Figs. 4 and 6, revealing the clusters C2, C4 and C5 as the most distant in term of processes within the studied area. In particular for Cluster C2, which is partially controlled by the litter amount, more investigation is needed regarding the inhibiting role.

4 Conclusions

The current work provides a successful extension of earlier relevant research issues (Fang et al., 1998; Richter et al., 1996) by discussing ongoing long-term CO₂ efflux measurements and multivariable environmental properties in a western German forest ecosystem.

For the period 2011 to 2012, data from ten selected measurement sites in the spruce-dominated forest floor of the Wüstebach catchment have shown a spring mean soil CO₂ efflux ranging from 1.2 to 3 μmolm⁻²s⁻¹ (1.7 to 4.5 μmolm⁻²s⁻¹ in summer) associated with a large range of mean volumetric soil moisture ranging from 12 % to 33 % (8 % to 30 % in summer), while the mean soil temperature remain around 8 °C (12 °C in summer). This less pronounced seasonal trend hides complex interactions between environmental factors, time-dependent factors and the CO₂ efflux rate (Metcalfe et al., 2007). A multivariate clustering of the measurement sites decreased the com-

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plexity level of the environmental control on CO₂ efflux and allowed concordant evaluations of a simple nonlinear model of time-dependent rating of specific-site CO₂ production/transport compared to simulation issues with the HYDRUS-1D model system. Although the uncertainty increased significantly from the nonlinear time-dependent rating model to the HYDRUS-1D simulations, the comprehensible linkage between the different results and the underlying approaches was not affected.

The results indicate that CO₂ efflux from the sub-surface floor of the study area is mainly controlled by soil temperature, moisture condition, root biomass and litter distribution. Four different process-based clusters with very clear physical and biochemical conditions (e.g., permanent moisture condition, accumulated litter amount, high changes in the air-filled pores) were found relevant in explaining the spatio-temporal variability of CO₂ efflux and providing reference characteristic values for the investigated area. Parameters such as the velocity constant of water sorption and desorption were specified for the clusters, accounting for the link between soil moisture and changes in soil CO₂ diffusivity. The results provide many other pattern characteristics such as the molecular diffusion coefficient of carbon dioxide in air, the molecular diffusion coefficient of carbon dioxide in water, the optimal CO₂ production by soil microorganisms for the entire soil profile and the optimal CO₂ production by plant roots for the entire soil profile.

Finally it should be remembered that the specific-site rating factor approach used in this study produced comprehensible, valid and more certain results compared to using the HYDRUS-1D.

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Table 1. Descriptive statistics ($n = 984$ observations) for 10 sites (M1, M8, WA1, WA6, WA7, WA10, WA11, WA15, WB3, WB4) from 2006–2012 along two transects (cf. Fig. 1 for the locations of measurement sites). The symbol (–) means that the dynamic variables were not tested for normality.

Variables	Min.	Max.	Mean	Std. deviation	Coef. of variation	Normally distributed
Litter thickness [m]	0.02	0.08	0.03	0.02	0.57	no
Bulk density [g cm^{-3}]	0.67	0.91	0.79	0.08	0.10	yes
Root biomass [g m^{-2}]	28.6	177.7	113.2	47.9	0.42	yes
Organic matter [g m^{-2}]	7330.2	12511.8	10833.6	1513.0	0.14	yes
Soil moisture at 15 cm depth [% Vol.]	2.03	54.77	22.78	–	–	–
Soil temperature at 11 cm depth [$^{\circ}\text{C}$]	0.00	15.80	8.58	–	–	–
CO_2 efflux [$\mu\text{mol m}^{-2} \text{s}^{-1}$]	0.02	8.74	2.51	–	–	–

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Table 2. Potential clusters for characterizing the patterns of CO₂ efflux in the study area.

