MODELING SOIL CO_2 PRODUCTION AND TRANSPORT TO INVESTIGATE THE INTRA-DAY VARIABILITY OF SURFACE EFFLUX AND SOIL CO_2 CONCENTRATION MEASUREMENTS IN A SCOTS PINE FOREST (PINUS SYLVESTRIS, L.)

Stéphanie Goffin[a,]*, Christophe Wylock[b], Benoit Haut[b], Martin Maier[c], Bernard Longdoz[d,e], Marc Aubinet[a]

[a]Université de Liège–Gembloux Agro-Bio Tech, Unit of Biosystem Physics, 5030 Gembloux, Belgium

[b]Université Libre de Bruxelles (ULB), Transfers, Interfaces and Processes (TIPs), 50 av. F.D. Roosevelt CP 165/67, 1050 Brussels, Belgium

[c]University of Freiburg, Chair of Soil Ecology,79085 Freiburg im Breisgau, Germany

[d]INRA, UMR d'Ecologie et Ecophysiologie Forestières, UMR1137, Champenoux, F-54280, France

[e]Université de Lorraine, UMR d'Ecologie et Ecophysiologie Forestières, UMR1137, Vandoeuvre Les Nancy, F-54500, France

* Corresponding author: stp.goffin@gmail.com / Tel: +32 81 62 24 90 / Fax: +32 81 62 24 39

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

MODELING SOIL CO_2 PRODUCTION AND TRANSPORT TO INVESTIGATE THE INTRA-DAY VARIABILITY OF SURFACE EFFLUX AND SOIL CO_2 CONCENTRATION MEASUREMENTS IN A SCOTS PINE FOREST (PINUS SYLVESTRIS, L.)

Stéphanie Goffin[a,*], Christophe Wylock[b], Benoit Haut[b], Martin Maier[c], Bernard Longdoz[d,e], Marc Aubinet[a]

[a]Université de Liège–Gembloux Agro-Bio Tech, Unit of Biosystem Physics, 5030 Gembloux, Belgium

[b]Université Libre de Bruxelles (ULB), Transfers, Interfaces and Processes (TIPs), 50 av. F.D. Roosevelt CP 165/67, 1050 Brussels, Belgium

[c]University of Freiburg, Chair of Soil Ecology,79085 Freiburg im Breisgau, Germany

[d]INRA, UMR d'Ecologie et Ecophysiologie Forestières, UMR1137, Champenoux, F-54280, France

[e]Université de Lorraine, UMR d'Ecologie et Ecophysiologie Forestières, UMR1137, Vandoeuvre Les Nancy, F-54500, France

* Corresponding author: stp.goffin@gmail.com / Tel: +32 81 62 24 90 / Fax: +32 81 62 24 39

Abstract

Aimed:

The main aim of this study is to improve the mechanistic understanding of soil CO_2 efflux (F_s), especially its temporal variation at short-time scales, by investigating, through modeling, which underlying process among CO_2 production and its transport up to the atmosphere is responsible for observed intra-day variation of F_s and soil CO_2 concentration [CO_2].

Methods:

In this study, a measurement campaign of F_s and vertical soil [CO_2] profiles was conducted in a Scots Pine Forest soil in Hartheim (Germany) and used to develop a model testing several hypotheses. A reference model taking into account a purely diffusive CO_2 transport and a temperature-dependent CO_2 production is compared to models with a more complex description of either CO_2 production or CO_2 transport. For transport, the introduction of advection and the dispersion is investigated. For the production, the emergent hypothesis of the phloem pressure concentration wave (PPCW) influence is tested.

Results:

We show that intra-day variation of F_s and [CO_2] is better represented when the more complex CO_2 production expression is taken into account compared to the more detailed description of CO_2 transport.

Conclusion:

We conclude that focus should be placed on the potential factors affecting the CO_2 production, rather than on the transport process description

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Keywords: Soil CO_2 efflux, Production, Transport, Process-based Model, Intra-day Variability

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Introduction

Soil CO_2 efflux (F_s) is the largest source of CO_2 emissions from terrestrial ecosystems (Ryan and Law, 2005). In 2008, the global F_s was estimated at $98\pm12 PgC yr^{-1}$ (Bond-Lamberty and Thomson, 2010) which is about 15 times greater than fossil fuel emissions (Denman et al., 2007). In the context of climate change, it is crucial to understand the mechanisms driving F_s to predict future atmospheric CO_2 concentrations. Even though F_s studies have received attention in recent years, its future response to climate change is far from being clear because of the complexity of controlling mechanisms that interact over several temporal (hours to millennia) and spatial scales (Vargas et al., 2011).

F_s is the result of two main processes: the production of CO_2 (P) within the soil and its transport from the production location up to the atmosphere (Fang and Moncrieff, 1999). Therefore, F_s involves both biological and physical mechanisms. The level of complexity to describe F_s depends on both the spatial and temporal scales of interest (Vargas et al., 2011). For example, at large temporal time scales, transport processes are negligible so it can be assumed that F_s represents CO_2 production (Luo and Zhou, 2006). On the contrary, at short time scale, transport processes can become more significant and can be responsible for a discrepancy between F_s and CO_2 production (Fassbinder et al., 2012; Risk et al., 2012; Gamnitzer et al., 2011; Philips et al., 2010).

Recently, the availability of automated F_s measurement systems has highlighted the F_s intra-day variations and facilitates the identification of their driving factors. There is now evidence that F_s presents clear intra-day cycles that can be large and change abruptly from day to day (Marron et al., 2009; Riveros-Iregui et al., 2008; Doff Sotta et al., 2004; Davidson et al., 2000). The processes responsible for those intra-day variations are still debated. Do those variations come from CO_2 production or CO_2 transport variation within the day?

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

There are two kinds of automatic systems measuring F_s: surface and subsurface approaches (Pumpanen et al., 2010; Savage and Davidson, 2003). Each approach has its own advantages and disadvantages that are largely mentioned in Goffin et al. (2014). The surface approach uses automatic chamber systems to measure F_s at the soil surface. Such measurements integrate all biophysical processes that contribute to F_s without distinguishing CO_2 transport and production. Even if automatic chamber systems offer the possibility to probe a wide spatial coverage (Risk et al., 2008) when multiplying the measurement points, they give no information about the vertical distribution of CO_2 sources (Goffin et al., 2014; Davidson et al., 2006b; Jassal et al., 2004; Hirano et al., 2003; Tang et al., 2003). The subsurface approach consists of the measurement of soil CO_2 concentration vertical profile using gas wells (Hirsch et al., 2004; Risk et al., 2002) or solid state CO_2 sensors (Goffin et al., 2014, Riveros-Iregui et al., 2008; Hirano et al., 2003; Tang et al., 2003). This method allows determining the location of CO_2 production within the soil profile, distinguishing CO_2 production from its transport, but it requires good estimates of multiple soil physical factors (Maier et al., 2014; Vargas et al., 2011; Turcu et al., 2005). Despite limitations of both methods, when used in combination, they can provide modelers the opportunity to answer some questions related to F_s underlying processes.

