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

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Abstract. CO_2 production and transport from forest floors is an important component of the carbon cycle and is closely related to the global atmosphere CO_2 concentration. If we are to understand the feedback between soil processes and atmospheric CO_2, 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 measurement sites led to the detection of site clusters along two CO_2 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 CO_2 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 soil moisture dependency parameter, 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 calibrated based on observed soil temperatures. The results were used to adjust CO_2 productions by soil microorganisms and plant roots under optimal conditions for each cluster. Although the uncertainty associated with the HYDRUS-1D simulations is higher, the results were consistent with both the multivariate clustering and the time-dependent rating of site production.

Finally, four clusters with significantly different environmental conditions (i.e. permanent high soil moisture condition, accumulated litter amount, high variability in soil moisture content, and dominant temperature dependence) were found to be relevant in explaining the spatio-temporal variability of CO_2 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 CO_2 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 CO_2 from the soil surface is the result of a number of complex processes, including CO_2 production, gas transport and interactions between physical and biological factors within the soil (Moncrieff and Fang, 1999). 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., 2005). Soil respiration is often measured as a flux of carbon dioxide from the soil surface, i.e. as soil CO_2 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).

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 CO_2 transport to the atmosphere is controlled by the rate of CO_2 production in the soil, the CO_2 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). The effects of soil temperature and soil moisture on CO_2 effluxes are nonlinear 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 (Fiener et al., 2011; Hashimoto et al., 2009; Niinistö et al., 2011; Shi et al., 2006) have based CO_2 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 CO_2 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 CO_2 efflux and the soil moisture dependency parameter that characterizes a specific location. Richter et al. (1996) used a combination of the Arrhenius law and the Walker's empirical formula (Walker and Allen, 1984) to express temperature and moisture dependency through soil layers. This combination of laws could be used as a rating factor of soil CO_2 efflux in regions where dependence on soil moisture is high.

Only a small number of studies have based a direct estimation of CO_2 efflux on soil moisture content. For example, Xu and Qi (2001) applied soil moisture thresholds depending on site conditions to inter-seasonal CO_2 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 CO_2 efflux for soil volumetric moisture $< 19\%$ 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 CO_2 efflux but poor predictors of the spatial variations of soil CO_2 efflux. In a study in a temperate forest Sitka spruce stand, Saiz et al. (2007) showed that soil temperature is the dominating factor, but soil moisture is more variable and had an overall negative effect on soil respiration.

By assuming that the influence of soil moisture and temperature was negligible, Fang et al. (1998) followed ideas developed by Sokal and Rohlf (1995) in which root and microbial respiration are considered as predictor variables when characterizing the spatial variability of CO_2 efflux in a forest ecosystem in a Florida slash pine plantation. They developed a simple model to specify the spatial variation in CO_2 efflux

by further assuming that (1) live and dead biomass dominate the distribution of CO_2 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 CO_2 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 possible with a relatively small number of process-based models (e.g. SOILCO2, PATCIS, HYDRUS-1D) (Fang and Moncrieff, 1999; Šimůnek et al., 2005; Šimůnek and Suarez, 1993a, b). In these models, CO_2 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. CO_2 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 CO_2 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, but can be improved. Furthermore, the complexity of the models hampers the understanding of the processes and variables included in the model (Pumpanen et al., 2003). While applying HYDRUS-1D for the simulation of soil respiration in an agricultural field, Buchner et al. (2008) showed that HYDRUS-1D is well suited for modelling and that CO_2 efflux strongly depends on soil hydrological properties which determine degradation as well as transport rates within the soil.

The spatio-temporal variability of soil respiration is analysed in a number of studies ranging from global to local scales. Reichstein et al. (2003) analysed 17 sites in Europe and North America with different site properties. Within the EUROFLUX project, Morales et al. (2005) applied different models for a number of sites spread over Europe to determine model applicability to this data set. From this study, not too much can be learned concerning the effect of site conditions on soil respiration. Kang et al. (2003) studied the effect of local topographic and climatic conditions on soil respiration in Korea. They compared six slopes with different aspect, elevation, and rainfall and found again that temperature is the most important driver. Pacific et al. (2009) investigated how large the effect of local-scale topography is on soil respiration. They analysed two different positions along a transect

from the riparian zone of a river to the drier hill slope for two short periods (less than 3 months) in a wet and a dry year. They found a strong influence of the hill slope position on soil respiration which is further modified by climate conditions. Because the measurement periods were rather short and they did not attempt to model the data, the findings cannot be transferred directly to other sites.

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 viable, it indicates that a high level of complexity may exist and affect the specification of CO_2 variability within the study area. Multivariate analyses, such as multiple factor analyses, may potentially provide linkages between environmental properties and CO_2 efflux and account for similarities and dissimilarities between the investigated measurement sites.

The objective of this study is to analyse and understand the spatio-temporal variability of CO_2 efflux patterns and their determining factors from measurement sites with significantly different environmental properties, qualified as specific sites. This objective is met by applying multivariate data analysis techniques to develop a simple nonlinear model describing a time-dependent rating of site-specific CO_2 production and transport and comparing results with the output of the process-based HYDRUS-1D model system.