Cluster 1 (C1)	Cluster 2 (C2)	Cluster 3 (C3)	Cluster 4 (C4)	Cluster 5 (C5)	Cluster 6 (C6)
M1	M8	WA1 WB3	WA6 WA7	WA10 WA15 WB4	WA11

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Table 3. Factor parameters obtained for the different clusters (cf. Eq. 4). k_0 = reaction rate at reference temperature to $[T^{-1}]$, ΔE = activation energy $[J\ mol^{-1}]$, α = velocity constant for sorption and desorption $[S^{-1}]$, a = cluster constant, b = root biomass factor, c = litter layer factor, d = organic matter factor.

	k_0 (10^8)	ΔE (10^4)	α (10^{-4})	a (10^4)	b	c (10^4)	d (10^4)
Cluster 1	11.7	7.1	-2.7	0.2	-34.8	-12.3	-0.4
Cluster 2	316.2	9.0	-3.1	0.7	16.5	106.4	-17.6
Cluster 3	11.1	6.8	-2.7	0.2	-29.9	-21.8	-0.1
Cluster 4	100.6	7.3	-1.8	-13.8	691.2	-2844.6	-6.4
Cluster 5	13.4	6.8	56.3	8.3	-446.5	60.1	0.3
Cluster 6	8.2	7.1	-2.6	0.2	-36.7	-12.7	-0.3

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Table 4. Pearson correlations between parameters of the modified Fang et al. (1998) model (Eq. 4). Correlations are underlined while values in italic are the significance of the correlations under alpha = 0.05. Values in bold highlight correlations with significance < 0.05.

Variables	k_0	ΔE	α	a	b	c	d
k_0		<i>0.001</i>	<i>0.620</i>	<i>0.756</i>	<i>0.639</i>	<i>0.911</i>	<i>< 0.0001</i>
ΔE	<u>0.978</u>		<i>0.514</i>	<i>0.837</i>	<i>0.717</i>	<i>0.926</i>	<i>0.001</i>
α	<u>-0.259</u>	<u>-0.337</u>		<i>0.208</i>	<i>0.191</i>	<i>0.705</i>	<i>0.552</i>
a	<u>-0.164</u>	<u>-0.109</u>	<u>0.600</u>		<i>< 0.0001</i>	<i>0.013</i>	<i>0.645</i>
b	<u>0.246</u>	<u>0.191</u>	<u>-0.618</u>	<i>-0.996</i>		<i>0.018</i>	<i>0.534</i>
c	<u>-0.060</u>	<u>0.050</u>	<u>0.199</u>	<i>0.904</i>	<i>-0.889</i>		<i>0.809</i>
d	<u>-0.997</u>	<u>-0.973</u>	<u>0.308</u>	<u>0.241</u>	<u>-0.322</u>	<u>0.128</u>	

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B. Diekkrüger

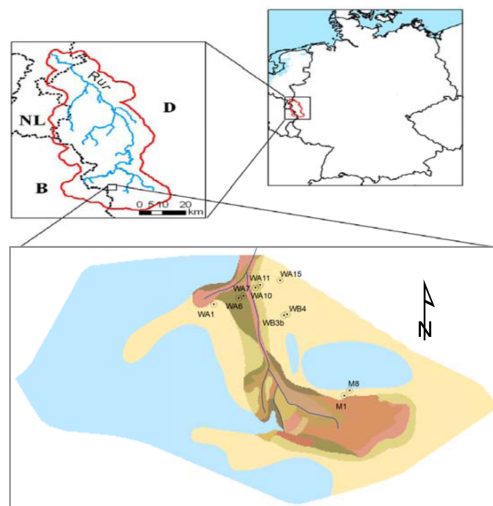
Table 5. Estimated parameters of the HYDRUS-1D model: air diff. = molecular diffusion coefficient of carbon dioxide in air [$\text{mm}^{-2}\text{s}^{-1}$]; water diff. = molecular diffusion coefficient of carbon dioxide in water [$\text{mm}^{-2}\text{s}^{-1}$]; OCDP microorganisms = optimal CO_2 production by soil microorganisms for the entire soil profile [$\mu\text{mol m}^{-2}\text{s}^{-1}$]; OCDP roots = optimal CO_2 production by plant roots for the entire soil profile [$\mu\text{mol m}^{-2}\text{s}^{-1}$].