Today, the scientific community agrees on the necessity of understanding soil respiration (CO_2 production) in a more mechanistic way, i.e. moving towards process-based model (Vargas et al., 2011; Kuzyakov and Gavrichkova 2010; Bahn et al., 2008; Davidson et al., 2006b; Jassal et al., 2004) to be able to reproduce observations like intra-day Fs variations and increase the reliability of Fs prediction under climatic change. The more basic models are driven primarily by temperature and soil water content relationships (Janssens et al., 2003; Davidson et al., 2002). A widespread temperature model is the Q_{10} law but Davidson et al. (2006a) highlighted its limits, by pointing out that the spatial and temporal Q_{10} variability indicates that unidentified factors influencing soil respiration covary with temperature. The Q_{10} decrease in trenched plots (Epron et al., 1999; Boone et al., 1998) and during autumn (Davidson et al., 2006a) suggests that substrate supply to roots may constitute a major controlling factor. Recently, evidences of newly photosynthetic assimilates impacting soil respiration within a very short time scale was reported in tree girdling, shading or labeling experiments (Kuzyakov and Gavrichkova, 2010; Mencuccini and Hölttä, 2010; Bahn et al., 2009; Ekblad and Högberg, 2001; Bahn et al.,2008; Wan and Luo, 2003; Högberg et al., 2006).

Regularly, the intra-day cycles of F_s are also decoupled from any measured temperature (air, soil at multiple depths) (Vargas et al., 2011; Bahn et al., 2008; Tang et al., 2005; Doff Sotta et al., 2004) or correlated to a shallow soil temperature while the production area extends over several horizons (Goffin et al., 2014; Vargas et al., 2011). For example, in a temperate Scots Pine Forest in Germany, the intra-day fluctuations of CO_2 production (P) in Ah horizon (0-20 cm) was strongly correlated with those of the temperature measured at -3 cm when this last influences only the thin shallow part of the Ah enzymatic and root activity (Goffin et al., 2014).. These inconsistencies should probably be attributed to the influence of assimilated carbon availability on P or complex soil CO_2 transport processes comparing to diffusion. Therefore, the intra-day cycle of the aerial climatic variables influencing these availability and processes, constitutes a trail of research increasingly suggested in the literature to explain the intra-day F_s cycles. Among the aerial variables, it is necessary to distinguish those impacting CO_2 transport processes from those impacting CO_2 production.

The aerial variables that could impact CO_2 production are especially photon photosynthetic flux density (PPFD) and vapour pressure deficit (VPD). They are mainly those related to photosynthesis which impacts the substrate supply by roots. On short timescales (from hours to weeks), photosynthesis can act through two different mechanisms on the substrate supply

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

in the rhizosphere: (i) the direct transport of assimilates from leaves to the rhizosphere (through the phloem) (Wingate et al., 2010; Plain et al., 2009) and (ii) the indirect physicochemical effect on root activity through the phloem pressure-concentration waves (PPCW) (Thompson and Holbrook, 2003; Kuzyakov and Gavrichkova, 2010; Mencuccini and Hölttä 2010). The first mechanism driven by PPFD, typically influences the substrate supply to roots with a daily to weekly time lag between leaf assimilation and rhizosphere production (Wingate et al., 2010; Plain et al., 2009; Ekblad et al., 2005), while the second mechanism can act with very shorter time lag (hours). The influence of the PPCW on the regulation of the substrate supply in the rhizosphere is increasingly reported in the literature. An increase in photoassimilate production and transpiration rate (linked to VPD) creates an increase in the turgor pressure at the upper loading phloem end. The pressure propagation through the phloem leads to expulsion of the sucrose molecule from the opposing phloem end (Gavrichkova and Kuzyakov, 2012; Mencuccini and Hölttä 2010). The photoassimilate production depends mainly on the photosynthetically active radiation (PAR), the air temperature and the vapour pressure deficit (VPD). All these variables present an intra-day cycle.

The aerial variables that could impact the soil CO_2 transport processes are those related to non-diffusive transfers induced by atmospheric turbulence (wind conditions). These transfers are in increasing recognition of the importance in several ecosystem types (Goffin et al., 2014; Maier et al., 2012; Bowling and Massman, 2011; Maier et al., 2010; Seok et al., 2009; Flechard et al., 2007; Takle et al., 2004) and are clearly defined in Maier et al. (2012) clarifies it by identifying its two components, advection and dispersion, and emphasizing the difference between them. The advection refers to the CO_2 transported vertically by the air mass flow in the soil which results from pressure fluctuations at the soil surface. As a result of the alternating direction of the pressure fluctuation, the advection is alternately up and down so that the net vertical air flow into/out of the soil is zero, although air flow occurs within soil pores (Maier et al., 2012). By cons, the dispersion can be conceptually described as an enhancement of diffusion following air movement in the soil. Basically, the speed of vertical air movement during advection is not horizontally homogeneous due to friction on pore walls, dead end pores, etc. In addition to the vertical CO_2 gradient, this creates horizontal heterogeneity in soil CO_2 concentration and leads to horizontal diffusion. Maier et al. (2012) showed that this last process combined with vertical advection leads to a net CO_2 vertical flux named dispersion. The dispersion enhances always vertical diffusion due to the fact that CO_2 molecules preferentially use upward movement of the oscillating air column (Maier et al., 2012). Again, atmospheric turbulence, and then soil CO_2 vertical transport related, underlies an intra-day cycle.

In this study, modelling is used to test whether transport or production processes of soil CO_2 is responsible for short-term (intra-day) variations observed in efflux and soil concentration measurements. In this framework, the model outputs simulating CO_2 production and its transport within the soil are compared with a measurement dataset. A reference model including a purely diffusive CO_2 transport and a temperature sensitivity of CO_2 production was compared to models taking into account turbulence-induced transport (advection or dispersion) or a rapid influence of photosynthetic activity on soil CO_2 sources.

Material and Method

Site description

A dataset from the Hartheim permanent forest meteorological experimental site (47°56’04’’N 7°36’02’’E, 201 m a.s.l) was used to develop our modelling approach. The site consists of a 50 year-old Scots pine stand (*Pinus sylvestris* L.) located in the Upper Rhine Valley (Holst et al, 2008). This stand is characterized by a sparse canopy and a dense understory. Climate

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

conditions are temperate: annual mean air temperature of 10.3°C and a mean annual total of precipitation of 642 mm (Holst et al., 2008). The soil is a carbonate-rich (pH=7.8-8.2), two-layer Haplic Regosol (calcaric, humic) (FAO, 2006). The texture of the Ah horizon is silt loam (0-20 cm), followed by a transitional horizon AhC (20-40 cm) with less silt and more gravel. The underlying layer (horizon C, 40-80 cm) is clearly stratified comprising alluvial sand and gravel. The humus type is mull. The O_L horizon thickness varies between 1 and 3 cm. A detailed site description is given in Holst et al (2008).