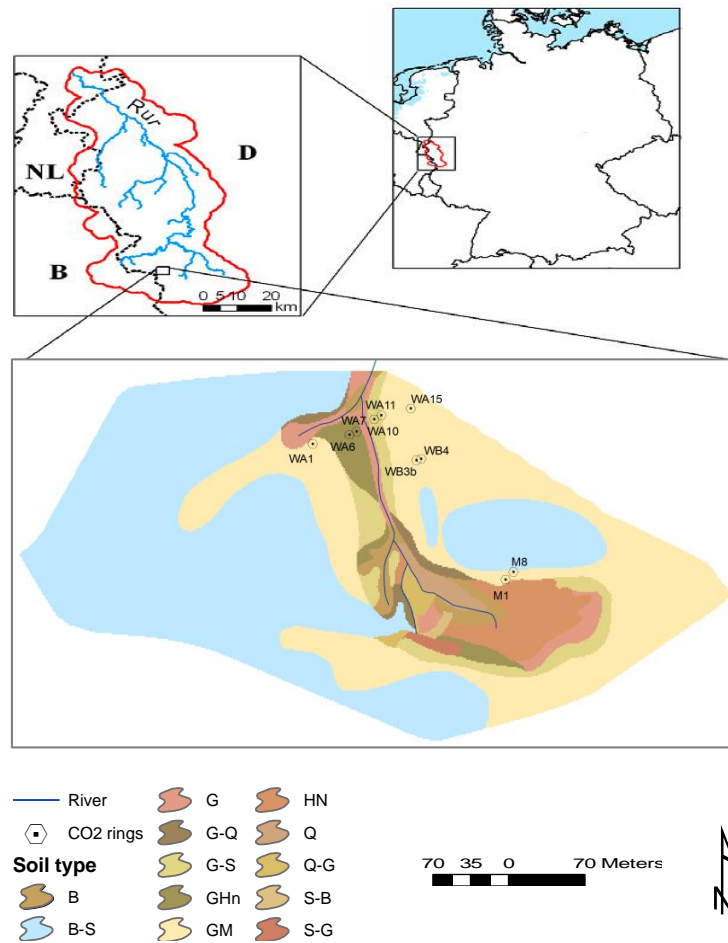## 2 Materials and methods

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 Erkensruhr River in western Germany. The catchment has a warm temperate oceanic climate with a mean annual temperature of 7 °C, 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 1–3 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 and data processing

In this study, soil CO_2 efflux was measured on a weekly basis using a closed dynamic chamber system (LI-8100, Li-Cor Inc., Lincoln, Nebraska, USA). The CO_2 efflux from the soil was estimated by placing the chamber on PVC collars (20 cm diameter) and measuring the increase of CO_2 within the chamber. The insertion depth of the collars was 5–8 cm into the forest floor. Along with soil CO_2 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. Measurements in the depth of 11 cm were available for the whole measurement period, while soil temperature measurements in 5 cm depth were limited to the period 2008–2010. Dwersteg (2012) analysed the differences in correlation between 5 and 11 cm using an Arrhenius relationship. She found that the coefficient of determination slightly reduces from 0.9 to 0.85 when data are used from 11 cm depth instead of 5 cm. Because of the variability in the thickness of the litter layer, Dwersteg decided to use 11 cm depth in order to always be in the mineral soil. This is similar to the approach of Saiz et al. (2007) who compared soil temperature measurements in 2 and 10 cm soil. 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). A total of 80 single points along two different transects across the investigated catchment river and at a grid set-up in the southern part of the catchment were monitored from 2006 to 2012 (cf. Dwersteg, 2012 for more details). In the present study, our objective is to analyse how the heterogeneity of the catchment is affecting the CO_2 pattern, so 10 measurements sites were selected according to different site properties. To confirm the selection process, the measurements of the 10 selected sites were grouped using a cluster analysis to show consistencies with the selection criteria, such as topography, soil type and proximity to the river. It should be noted that in our approach a high number of clusters is expected.

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 (8 cm diameter), and detailed soil profiles for bulk density were generated for each soil type (in total eight 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 matter content in the soil or litter was determined using a Carbon/Nitrogen/Sulphur analyser (CNS-2000, Leco, St. Joseph, Michigan, USA). Soil bulk density was determined by retrieving undisturbed cores of known

Figure 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).