	M1 (C1)	M8 (C2)	WA1 (C3)	WA7 (C4)	WA10 (C5)	WA11 (C6)
Air Diff.	2 479 380	129 238	1 862 439	157 731	2 284 559	1 982 122
Water Diff.	107.75	89.75	110.00	90.65	162.65	105.95
OCDP microorganisms	10.40	9.48	11.31	6.32	10.65	7.27
OCDP roots	13.42	7.80	9.74	10.49	11.90	7.33

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Site	Soil type	Slope (%)	Elevation (m)
WA1	S-B: Gleyic Cambisol	8.84	600
WA6	S-G: Stagnic Eutric Gleysol	5.59	598
WA7	S-G: Stagnic Eutric Gleysol	5	598
WA10	B-S: Cambisol	5.3	597
WA11	B-S: Cambisol	7.29	598
WA15	S-B: Gleyic Cambisol	12.87	601
WB3	S-B: Gleyic Cambisol	12.75	604
WB4	S-B: Gleyic Cambisol	14.25	605
M1	S-B: Gleyic Cambisol	7.29	616
M8	S-B: Gleyic Cambisol	7.29	617

Fig. 1. Location of the measurement sites (M1, M8, WA1, WA6, WA7, WA10, WA11, WA15, WB3b, WB4) in the Wüstebach catchment, Germany, as used in this study (modified from Sciuto and Diekkrüger, 2010).

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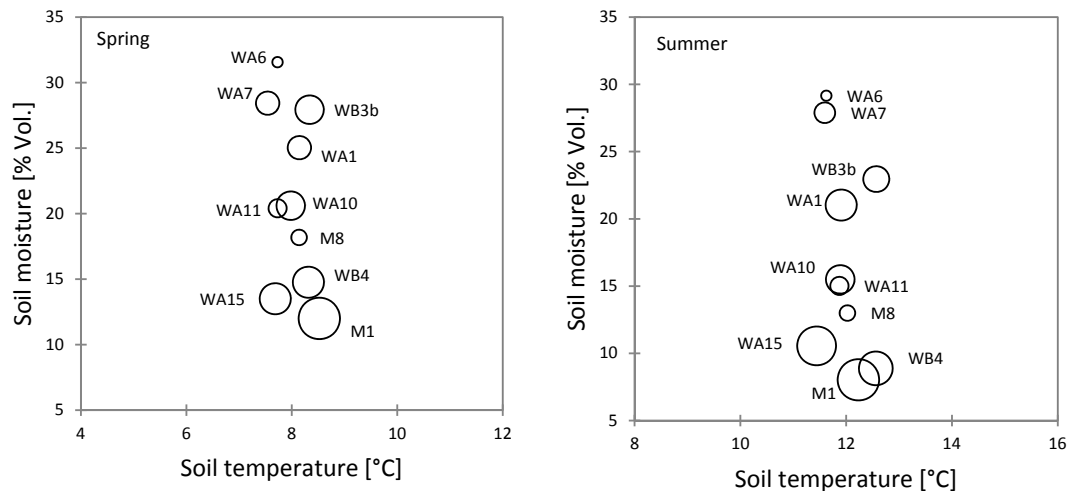


Fig. 2. 3-D plot of CO_2 efflux dependency on soil temperature and soil moisture and likely clustering based on average values observed from 2011 to 2012. The circle sizes indicate the rate of CO_2 efflux at a given site.