An *in-situ* measurement campaign with detailed subsurface vertical profile of soil water content (SWC), temperature (T), air [CO_2] and surface CO_2 effluxes (F_s) was performed at the Hartheim site from August 25 to September 15, 2010. The temporal resolution of these measurements was 30 min. In addition, soil physical characteristics (porosity, diffusion coefficient, air permeability) were measured in laboratory on soil samples collected in each horizon of the site. The detailed description of the *in situ* and the laboratory measurements can be found respectively in Goffin et al., (2014) and Maier et al., (2012). A brief description is given in the following paragraphs.

Field Measurements

Profiles of [CO2], SWC, T

The soil air CO_2 concentration ([CO_2]) profile was measured using solid-state non dispersive infrared CO_2 sensors (GMP343, diffusion model, Vaisala Oy, Helsinki, Finland) inserted in the soil at -5, -25, -50 and -95 cm depth. Another probe was placed on the forest floor, just above the litter surface.

The soil water content (SWC) profile was determined using both volumetric soil moisture sensors inserted horizontally at -7, -20 and -30 cm depth (Theta Probe ML1, Delta-T Devices,

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Cambridge UK) and matric potential sensors (EcoTech Gmbh, Bonn, Germany) at 20, 50 and 70 cm depth.

The soil temperature (T) profile was recorded using PT100 (Heraeus Sensor Technology, Kleinostheim, Germany) at -1, -3, -5, -10, -20, -40, -50, -70 and -120 cm depth. Additionally, air temperature was also available. The soil sensors were installed during the winter 2009, leaving a large part of the 2010 growing season for fine root biomass recovering before the beginning of the measurement (27th August 2010).

Surface CO_2 efflux (Fs)

F_s were measured using four open chamber systems (or steady-state flow-through chambers). The detailed experimental design and operating method was given in Marron et al. (2009). The chambers were mainly constituted by a collar (stainless steel, 20 cm diameter, 12.5 cm high) and a mobile lid. The recommendations of Rayment and Jarvis (1997) about the chamber design were taken into account, *i.e* (i) steady state for chamber CO_2 concentration can be ensured with a value close (few µmol/mol) to the atmosphere, (ii) turbulent conditions at the soil surface inside the chamber must be as close as possible to the outside conditions, (iii) the pressure difference between the outside and inside of the chamber must be minimal (<0.1 Pa, as shown in Longdoz et al., 2000). To measure F_s every 30 min, six collars were partially pushed into the soil on 23 August 2010 and were alternatively covered, from 25 August to 15 September 2010, with one of the four mobile lids. After the two main rain events occurring during the campaign, only two of the four lids were moved to other collars in order to, on the one hand, avoid a permanent soil covering and its environment modification and on the other hand, ensure a relative continuity in the measurements. For this purpose, there were three sequences of 7-day measurements with different sets of four collars (see Goffin et al., 2014). Due to technical issues, however, the measurements of F_s on collar 3 were excluded from the dataset. The flow rate through the system (2 l min^{-1}) was adapted to the inlet aperture (21.2 cm^2). The F_s (µmol m^{-2} s^{-1}) was calculated as:

$$F_s = \frac{([CO_2]_{outlet} - [CO_2]_{inlet}) * f}{S} \quad \textbf{(Equation 1)}$$

where $[CO_2]_{inlet}$ and $[CO_2]_{outlet}$ are CO_2 concentration in the inlet and outlet flows from the chamber, *f* is the air flow through the chamber (m^{3}s^{-1}) and *S* is the soil surface inside the chamber (m^{-2}).

Finally, the mean plot F_s were estimated throughout the study period (25 August to 15 September) as the average of the 5 remaining collars after gap filling according to Goffin et al (2014).

Standard deviation of horizontal wind speed and differential pressure

The standard deviation of horizontal wind speed ($\sigma_{h,tower}$) was calculated every second from high frequency (20 Hz) measurements of horizontal wind velocity component. The latter were monitored above the canopy during the entire measurement campaign with a sonic anemometer (CSAT3, sonic anemometer, Campbell Scientific, Inc, Logan, Utah, USA) located on a 30 m-height tower and used as a proxy for the turbulence at the soil surface. To ensure the quality of this proxy, a sonic anemometer was placed at the soil surface after the measurement campaign and the data from this one were compared to the data from the anemometer placed at the top of the tower. We have observed a significant positive correlation between turbulence conditions measured above and below the canopy (R^2=0,62, pvalue<0.001).

The differential pressure between soil interface and -25 cm depth was recorded using a sensitive piezo-resistive relative pressure sensor (GMSD 2.5MR,, Greisinger Electronic

GmbH, Regenstauf, Germany, sensitivity 0.1 Pa, accuracy 1%). Pressure was measured with a frequency of 20 Hz and recorded as minimum, maximum and mean differential pressure measured every 4 min during the period from September 8 to 16, 2010.

Laboratory Measurements

The relationships between soil relative diffusivity ($D_r=D_s/D_0$) and SWC, and between air permeability (K) and air-filled porosity (ε), as well as the retention curves and the total porosity were determined for each soil horizon from laboratory experiments performed on Hartheim soil samples. The methods are widely described in Maier et al., (2010) and (2012). The soil cylinders used for the physical parameters determination were sampled on the studied plot during the installation of the device for profiles ([CO_2], SWC, T) measurements and maintained intact before analyses.

The total porosity (Φ) of each horizon was calculated as the average value of all samples collected from the same horizon as mentioned in Goffin et al., (2014). Horizon specific relationship between D_r and SWC (see below Equation 6) and between K and ε (see below Equation 11) were determined from D_r and K measurements on several soil cores collected in each horizon and subjected, in laboratory, to several water treatments. For each horizon, linear regressions were then used to derive specific relationships between D_r and SWC and non-linear regressions to derive the relationships between K and ε. The regressions were performed with MATLAB by minimizing the mean square error (R2009b version, *The Mathworks*, Natick, USA).

Model

CO_2 transport and production within the gaseous phase in the soil were modelled using the gaseous CO_2 mass balance equation with separate soil layers. Under the assumption of horizontal homogeneity in the studied soil, the one-dimensional CO_2 mass balance equation on an infinitesimal depth soil element can be expressed as:

$$\varepsilon \frac{\partial [CO_2]}{\partial t} = -\frac{\partial}{\partial z}(F) + P$$ (**Equation 2),**

where ε is the air-filled porosity ($m^3 m^{-3}$), [CO_2] is the CO_2 concentration (µmol CO_2 m^{-3}), F represents the CO_2 fluxes caused by transport in the gaseous phase (µmol CO_2 $m^{-2}s^{-1}$), P represents the CO_2 production terms (sources) (µmol$m^{-3}s^{-1}$) mainly coming from the organic matter through the autotrophic and heterotrophic component of soil respiration and to a lesser extent by CO_2 exchanges with liquid phase, z is the depth (m) and t is the time (s) (z=0 at the bottom of the O_L horizon, z>0 above the bottom of O_L horizon pointing to the atmosphere and z<0 below O_L horizon pointing to the soil).