Site	Soil type	Slope (%)	Elevation (m)	Bulk density [g cm^{-3}]	Root biomass [g m^{-2}]	Organic matter [g m^{-2}]	Litter thickness [m]
WA1	S-B: Gleyic Cambisol	8.84	600	0.82	131.25	10029.67	0.02
WA6	S-G: Stagnic Eutric Gleysol	5.59	598	0.91	73.20	12272.50	0.02
WA7	S-G: Stagnic Eutric Gleysol	5	598	0.90	73.20	12272.50	0.02
WA10	B-S: Cambisol	5.3	597	0.67	177.73	10029.67	0.04
WA11	B-S: Cambisol	7.29	598	0.70	177.73	10029.67	0.02
WA15	S-B: Gleyic Cambisol	12.87	601	0.70	131.25	10029.67	0.02
WB3	S-B: Gleyic Cambisol	12.75	604	0.82	131.25	12511.83	0.03
WB4	S-B: Gleyic Cambisol	14.25	605	0.76	131.25	12511.83	0.02
M1	S-B: Gleyic Cambisol	7.29	616	0.76	28.58	11019.17	0.04
M8	S-B: Gleyic Cambisol	7.29	617	0.84	52.40	7330.17	0.08

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 detach roots from soil mineral particles. The washed root mass was then determined by classifying it into diameter classes and weighing it after being oven-dried at 70 °C for 48 h. The grain size distribution was analysed according to Köhn (ISO 11 277) and by using a

particle analyser (Analysette 22, Fritsch, Germany). Soil information for the model 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 site-specific CO_2 efflux

The combined effects of soil temperature and soil moisture were used as a time-dependent rating factor affecting a site-specific optimal CO_2 production and transport. This method is a generalized estimation approach to characterize CO_2 efflux within the catchment. In the method, observed soil temperature, soil moisture, soil parameters and soil CO_2 efflux are used to automatically solve a generalized equation where only site-specific CO_2 production and transport parameters are unknown. The classical law of Arrhenius, the empirical formula of Walker and Allen (1984), and a formula characterizing a site-specific CO_2 efflux developed by Fang et al. (1998) are combined to account for the temporal pattern of soil CO_2 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 site-specific CO_2 efflux from the soil surface at a certain time t and in a forest environment can be expressed as a sum of root and microbial respiration:

$$F^* = R_r + R_{ml} + R_{ms}, \tag{1}$$

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

$$F^* = a + bB\phi + cM_l - d\ln(M_s)/\phi, \tag{2}$$

where B is the biomass of live fine roots in the soil, ϕ is the soil total porosity, M_l 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).

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

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 parameter describing soil moisture dependency (T^{-1}), A is the humidity response function parameter set equal to 1 in the following

steps as in Richter et al. (1996), and R is the gas constant ($kJ\,(mol\,K)^{-1}$).

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

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).

2.4 HYDRUS-1D parameterization

HYDRUS-1D (Šimůnek et al., 2005) is a one-dimensional process-based model used in this study to simulate daily soil CO_2 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-1D 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.

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

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. $\beta = 0°$ for vertical flow, 90° for horizontal flow, and $0° < \beta < 90°$ 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 CO_2 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 CO_2 is considered as the sum of the production by soil microorganisms and by plant roots. HYDRUS-1D also assumes that the CO_2 transport in the unsaturated zone can occur in both the liquid and gas phases. Furthermore it is assumed that the CO_2 concentration in the soil is governed by two transport processes: convective and diffusive transport in both gas and aqueous phases, and CO_2 production and/or removal (Patwardhan et al., 1988).

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 1 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 CO_2 simulations were estimated and optimized from the soil moisture measurements using an inverse modelling approach included in HYDRUS-1D. The 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.

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

where, m_q and 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 jth 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), and v_j and $w_{i,j}$ are weights associated with a particular measurement set or point, respectively.

2.6 Uncertainty approach

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 between measured and simulated values within the range of 0 to 1. The ME describes the degree of accordance between observed and simulated values and varies between $-\infty$ and 1.

The index of agreement ranging between 0 and 1 is strongly influenced 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 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 % 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 CO_2 efflux

The measurements ($n = 984$ observations) analysed in this work are from 10 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 site-specific soil moisture and thus greatly affect the CO_2 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 site-specific behaviour. Nevertheless, this result should also be analysed 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.

Table 1. Descriptive statistics (n=984 observations) for 10 sites (M1, M8, WA1, WA6, WA7, WA10, WA11, WA15, WB3, WB4) from 2006 to 2012 along two transects (cf. Fig. 1 for the locations of measurement sites and for more details). 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^{-3})	28.6	177.7	113.2	47.9	0.42	yes
Organic matter (g m^{-3})	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 (°C)	0.00	15.80	8.58	–	-	–
CO$_2$ efflux (μmol m^{-2} s^{-1})	0.02	8.74	2.51	–	–	–

Figure 2 shows CO_2 efflux rates for the investigated sites with their dependence on soil temperature and soil moisture for seasonal means over the period 2011 to 2012. The circle sizes indicate the rate of CO_2 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 at relatively fix temperature ranges (seasonal means) shows that emission rates decrease with increasing soil moisture. A clear dependence of the CO_2 pattern on soil temperature (transition from spring to summer) is not necessarily shown, even if the humidity conditions are similar, which is likely for the sites WA6 and WA7 as they are close to the river bed (permanently wet). In addition, CO_2 emission rates 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 CO_2 efflux rate may also remain similar (e.g. M8). Thus, the CO_2 efflux rate remained, for instance, almost unchanged at 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, CO_2 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.