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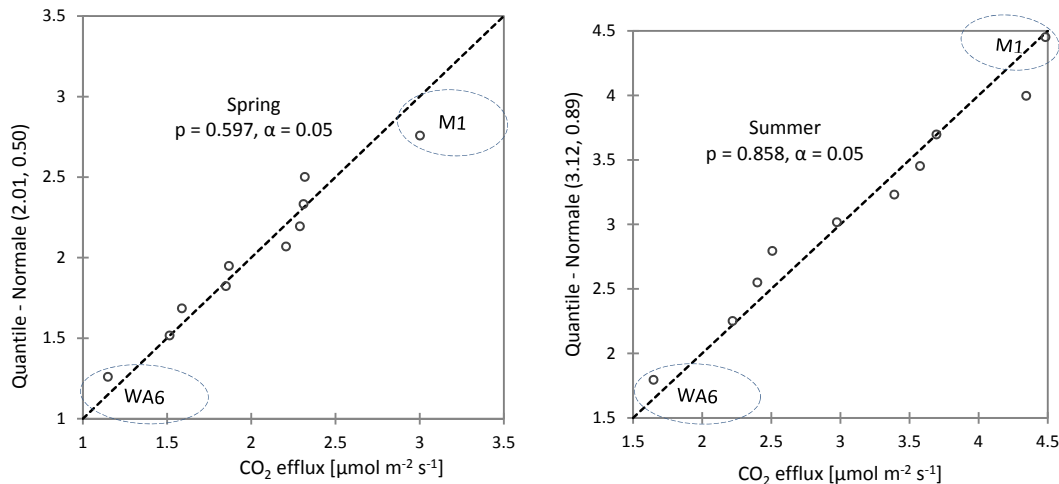


Fig. 3. Scattergram of observed vs. estimated quantiles for a normal distribution with the same mean and variance as from the observed CO₂ efflux and soil moisture. Analysis based on average values observed from 2011 to 2012. When the computed p value is greater than the significance level alpha, the parameter follows a normal distribution (Anderson–Darling test).

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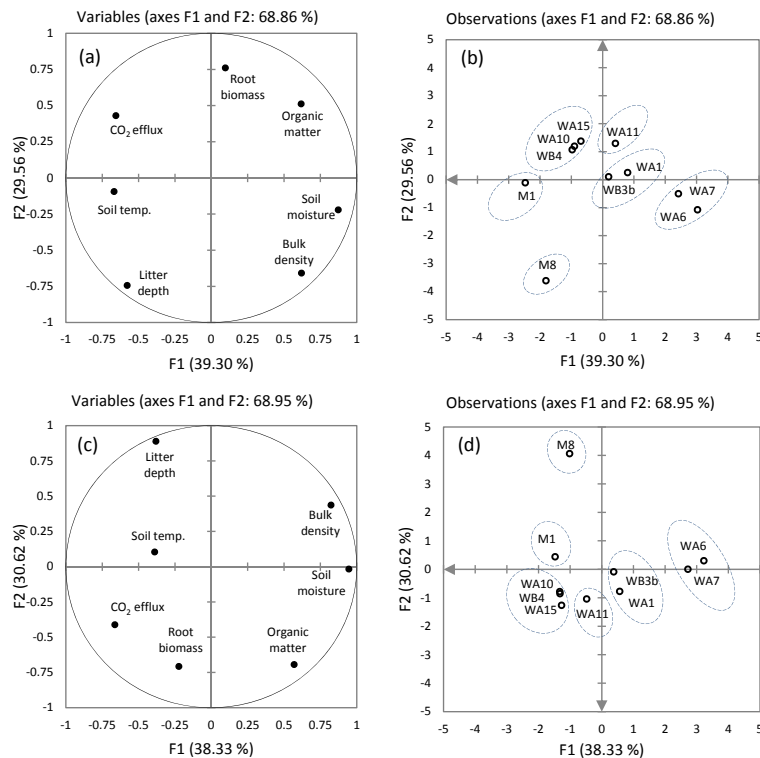
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Fig. 4. Multiple factor analysis (MFA) based on seasonal means of observed variables from 2011 to 2012, **(a)** and **(c)** correlations between variables and factors over spring and summer respectively, **(b)** and **(d)** dependence of measurement sites on the factors and clustering over spring and summer respectively.