In this study, the CO_2 exchanges between the gaseous and the liquid phase is negligible and were estimated to represent only few percent (<4%) of the biotic CO_2 sources (autotrophic and heterotrophic respiration). In this way, P term is simulated as biotic production only.

The air-filled porosity at each depth is computed from the difference between the horizon specific total porosity (*Φ*) and the volumetric soil water content (SWC) measured *in situ* according to Maier et al., (2010) and Goffin et al., (2014).

$$\varepsilon(t,z) = \Phi^{horizon} - SWC(t,z)$$ (**Equation 3)**

We tested several expressions of CO_2 production (*P*) and CO_2 transport (*F*) that differ in the underlying assumptions considered, respectively for both the production and transport of CO_2 within the soil.

The model is applied on the Haplic Regosol (calcaric, humic) (FAO, 2006) in Hartheim site consisting of 4 soil horizons: O, Ah, AhC and C. The soil was treated as a one-dimensional

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

structure, each horizon having its own physical and biological properties. The Ah horizon was split into two parts because of its large vertical heterogeneity of physical parameters, so that the modeled soil consisted of five parts: O_L (+2.5-0cm), Ah1 (0-10cm), Ah2 (10-20 cm), AhC (20-40cm) and C (40-80 cm).

Reference Model

In the reference model, the most commonly accepted processes of soil CO_2 transport and production are considered, namely a purely diffusive transport and production dependent on the local soil temperature only (Curiel Yuste et al., 2005; Davidson et al., 2006a).

Diffusion is reported to be the main transport mechanism in the soil (Pumpanen et al., 2008; Davidson et al., 2006b; Hirano et al., 2005; Jassal et al., 2005; Fang and Moncrieff, 1999). The CO_2 fluxes F can be expressed by Fick's first law.

$$F = -D_s \frac{\partial [CO_2]}{\partial z} \quad \textbf{(Equation 4),}$$

where D_s is the effective soil diffusion coefficient (m^2s^{-1}) which was determined, at each depth, as a function of the free air CO_2 diffusion coefficient in standard conditions (D_0=1.47*$10^{-5}m^2s^{-1}$ at 293.15 K and 101325 Pa), atmospheric pressure (p_{atm}, Pa), temperature at the corresponding depth (T, [K]) and the relative soil diffusion coefficient (D_r=D_s/D_0).

$$D_s(t,z) = D_r(t,z) * D_0 * \left(\frac{T(t,z)}{293.15}\right)^{1.75} * \left(\frac{p_{ref}}{p_{atm}(t)}\right) \quad \textbf{(Equation 5)}$$

$$D_r(t,z) = \alpha_1^{horizon} * SWC(t,z) + \alpha_2^{horizon} \quad \textbf{(Equation 6),}$$

where SWC(t,z) and T(t,z) are estimated from interpolation between *in situ* measurement point, α_1 and α_2 are parameters deduced in each horizon from experimental linear relationship between D_r and SWC obtained in laboratory on soil samples. More details are given in Goffin et al., (2014) and Maier et al., (2010).

Usually in temperate ecosystem, the CO_2 biotic production in the soil is represented as a function of soil temperature (Davidson and Janssens, 2006; Kätterer et al., 1998; Lloyd and Taylor, 1994). In the reference model, the CO_2 production in each layer and time step was adjusted according to the temperature at each depth following a Q_{10} equation (Moyes et al., 2010; Curiel Yuste et al., 2005)

$$P(t,z) = R_b(z) * Q_{10}^{\frac{T(t,z)-T_{ref}}{10}} \quad \textbf{(Equation 7),}$$

where R_b is the basal respiration rate (µmol CO_2 m^{-3}), representing the CO_2 production at the reference temperature T_{ref} (15°C), Q_{10} is a coefficient defining the temperature sensitivity of CO_2 production, constant over the profile.

The basal respiration rate decreases with depth (Moyes et al, 2010). We considered the decreasing basal respiration rates with depth by using two linear functions which intersect at the depth z_2. The depth z_2 should represent the limit between high and low organic content zones (normally close to the transition between Ah and C horizons). The following expressions were used:

$$R_b(z) = \begin{cases} R_b(z_1) + \dfrac{R_b(z_2) - R_b(z_1)}{z_2 - z_1}(z - z_1), z_1 > z > z_2 \\ R_b(z_2) + \dfrac{R_b(z_3) - R_b(z_2)}{z_3 - z_2}(z - z_2), z_2 \geq z > z_3 \end{cases} \quad \textbf{(Equation 8),}$$

with z_1=+0.025 m (the top of the litter layer), z_3=-0.8 m (the bottom of the C horizon) $R_b(z_3)$=0 (no production below C horizon). Q_{10}, $R_b(z_1)$, $R_b(z_2)$ and z_2 are parameters determined by adjustment of the model outputs to the *in-situ* measurements (CO_2 concentration and efflux).

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Boundary and initial conditions

The initial CO_2 concentration profile in the soil (t=0) was interpolated between the concentrations measured at several depths at the beginning of the measurement campaign.

The top boundary condition (at z_1=+0.025 m) for [CO_2] was equal to the value measured at the soil-air interface. At the bottom of the domain (z_3=-0.8 m), it was considered that the CO_2 vertical gradient was negligible so that the mass fluxes were zero.

Model including advection

Many authors reported the importance of considering advection in conjunction with diffusion to characterize vertical gas transport in the soil (Bowling and Massman, 2011; Seok et al., 2009; Flechard et al., 2007; Fang and Moncrieff, 1999). The flux induced by the pressure fluctuation (advective transport) at the soil surface is taken into account and coupled with diffusion so that, F (in Equation 2) can be expressed according to Equation 9.

$$F = -\frac{K}{\eta}[CO_2]\frac{\partial p}{\partial z} - D_s\frac{\partial [CO_2]}{\partial z} \quad \textbf{(Equation 9),}$$

where p is a differential pressure relative to a reference pressure p_{ref}=101325 Pa (the absolute pressure in the soil is then given by $p+p_{ref}$), K is the air permeability (m^2) and $\eta=1.8*10^{-5}kgm^{-1}s^{-1}$ is the air dynamic viscosity.

Since the soil is a porous medium, Darcy law is used to compute the pressure fields. It leads to the following Partial Differential Equation (PDE) to determine the air pressure in the soil:

$$\varepsilon\frac{\partial p}{\partial t} = \frac{K}{\eta}\frac{\partial}{\partial z}((p+p_{ref})\frac{\partial p}{\partial z}) \quad (\textbf{Equation 10})$$

The air permeability (K) was determined, in each horizon except in C one, as a function of the air-filled porosity.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

$$K(t,z) = \alpha_3^{horizon} * (\varepsilon(t,z))^{\alpha_4^{horizon}}$$ **(Equation 11),**

where α_3 and α_4 are parameters deduced from relationship between air permeability and air-filled porosity measured in laboratory on the same soil samples as those used to determine D_r. In the C horizon, because the relationship could not be deduced from the laboratory measurements, the average value measured on all the soil samples collected in C horizon was used independently of air-filled porosity.