In summary, site WA6 is characterized by very low CO_2 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 behaviours of the other sites, if existing, remain unclear.

Combining information from Fig. 2 and calculated mean efflux values, it can be seen that

1. a seasonal (spring) mean soil CO_2 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 remains relatively close to 8 °C

2. a seasonal (summer) mean soil CO_2 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. CO_2 efflux, soil moisture and soil temperature) from 2011 to 2012 were combined as multivariate data for a multiple factor analysis. In Fig. 3, the results show two main axes (factors F1 and F2) controlling about 70 % of the total observed variance. CO_2 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. CO_2 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. CO_2 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 relatively constant and low emission rate at the site M8 results mainly from the litter depth. The figures show that if the

Table 2. Potential clusters for characterizing the patterns of CO_2 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	WA6	WA10	WA11
		WB3	WA7	WA15	
				WB4	
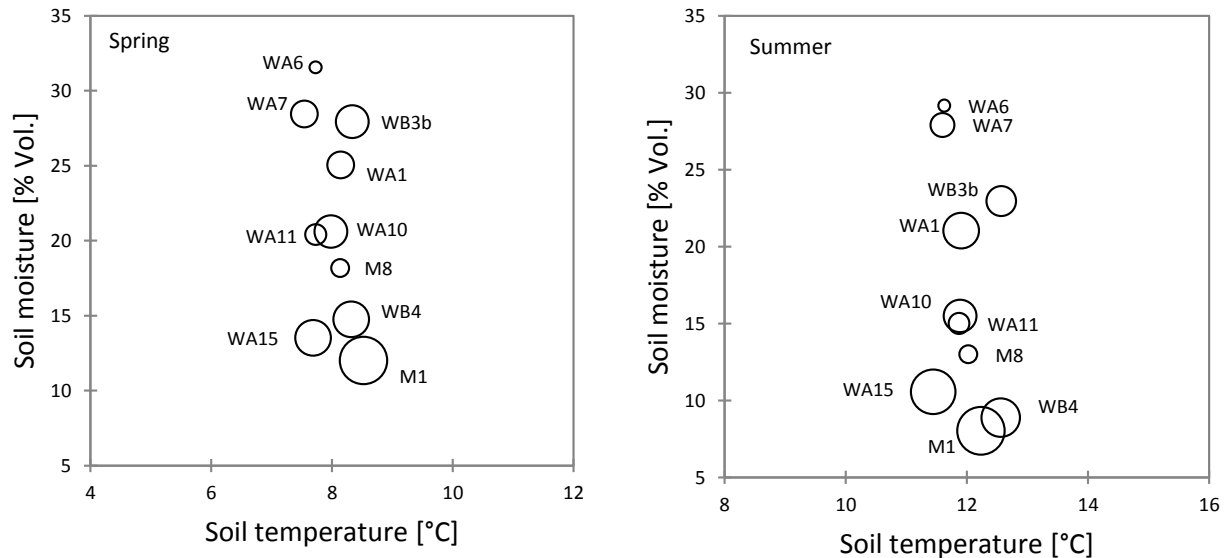
Figure 2. 2-D plot of CO_2 efflux dependency on soil temperature and soil moisture and likely clustering based on average values observed from 2011 to 2012. The circle sizes indicate the rate of CO_2 efflux at a given site.

litter is a factor that indirectly and positively influences the CO_2 efflux through microorganism respiration, it could be at the same time a factor that regulates the emission rate (negative correlation between the litter depth and CO_2 efflux). The site WA11 is mainly controlled by the root biomass. The sites WA10, WA15 and WB4 gathered in Cluster 5 (Fig. 3 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. Clusters C2, C4 and C5 are the most geometrically distant in reference to the Fig. 3 and should lead to significantly different site-specific parameters shown in Eq. (4) (e.g. reaction rate at reference temperature, activation energy, parameter describing soil moisture dependency, cluster constants).

3.2 Site cluster weighting and characterization

Figure 4 shows the estimated and observed soil CO_2 efflux and the quality measure displayed in the bottom table. As mentioned in Sect. 2, the estimations are based on a non-linear time-dependent rating of site-specific models (Eq. 4).

The estimation quality remains on average with coefficients of determination ranging from 0.43 to 0.65, model efficiencies from 0.36 to 0.51, and indices of agreement from 0.73 to 0.82. Uncertainty quality measures are relatively high, with more than 50 % of the measurements captured by the 95 % prediction band, ranging from 53 to 60 %. The R factor ranges between 0.53 and 1.09. 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 site-specific parameters are shown in Table 3. This table shows the large dissimilarities between clusters C2, C4 and C5/C6, compared to the others. These results are consistent with the multiple factor analysis discussed in the Sect. 3.1, in which 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 average data, while the parameter estimations are based on the weekly scale data.