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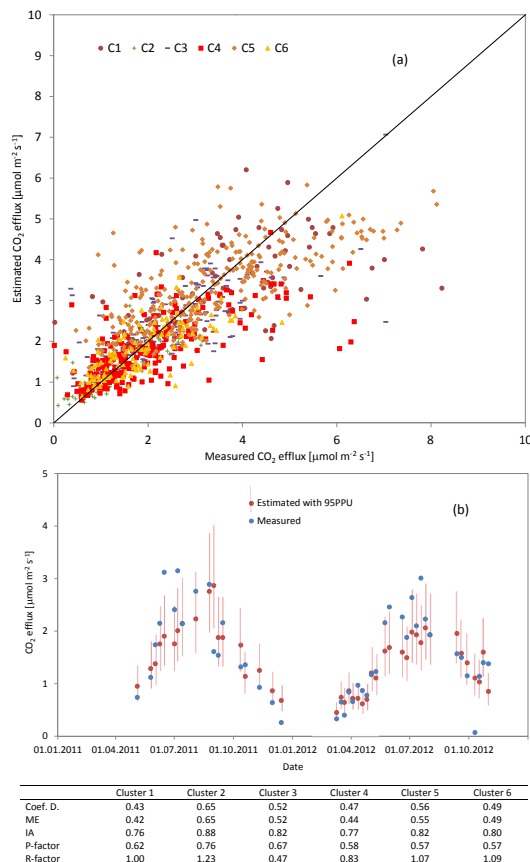


Fig. 5. Estimated vs. observed CO₂ efflux based on the time-dependent rating of specific-site production and transport approach. **(a)** Scatter plot of simulated vs. measured CO₂ efflux for all clusters from 2006 to 2012, **(b)** simulated vs. measured CO₂ efflux with associated 95 percent prediction uncertainty (95PPU) from 2011 to 2012 for the site M8 (cluster C2). C1...6 means clusters 1...6.

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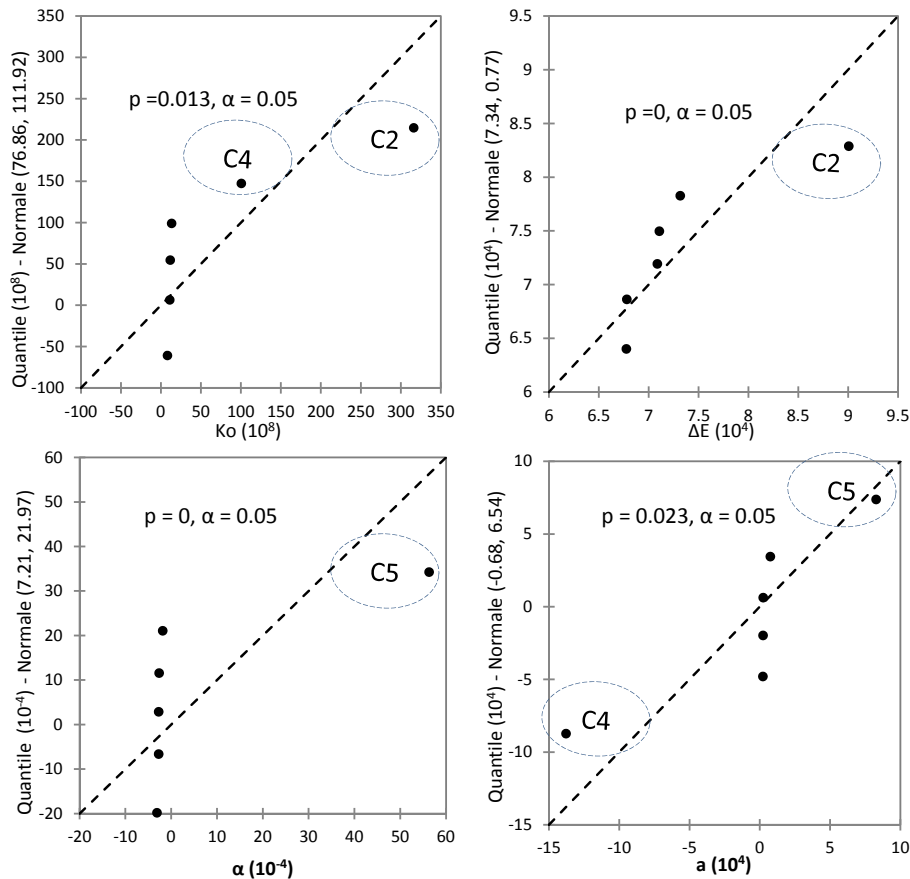


Fig. 6. Scattergram of parameter quantiles according to the Anderson–Darling test (see Table 3 for the parameter units). When the computed p value is greater than the significance level α , the parameter follows a normal distribution.