Boundary and initial conditions

Additional boundary conditions should be added for pressure. At the top of the domain, the differential pressure p (Equation 9) is assumed to be proportional to the standard deviation of horizontal wind speed fluctuation ($\sigma_{u,tower}$) calculated every second from data collected at 20 Hz at the top of the tower (Subke et al, 2003), :

$$p\big|_{z=0.025,t} = \Delta p_{\text{int}} = \alpha_5 * \sigma_{u,tower}$$ **(Equation 12),**

Where Δp_{int} is the differential pressure (p-p_{ref}) at the boundary between litter layer and atmosphere and α_5 is a parameter that should be determined by comparison between simultaneous measurements of $\sigma_{u,tower}$ and Δp_{int}. Unfortunately, Δp_{int} was not directly measured but the pressure difference between soil interface and -25 cm depth was. The maximum and minimum values of this difference were recorded every 4 min from high frequency data. Assuming no more pressure fluctuation at -25 cm depth, the gap between these maximum and minimum values ($\Delta p_{int\text{-}25}$) can be used as a proxy of the pressure fluctuation at the soil interface (Δp_{int}).

At the bottom of the domain, it was assumed that the pressure fluctuation cannot penetrate further in the soil, leading to the following condition:

$$\left.\frac{\partial p}{\partial z}\right|_{z=-0.8,t} = 0 \quad \textbf{(Equation 13)}$$

The initial differential pressure is set to 0.

Model including dispersion

The dispersion process is reported to influence soil gas transport, more specifically to enhance the gas exchange in the soil (Maier and al., 2012; Bowling and Massman, 2011; Takle et al., 2004). This process is difficult to model with a mechanistic description but this difficulty can be circumvented by considering that it can be expressed as an increase of the soil diffusion coefficient due to turbulence (Maier and al., 2012; Bowling and Massman, 2011). The dispersion potentially affected the uppermost few centimeters of the humus layers (Maier et al., 2012) and therefore we test it by introducing a turbulence-dependency of the soil diffusion coefficient in the litter (O_L horizon). In that way, Equation 5 is written in O_L as indicated in Equation 14.

$$D_s^{O_L}(t,z) = D_r^{O_L}(t,z) * D_0 * \left(\frac{T(t,z)}{293{,}15}\right)^{1.75} * \left(\frac{p_{ref}}{p_{atm}(t)}\right) * \left(1+\frac{u*(t)}{\alpha_6}\right) \quad \textbf{(Equation 14),}$$

where u* is the friction velocity measured above the canopy [ms^{-1}] and α_6 a parameter [ms^{-1}] reflecting the influence of turbulence on soil CO_2 transport. The u* is taken above the canopy because: (i) it can be considered as a good proxy for turbulence intensity at soil level given the good correlation between u* measured above and below the canopy at Hartheim site (data not shown), and (ii) this measurement was available throughout the measurements campaign.

From Figure 8 in Maier et al., (2012), the increase of the diffusion coefficient due to dispersion may reach, in a laboratory experiment on several Hartheim soil samples, more than 30% in high turbulence level. The latter corresponds to a friction velocity artificially induced at the sample surface ($u*_{floor}$) of 0.34 ms^{1}. They have even observed on one sample an extreme increase of 85% at this turbulence level. In view of these results and given the relationships between the friction velocities at the forest floor and at the top of the tower (data not shown), the potential fitting range of α_6 should be between 3 (great influence of dispersion) and 8 (moderate influence of dispersion).

Model including the photosynthetic substrate supply through phloem pressure concentration waves

Phloem movements in a plant are closely related to the water movement, in the opposite direction, through the xylem. Therefore, the phloem transport depends indirectly on the plant transpiration (TR) which can be approached by the vapour pressure deficit (VPD). To date, no equation describes the phloem pressure concentration wave in a mechanistic way (Mencuccini and Hölttä 2010). Here, the influence of such phenomenon is empirically tested using a linear influence of the vapour pressure deficit (VPD, [hPa]) on soil CO_2 production, so that the latter can be expressed as indicated in Equation 15.

$$P(t,z) = R_b(z)Q_{10}^{\frac{T(t,z)-T_{ref}}{10}} + (\alpha_7 * VPD(t) + \alpha_8) \quad (\textbf{Equation 15})$$

Where α_7 and α_8 are parameters.

In this way, Equation 15 is expressed as a Q_{10} law to which a residual influence of VPD is added. This equation was applied only in O_L, Ah_1 and Ah_2 horizons where are located most of the roots (Goffin et al, 2014). In the other horizons, CO_2 production remains expressed by Equation 7.

Model Calibration Procedure

As mentioned above, some parameters of the production expression ($R_b(z_1)$, $R_b(z_2)$, z_2, Q_{10}) have to be calibrated. This task has been performed using a least-square fitting method. It consists to minimize a cost function C_F which corresponds to the average quadratic difference

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

between the experimental measurements and the simulation outputs obtained for a given set of parameters.

$$C_F(M) = \sum_i \sum_j ((Y_{\exp}(z_i, t_j) - Y_{sim}(z_i, t_j, M))^2 \quad \textbf{(Equation 16)}$$

Where Y is a calibration variable and M a given set of parameters. The final calibrated values for the parameters are those which minimize the cost function.

$R_b(z_1)$, $R_b(z_2)$, z_2, and Q_{10} are fitted by minimizing the cost function for $Y = [\mathrm{CO}_2]$, $z_i = \{-0.05\,;\ -0.25\,;\ -0.50\,\}$ and t_j from 0 to 15 days.

Numerical procedure and post-processing

To simulate the time evolution of the CO_2 concentration profile and CO_2 fluxes, Equation 2 was solved numerically using the respective initial and boundary conditions with the commercial software COMSOL Multiphysics 3.5. This software enables to solve partial differential equations using the finite element method.

The one-dimensional computational domain is meshed using regularly spaced elements. Various mesh sizes have been assessed and it has been found that an optimum mesh size is 10^{-3} m because further refinement of the mesh no longer influences the simulated concentration profiles. The direct solver UMFPACK was used to resolve the equation system with Quadratic Lagrange elements for the spatial discretization and the Backward Differentiation Formulas (BDF) method for the time discretization.

The minimization of the cost function (Equation 16) is realized using *fminsearch* function of COMSOL which performs unconstrained nonlinear minimizations using a Nelder-Mead algorithm.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Results and Discussion

First, the results of the reference model are presented with their own pros and cons. Then the models taking into account more complex transport or production expressions are respectively presented emphasizing the improvement compared to the reference model.