Table 3. Factor parameters obtained for the different clusters (cf. Eq. 4). $k_0 =$ reaction rate at reference temperature T_0 (T^{-1}), $\Delta E =$ activation energy ($\mathrm{J\,mol}^{-1}$), $\alpha =$ parameter describing soil moisture dependency (T^{-1}), $a =$ cluster constant, $b =$ root biomass factor, $c =$ litter layer factor, $d =$ organic matter factor.

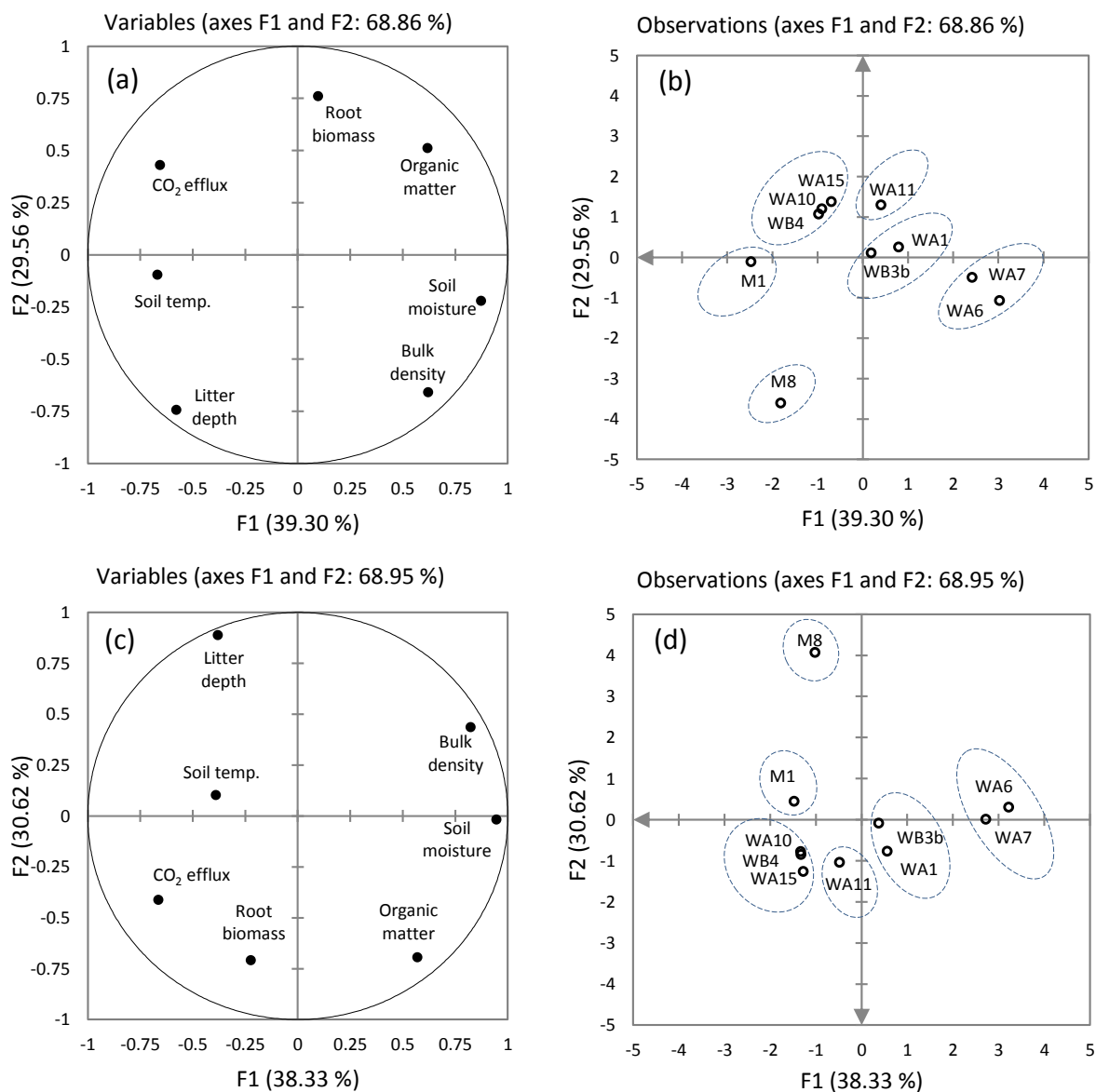|	k_0 (10^8)	$\Delta E (10^4)$	α (10^{-4})	a (10^{-2})	b (10^{-2})	c (10^{-2})	d (10^{-2})
Cluster 1	12.22	7.12	−2.78	2443546.23	2978.67	30088896.19	471.59
Cluster 2	316.17	9.00	−3.09	39840964.13	10332.46	1551055746.34	0.10
Cluster 3	11.12	6.78	−2.74	432919.94	97620.17	0.10	627307.69
Cluster 4	13.41	6.78	56.32	818192.95	0.10	0.10	0.00
Cluster 5	8.16	7.09	−2.63	640958.13	13557.46	26824424.54	7480.35
Cluster 6	68.68	7.23	−1.85	0.88	1583662.25	39.94	5289549.76