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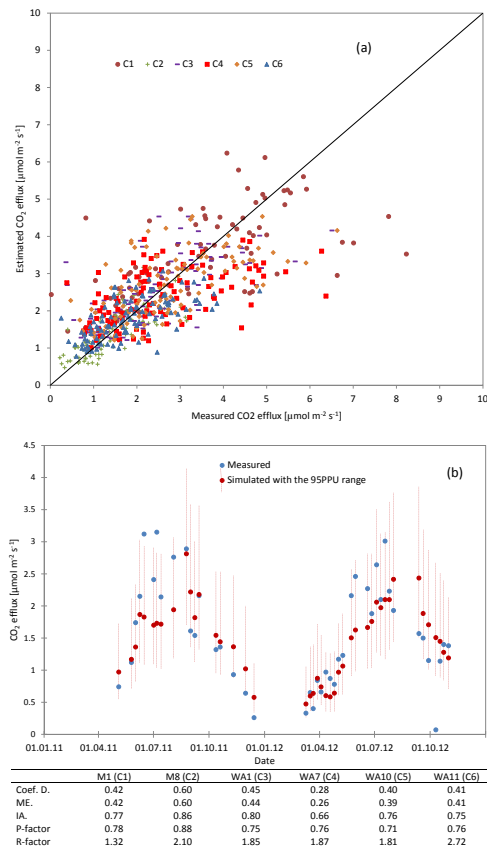


Fig. 7. Simulated vs. observed CO₂ efflux for selected sites from the clusters using HYDRUS-1D. The simulation quality measures are displayed in the associated table. **(a)** Scatter plot of simulated vs. measured CO₂ efflux for all clusters from 2006 to 2012, **(b)** simulated vs. measured CO₂ efflux with associated 95 % prediction uncertainty (95PPU) from 2011 to 2012 for the site M8 (cluster C2). C1... 6 means clusters 1... 6.

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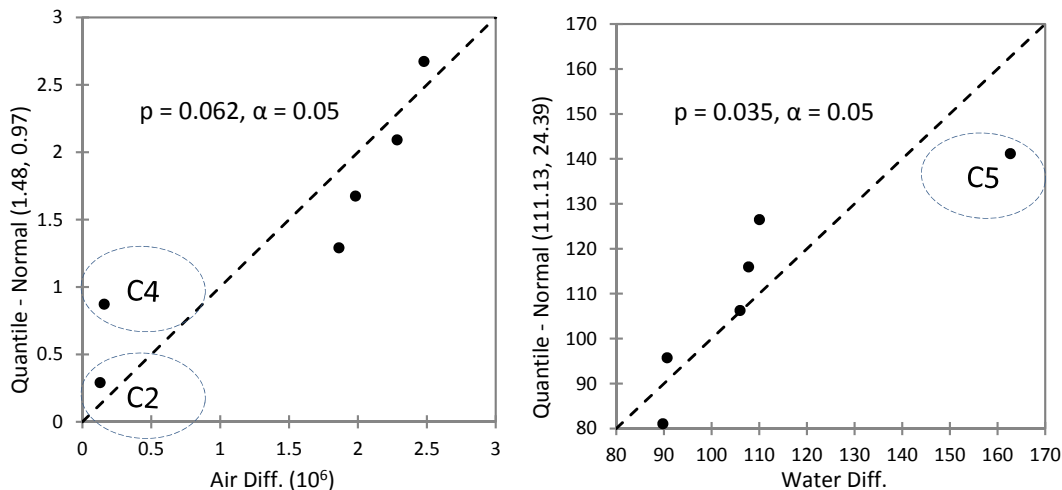


Fig. 8. Scattergram of parameter quantiles according to the Anderson–Darling test (see Table 5 for the parameter units). When the computed p value is greater than the significance level alpha, the parameter follows a normal distribution. Air diff. follows a normal distribution, while water diff. is not.

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