Reference model

Parameter values of Equation 6 (α_1 and α_2) were obtained by laboratory measurements and are presented in Table 1. The parameters of Equations 7-8 (Q_{10}, $R_b(z_1)$, $R_b(z_2)$ and z_2) were calibrated using experimental data of soil CO_2 concentration measured in Hartheim from August 27 to September 14, 2010.

Calibration values

The calibrated parameters are presented in Table 2. The basal respiration rate values ($Rb(z_1)$ and $Rb(z_2)$) are consistent with the CO_2 production values reported in Goffin et al, (2014) on the same site. These calibrated parameters suggested that the CO_2 production within the entire soil profile (from the air/soil interface to z=-0.8 m) at 15°C was equal to 5.57 µmol CO_2 $m^{-2}s^{-1}$ and that 90% of the CO_2 was produced above -30 cm depth which is close to values reported in Goffin et al., (2014). The Q_{10} obtained is within the range commonly reported in the literature i.e. from 1 to 10 (Luo and Zhou, 2006; Davidson et al., 2006a; Fang and Moncrieff, 2001). Nevertheless, Davidson et al. (2006a) speculate that a Q_{10} value above 2.5 probably indicates that some unidentified process of substrate supply should be considered. In addition, it was expected that the depth z_2 represents the boundary between high and low organic content and root zones. This is the case as the calibrated value is close to the estimated depth transition between AhC and C horizons (-0.40 m) below which Goffin et al. (2014) showed a clear depletion in C organic and root content.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Time evolution

The time evolution of simulated F_s and soil $[CO_2]$ are compared to measurements, in Figure 1 and Figure 2 respectively.

The magnitude and the inter-day variability in F_s and soil $[CO_2]$ at each depth are relatively well represented by the reference model. But, the amplitude and the phase of the intra-day pattern of surface variables (F_s and $[CO_2]$ at -5cm depth) are poorly reproduced.

This version of the model explains 61%, 92%, 75% and 70% of the inter-day variation of F_s, $[CO_2]$ at -5 cm, $[CO_2]$ at -25 cm and $[CO_2]$ at -50 cm depth, respectively. The inter-day variation was estimated using the daily average of the above variables. The amplitude of intra-day variation of F_s and $[CO_2]$ at -5 cm depth ($[CO_2]_{-5cm}$) are significantly smaller in the simulation than in the measurements. Indeed, the F_s and $[CO_2]_{-5cm}$ intra-day amplitude, averaged on data collected over the days where there is a well-marked daily cycle (from 31/08/2010 to 6/09/2010 & from 10/09/2010 to 12/09/2010 & from 13/09/2010 to 15/09/2010), are 1.6 (Standard Error, SE=0.1) $\mu molCO_2m^{-2}s^{-1}$ and 10998 (SE=402) $\mu molCO_2m^{-3}$, respectively. Those values are significantly larger than the simulated values of 1.06 (SE=0.05) $\mu molCO_2m^{-2}s^{-1}$ and 7335 (SE=560) $\mu molCO_2m^{-3}$, respectively for F_s and $[CO_2]_{-5cm}$. The phase difference between simulation and measurement is not constant in time. The phase difference is especially marked during sunny days without rain. The simulated F_s tends to be ahead of the measured one, with an averaged phase advance of 2.5 hours. Conversely, the simulated $[CO_2]_{-5cm}$ tends to be delayed from the measured one, with an averaged delay of 6h.

The differences between measurements and model simulations (amplitude and phase) cannot be reduced by changing the values of calibrated parameters, except by unreasonably increasing the Q_{10} value (>10). In that case, however, the inter-day variability of F_s and $[CO_2]$

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

is no longer adequately represented. Such important difference between temperature sensitivity on hourly and daily basis is difficult to explain in a mechanistic way, so that other variables should affect the F_s and $[CO_2]$ within short-timescales.

As shown above, the model failed to reproduce concentrations and fluxes in the two first shallowest horizons (O_L & Ah) where more than 76% of the CO_2 was produced. The model modification aims at improving this description. Below, we will focus only on those variables.

Model with advection

Parametrization

The parameter α_5 was determined using simultaneous data of $\sigma_{u,tower}$ and $\Delta p_{int-25,}$ the latter being assumed to represent $\Delta p_{int.}$ Two values were obtained, $\alpha_5 = 0.89$ and $\alpha_5 = 2.66$, using respectively for the comparison, the maximum and the mean value of $\sigma_{u,tower}$ recorded every 240 seconds (to match frequency of Δp_{int-25} data). These values best represent the average behavior and the extreme values of Δp_{int-25}, respectively. These values are higher than those reported by Subke et al., (2003) (up to 0.87) but do not seem aberrant. In addition, it is difficult to discuss the value of such parameter, as it is highly sensitive to the location of measurements (Subke et al., 2003). Given the challenge of measuring pressure fluctuation *in situ* (Maier et al., 2010), it is necessary to use a proxy. In this case, it seems particularly important to test the sensitivity of the model to the proxy. Below, the impact of the Equation 12 parameters (α_5 and frequency of p) is evaluated on the instantaneous value of F_s, because the advection primarily impacts this variable.

Impact of α_5

The value of the parameter α_5 determines the amplitude of the pressure fluctuations. Several values of α_5 going from $\alpha_5 = 0$ (corresponding to reference model) to $\alpha_5 = 20$(extremely

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

high amplitude of pressure fluctuation) have been tested (with a $\sigma_{u,tower}$ varying at 1 Hz) during the most turbulent days of the measurement campaign ([8/09/2010-10/09/2010[).

Figure 3 shows, for different α_5 values, the maximum instantaneous contribution of advection (F_{adv}) to F_s according to the amplitude of pressure fluctuation at the interface Δp_{int}. As expected, F_{adv}/F_s increases with Δp_{int} (or α_5), i.e. with the strength of turbulence. We can observe that the contribution of advection is very low for the α_5 range expected in Hartheim. The considered extreme value of $\alpha_5 = 2.66$ leads to a maximum advective contribution of only 3.8% and this percentage is even lower for $\alpha_5 = 0.89$ (average behavior). To reach a 10% advective-contribution to F_s, Δp_{int} must exceed 17.3 Pa ($\alpha_5 > 6.9$). Such Δp_{int} has not been observed in situ in Hartheim and is likely extremely rare at other sites as well. Takle et al., (2003 and 2004) measured high frequency (2Hz) pressure variation and reported values below 5 Pa. Using 1 Hz for p variations, advection does not seem to be a significant CO_2 transport mechanism in the soil.

Impact of frequency

The impact of pressure fluctuation frequency was tested, away from natural wind time evolution, by applying a sinusoidal Δp_{int} with amplitude of 5 Pa and different frequencies: 0.2 Hz, 1 Hz, 10 Hz, 20 Hz and 50 Hz. The chosen amplitude represents an extreme value observed *in situ* by Takle et al., (2004).