Figure 3. Multiple factor analysis (MFA) based on seasonal means of observed variables from 2011 to 2012. **(a)** and **(c)** are the correlations between variables and factors over spring and summer, respectively; **(b)** and **(d)** are the dependence of measurement sites on the factors and clustering over spring and summer, respectively.
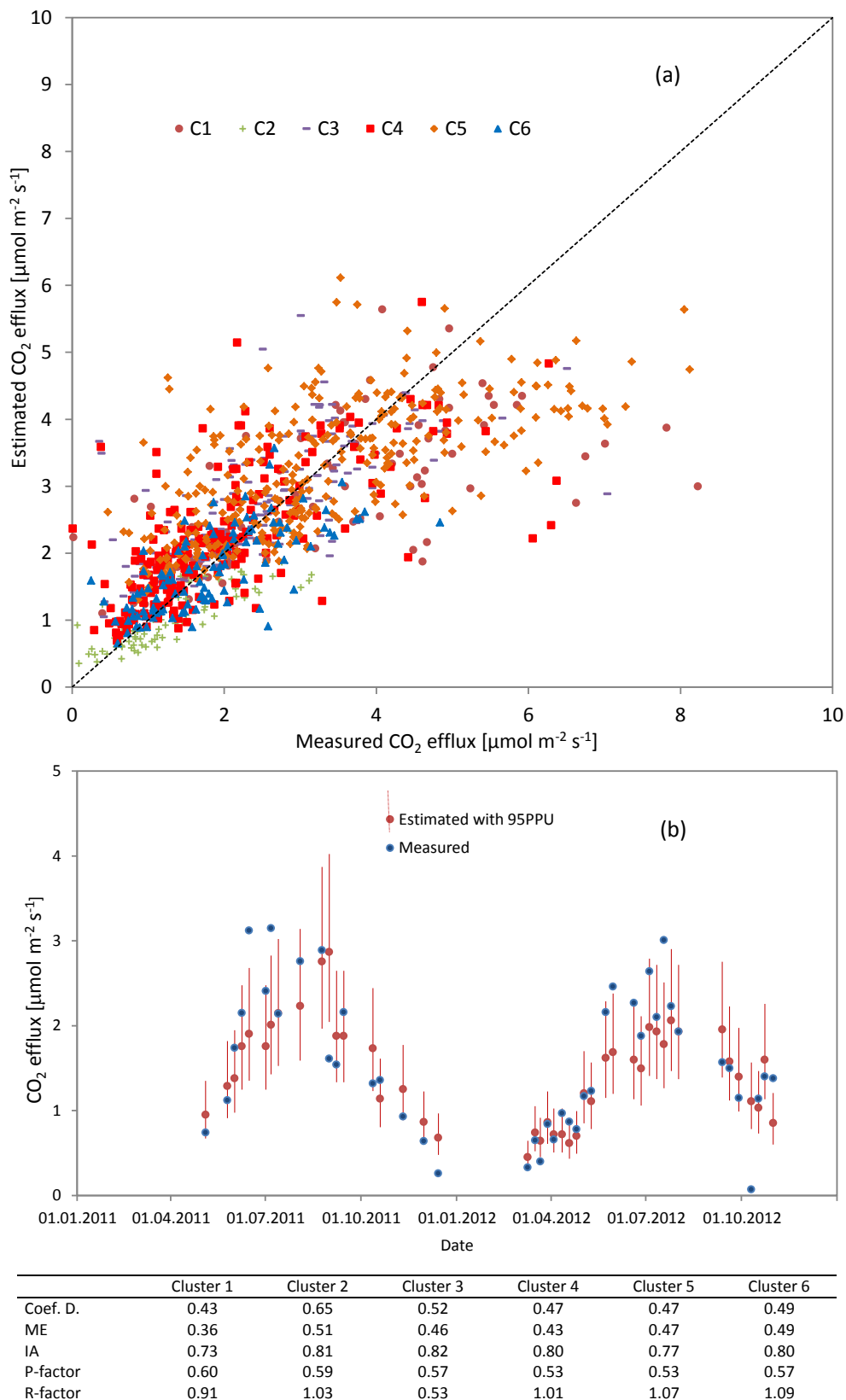
Figure 4. Estimated vs. observed CO_2 efflux based on the time-dependent rating of site-specific production and transport approach (Eq. 4). **(a)** Scatter plot of simulated vs. measured CO_2 efflux for all clusters from 2006 to 2012, **(b)** simulated vs. measured CO_2 efflux with associated 95 percent prediction uncertainty (95PPU) from 2011 to 2012 for the site M8 (cluster C2). C1…6 means clusters 1…6.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6
Coef. D.	0.43	0.65	0.52	0.47	0.47	0.49
ME	0.36	0.51	0.46	0.43	0.47	0.49
IA	0.73	0.81	0.82	0.80	0.77	0.80
P-factor	0.60	0.59	0.57	0.53	0.53	0.57
R-factor	0.91	1.03	0.53	1.01	1.07	1.09

Combining information drawn from Fig. 4 and Table 3, it appears that clusters C1, C2, C4 and C5 may be seen as representative when characterizing the spatio-temporal pattern of CO_2 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. 3 and does not display any clear characteristic values in Table 3.