The ratio between instantaneous F_{adv} and the diffusive component of F_s (F_{diff}) was sampled at 100 Hz during 3600 seconds (i.e. with frequency of sampling>frequency of imposed Δp_{int}). The frequency of pressure fluctuation has a significant influence on instantaneous F_{adv} value, so that F_{adv} could become very high compared to the diffusive flux (F_{diff}). Indeed, F_{adv} can largely exceed $F_{diff,}$ the former becomes twice as high as the latter already at a frequency of 10

Hz. Of course, it is only instantaneous F_{adv}/F_{diff} ratio recorded at a given instant and given the natural oscillating character of F_{adv} (positive and negative), this ratio is inevitably lower when it is temporally integrated. The next paragraph presents a quantification of the impact of the temporal integration.

In view of the advection study, the amplitude of p fluctuation had a lower impact on instantaneous fluxes than the frequency of its variation.

Time evolution: high frequency recording

The preceding simulation suggests that, compared with the reference model, the introduction of advection did not reduce the phase and amplitude divergences observed between measurements and simulation outputs. In fact, the effects of advection are observable only on very short timescales (tenth of seconds). To illustrate this effect, a simulation with extreme turbulence conditions (frequency=50Hz and $\alpha_5 = 2.66$) was performed with high-frequency recording (50 Hz) during 3600 s.

Figure 4 represents the time evolutions of instantaneous F_{diff} and F_{adv}, the surface [CO_2] at 0 cm (just below the O_L horizon) and the amplitude of pressure fluctuations at soil/atmosphere interface for both the reference model and the model including advection.

In these conditions, the instantaneous absolute value of F_{adv} can largely exceed F_{diff} (up to three times larger). In addition, advection modifies F_{diff} (up to 4%). It’s because advection disturbs [CO_2] vertical gradient, soil diffusion coefficient remaining unchanged between the two models. Nevertheless, the [CO_2] disturbance is insignificant since the introduction of advection induced only concentration variations of maximum 0.26 and 0.05% at +2 cm (in O_L) and 0 cm (below O_L), respectively.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

As mentioned above, the advection acts only on very short timescales. To illustrate this, we integrated F_{adv} ($int(F_{adv})$) and F_{diff} ($int(F_{diff})$) over several integration times and calculated the ratio between these variables. Figure 5 represents the maximum ratio between $int(F_{adv})$ and $int(F_{diff})$ obtained during the 3600 s according to the considered integration time (horizontal axis). The contribution of advection drops rapidly and becomes almost zero already for an integration time of 10 seconds. Surface fluxes measurement typically lasts few minutes and therefore such measurement should not reflect the advective process. This last should be taken into account only in studies focusing on mechanisms with a time characteristic around or lower than one second.

In summary, considering the advection to characterize the soil CO_2 transport considerably lengthens the computation time of modeling without improving the prediction of measurements (half-hour integrated). The only significant effect was observed on the instantaneous value of fluxes, but as soon as they are integrated over few seconds, the impact of advection becomes negligible. In addition, we emphasized that the frequency of p fluctuations is more important than its amplitude to more accurately quantify the potential impact of advection on F_s at very short time scale.

Effect of dispersion

Time evolution

The time evolutions of the diffusion coefficient in the litter ($D_s(O_L)$) and the $[CO_2]_{-5cm}$ are represented in Figure 6 respectively for the reference model and the model with dispersion (using $\alpha_6 = 3$). In addition, the measured $[CO_2]_{-5cm}$ is presented to prove the reliability of the model outputs. The general evolution of this measured $[CO_2]_{-5cm}$ has been analyzed in Goffin et al. (2014) and is due to soil temperature and water content. Especially the drop around the 7th-8th September corresponds to a rain event inducing in a cascade effect D_s decrease, CO_2

blockage and $[CO_2]_{-5cm}$ increase. Introducing a $D_s(O_L)$ dependence to the friction velocity (u*) can change the dynamics of soil CO_2 concentration and, to a lesser extent, of F_s.

In the model that includes dispersion, the $D_s(O_L)$ increases as soon as the friction velocity increases (during daytime), thus facilitating the $[CO_2]$ transport. This implies a topsoil $[CO_2]$ decreases during daytime. In such situations, the amplitude of intra-day variation of simulated $[CO_2]$ and F_s increases compared to the one obtained with the reference model (Figure 6). The impact of dispersion is less clear on simulated F_s than on soil $[CO_2]$. This is because the dispersion impacts the underlying variables of F_s (D_s and $[CO_2]$) in opposite direction. Furthermore, the dispersion especially impacts the litter $[CO_2]$ dynamics, but its effect is still visible in the lower layers. For example, the dispersion with $\alpha_6 = 3$ increases the amplitude of intra-day variation of $[CO_2]$ in the litter, at – 5cm, -25 cm, -50 cm respectively by 59%, 41%, 12% and 2%, in comparison with the reference model. In contrast, the amplitude of intra-day variation of F_s increases by only 1% (Figure 7).

The amplitude of intra-day variation of $[CO_2]_{-5cm}$ features similar values to the measured one for α_6 included between 2 and 3 (Figure 7).

When dispersion is included in O_L, it can increase the intra-day variation of F_s and $[CO_2]$, the latter becoming closer to those measured, but the phase difference observed between simulation and measurement remains as well for F_s and CO_2. Therefore, this phenomenon helps but does not explain suitably the anomalies observed in 0. Nevertheless, those simulations highlights the dispersion impact on topsoil $[CO_2]$, even with $D_s(O_L)$ increases similar to those observed in laboratory by Maier et al., (2012). Quantifying the impact of turbulence on topsoil $[CO_2]$ is really important for the Flux Gradient Approach (Goffin et al., 2014) which is a measurement technique that is increasingly being used. To go further in this direction, it is essential to establish experimentally and *in situ* relationships between turbulence at the forest floor and the soil diffusion coefficient (Schwen et al, 2011; Lehmann et al, 2000; Van Bochove et al, 1998).

Model including the phloem pressure concentration waves

The inclusion of turbulence-induced transport in the Model did not elucidated sufficiently the phase and amplitude differences observed between the reference model and the measurements. Therefore, it seems that the expression of CO_2 production should be questioned. An impact of the pressure concentration wave could modify the simulation in the right direction because it includes (i) the influence of photosynthetic activity that depends on aerial variables presenting an intra-day cycle and (ii) a time lag between the aerial variables and its action on $[CO_2]$ production (Kuzyakov and Gavrichkova, 2010; Mencuccini and Hölttä 2010).

The parameters α_7 and α_8 in Equation 15 have not been directly calibrated on CO_2 production measurements but their value was set to improve the representation of the temporal evolution of measured variables. Giving a more accurate value of those parameters would need a specific study with additional data compared to those collected in this study.