2. As previously found, Cluster C2 is minimally affected by the time-dependent rating factor but highly influenced by the combined effects of root biomass and litter depth. The effects of the litter depth are predominant and expressed as an inhibiting factor for CO_2 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. As discussed in Sect. 3.1, if the litter is a factor indirectly and positively influencing the CO_2 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 CO_2 efflux). As already mentioned, different depths 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).

3. Cluster C4 was found to be minimally 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 value as for the parameter describing soil water dependency (Table 3).

4. Clusters C5 and C6 are highly influenced by the combined effects of the time-dependent rating factor and the root biomass. This result is explained by the low value obtained for the parameter describing soil moisture dependency and the specific value obtained for the cluster constant (Table 3).

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-year experiment) on soil CO_2 efflux and found out that soil respiration was significantly reduced. Sulzman et al. (2005) studied the contribution of litter to total soil CO_2 efflux in an old growth 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 CO_2 efflux from surface litter at four rain forest sites in the eastern Amazon. They found that litter contribution showed no clear seasonal change, though experimental precipitation exclusion was associated with a 10-fold reduction in litter respiration relative to unmodified sites. These findings invite more attention and studies on how litter controls CO_2 efflux.

Table 4 shows Pearson correlations between the site-specific factors (cluster constant, root biomass factor, litter layer factor, organic matter factor). These correlations are overall insignificant, ensuring that the evaluated nonlinear model is not over-parameterized.

3.3 CO_2 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 CO_2 efflux for one site picked from each cluster presented in the previous sub-sections.

Figure 5 shows observations versus best simulations with the associated uncertainty ranges for the soil CO_2 efflux of the measurement sites picked up from the clusters. The table associated with Fig. 5 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).

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 site-specific CO_2 production and transport.

Table 5 shows calibrated values for site-specific CO_2 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 CO_2 production by soil microorganisms for the entire soil profile and the optimal CO_2 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 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
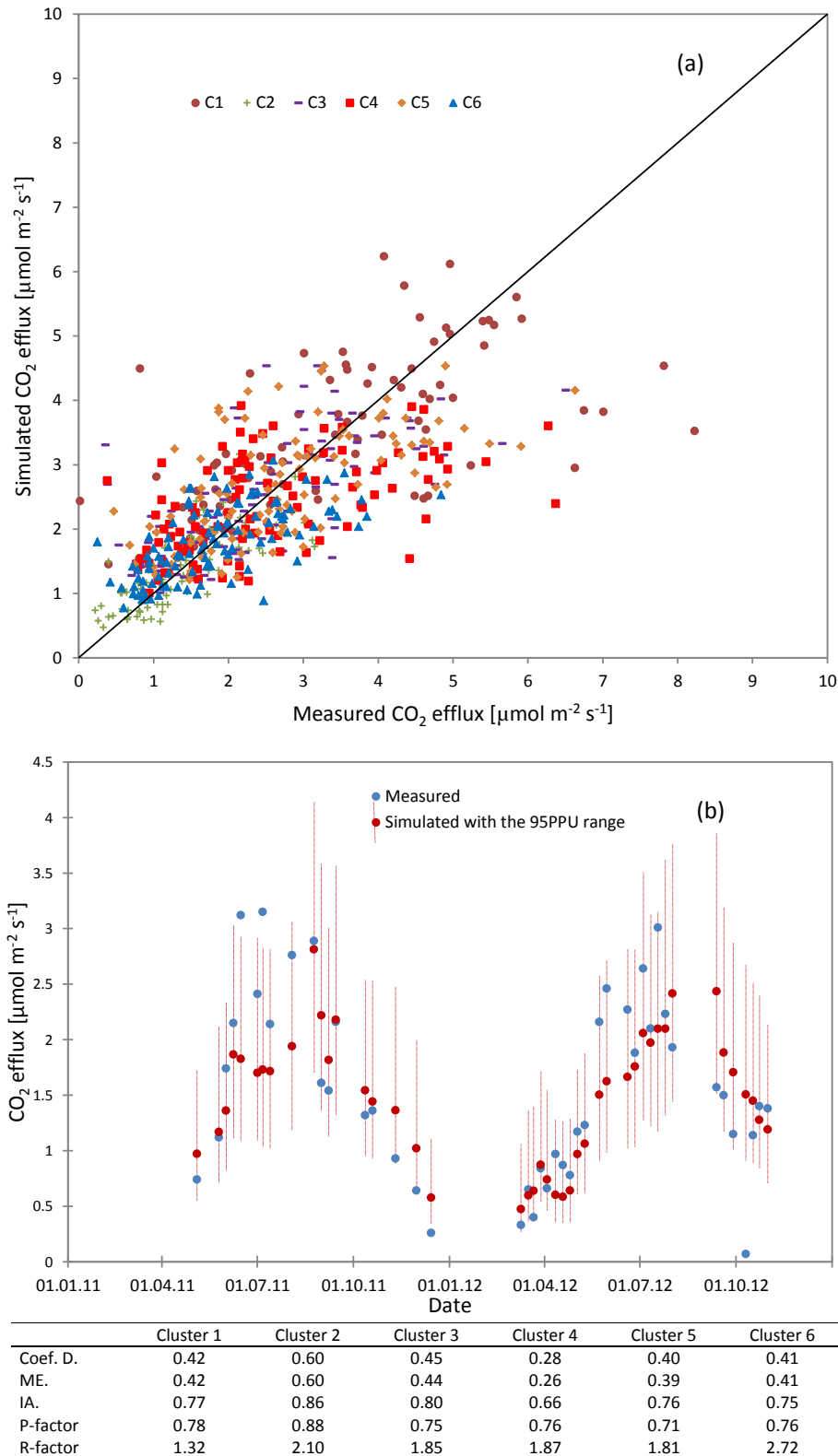
Figure 5. Simulated vs. observed CO_2 efflux for selected sites from the clusters using HYDRUS-1D. The simulation quality measures are displayed in the associated table. **(a)** Scatter plot of simulated vs. measured CO_2 efflux for all clusters from 2006 to 2012, **(b)** simulated vs. measured CO_2 efflux with associated 95 percent prediction uncertainty (95 PPU) from 2011 to 2012 for the site M8 (cluster C2). C1...6 means clusters 1...6.

	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6
Coef. D.	0.42	0.60	0.45	0.28	0.40	0.41
ME.	0.42	0.60	0.44	0.26	0.39	0.41
IA.	0.77	0.86	0.80	0.66	0.76	0.75
P-factor	0.78	0.88	0.75	0.76	0.71	0.76
R-factor	1.32	2.10	1.85	1.87	1.81	2.72

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		*0.982*	*−0.241*	*0.976*	*−0.023*	*0.980*	*−0.042*
ΔE	**0.982**		*−0.330*	*0.975*	*−0.078*	*0.977*	*−0.102*
α	−0.241	−0.330		*−0.211*	*−0.203*	*−0.219*	*−0.212*
a	**0.976**	**0.975**	−0.211		*−0.238*	*0.999*	*−0.256*
b	−0.023	−0.078	−0.203	−0.238		*−0.220*	*0.998*
c	**0.980**	**0.977**	−0.219	**0.999**	−0.220		*−0.238*
d	−0.042	−0.102	−0.212	−0.256	**0.998**	−0.238	

Table 5. Estimated parameters of the HYDRUS-1D model: Air Diff. = Molecular diffusion coefficient of carbon dioxide in air (mm^{-2} d^{-1}); Water Diff. = Molecular diffusion coefficient of carbon dioxide in water (mm^{-2} d^{-1}); OCDP microorganisms = Optimal CO_2 production by soil microorganisms for the entire soil profile (µmol m^{-2} s^{-1}); OCDP roots = Optimal CO_2 production by plant roots for the entire soil profile (µmol m^{-2} s^{-1}).

	M1 (C1)	M8 (C2)	WA1 (C3)	WA7 (C4)	WA10 (C5)	WA11 (C6)
Air Diff.	1 373 760	1 373 760	1 373 760	1 373 760	1 373 760	1 373 760
Water Diff.	152.9	152.9	152.9	152.9	152.9	152.9
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

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 partly consistent with conclusions drawn from Fig. 3 in Sect. 3.1, where attention was drawn to a likely inhibiting effect of the litter depth on the CO_2 production and transport with a direct link to very low air and heat circulation. This result helps make clear why the activation energy found in Sect. 3.2 (Table 3) is very high. The highest CO_2 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. 3 (Sect. 3.1).

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 CO_2 efflux measurements and multivariable environmental properties in a western German forest ecosystem.

For the period 2011 to 2012, data from 10 selected measurement sites in the spruce-dominated forest floor of the Wüstebach catchment have shown a spring mean soil CO_2 efflux ranging from 1.2 to 3 µmol m^{-2} s^{-1} (1.7 to 4.5 µmol m^{-2} s^{-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 remains around 8 °C (12 °C in summer). This less pronounced seasonal trend hides complex interactions between environmental factors, time-dependent factors and the CO_2 efflux rate (Metcalfe et al., 2007).

A multivariate clustering of the measurement sites decreased the complexity level of the environmental control on CO_2 efflux and allowed concordant evaluations of a simple nonlinear model of time-dependent rating of site-specific CO_2 production 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 CO_2 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 bio-chemical 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 CO_2 efflux and providing reference characteristic values for the investigated area. Parameters such as the one describing soil moisture dependency were specified for the clusters, accounting for the link between soil moisture and changes in soil CO_2 emission rate. The results provide many other pattern characteristics, such as the optimal CO_2 production by soil microorganisms for the entire soil profile and the optimal CO_2 production by plant roots for the entire soil profile.

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

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