The values of 0.35 $\mu molCO_2m^{-3}s^{-1}hPa^{-1}$ and -0.04 $\mu molCO_2m^{-3}s^{-1}$ was found respectively for α_7 and α_8 to represent the same magnitude of intra-day variation of F_s and $[CO_2]_{-5cm}$ measurements. With those values, the resulting VPD contribution to total CO_2 production can vary between 0 and 15% at 5 cm depth. Several time lags between the VPD and its action on CO_2 sources were tested. A consistent time lag of -2 hours was found to erase the important phase differences observed between simulated and measured $[CO_2]_{-5cm}$. Mencuccini and Hölttä 2010 reported time lag from few hours.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Figure 8 represents the time evolutions of F_s and $[CO_2]_{-5cm}$ and their averaged intra-day variation for the reference model, the model including the phloem pressure concentration wave (PPCW) and the measurements. In general, adding the influence of VPD in the surface horizons (O_L, Ah_1 and Ah_2) allowed improving the representation of the amplitude and the phase of surface $[CO_2]$ intra-day variation and the amplitude of F_s intra-day variation. With the introduction of the VPD influence, the average amplitude of $[CO_2]_{-5cm}$ and F_s intra-day variation became, respectively, 10818 (SE=351) $\mu molCO_2m^{-3}$ and 1.78 (SE=0.11) $\mu molCO_2m^{-2}s^{-1}$ and was thus not significantly different from the measured values. The phase shift with observations is largely reduced on most of the $[CO_2]_{-5cm}$ time series. Nevertheless, this last improvement is not large enough for F_s and the phase difference between simulated and measured F_s remains significant during the sunny days without rain (from 31/08/2010 to 6/09/2010, from 10/09/2010 to 12/09/2010, from 13/09/2010 to 15/09/2010). This can be explained by the fact that the PPCW is one of the mechanisms that could impact CO_2 production but there are still other mechanisms that could interact together on intra-day scale (Moyes et al., 2010) and influence CO_2 production. In this study, the PPCW seem to be the most appropriate mechanism to explain our measurements, but with the data available, we cannot investigate further. Indeed, there is a lack of experimental studies about the PPCW and the potential variables that could impact it. A constant (temporally and spatially) lag (2 hours here) between the VPD and its action on the CO_2 production is supposed here but is maybe not appropriate. Spatially, the PPCW lag should depend on the root position within the soil which is highly variable among the surface horizons (see Goffin et al., 2014). The PPCW should reach faster the surface horizons than the other ones. In addition, the production of photoassimilate depends not only on the VPD but also on the radiation. In this case, the influence of photosynthetic substrate supply to root should differ according to the radiation too. Then the time lag should not be constant over time and should depend on climatic conditions. Wingate et al. (2010) showed that the time lag for the direct transport of photoassimilates from the canopy to root depend on the climatic conditions. This should be also the case for the indirect physicochemical effect on root activity through the PPCW. Further investigations are required to understand the impact of photosynthesis substrate on soil respiration and propose a more mechanistic model.

Conclusions

The reference model took into account a purely diffusive transport of soil CO_2 and a production which depends on the temperature variation only. This model produced a good representation of the inter-day variability of F_s and $[CO_2]$ measurements, but it failed to accurately simulate their intra-day variability. Phase and amplitude differences were indeed observed on the intra-day variation of $[CO_2]$ and F_s compared to measurements. Adding the influence of turbulence-induced transport does not sufficiently improve the intra-day pattern of simulations. Advection was shown to disturb the instantaneous value of F_s with a higher sensitivity to the frequency of the pressure disturbance than to its amplitude. The impact of advection becomes negligible as soon as the fluxes are integrated over several seconds. Including dispersion in the O_L horizon was shown to significantly disturb the topsoil $[CO_2]$ concentration. The latter decreased during turbulent events (daytime) resulting in an increase of the intra-day dynamic of topsoil $[CO_2]$. The impact of dispersion decreased with depth, but was still visible below -50 cm depth. Dispersion allowed a better representation of soil $[CO_2]$ intra-day variation, but not of F_s ones and the phase differences remain. When a mechanism representing the PPCW was included, it was shown to modify the intra-day pattern of simulated $[CO_2]$ and F_s in the right direction. The influence of a rapid transport of the phloem pressure concentration waves could explain the intra-day variability of $[CO_2]$ and F_s measurement in Hartheim during the summer 2010. From this study, we can conclude that focus should be placed on the potential factors affecting the CO_2 production, rather than on the transport process description.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Acknowledgments

Stéphanie Goffin acknowledges the support of the Belgium National Fund for Scientific Research (FNRS), within the framework of her thesis (FRIA) and the FEDER (Fonds Européen de Développement Régional). Christophe Wylock acknowledges the support of the FNRS within the framework of his postdoctoral research. The authors are grateful to B. Clerc, P. Courtoisand J.M Gioria of the UMR1137 at INRA Nancy for the installation and maintenance of the experimental set-up during summer 2010.The authors wish to thank the reviewers for their comments.

Tables

Table 1: Values of underlying parameters of Equation 6 and 11 obtained from laboratory measurements

Table 2: Calibrated values for the parameters in Equation 7 and 8

Figures

Figure 1 : a) Time evolution of surface fluxes (F_s) measured (grey) and simulated with the reference model (black), b) Time evolution of the measured climatic conditions: rain and photosynthetically active radiation.

Figure 2: Time evolution of measured (grey) and simulated (black) CO_2 concentration at -5cm, -25 cm and -50 cm.

Figure 3: The maximum instantaneous advective contribution to F_s (F_{adv}/F_s) observed during the two most turbulent days of the measurements campaign according to Δp_{int} obtained for several tested $\alpha_{5.}$

Figure 4: Time evolution (high frequency recording) of the diffusive (F_{diff}) and advective (F_{adv}) components of F_s, [CO_2] below the O_L horizon and Δpint for the reference model and the model including advection with α_5=2.66 and the frequency of 50 Hz.

Figure 5: The maximum ratio between the integrated advective component (int(F_{adv})) and the integrate diffusive component (int(F_{diff})) of F_s obtained during the 3600 s according to the considered integration time (horizontal axis)

Figure 6: The time evolutions of the diffusion coefficient in the litter (D_s(OL)) for the reference model and the model including dispersion and the $[CO2]_{-5cm}$ for the reference model, the model including dispersion and the measurements.

Figure 7: Average inta-day variation of $[CO_2]_{-5cm}$ and F_s respectively for the measurement, the reference model and the model including dispersion with different value of α_6

Figure 8: a)-c) Time evolutions of respectivevly F_s and [CO_2] with the reference model, the model including the phloem pressure concentration wave and the measure, b)-d) the averaged intra-day variability respectively of F_s and [CO_2].

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

References

Bahn, M. et al., 2008. Soil Respiration in European Grasslands in Relation to Climate and Assimilate Supply. Ecosystems, 11(8): 1352-1367.

Bond-Lamberty, B. and Thomson, A., 2010. Temperature-associated increases in the global soil respiration record. Nature, 464(7288): 579-582.

Boone, R., Knute, J.N., Jana, D.C. and Jason, P.K., 1998. Roots exert a strong influence on the temperature sensitivityof soil respiration. Nature, 396(6711): 570-572.

Bowling, D.R. and Massman, W.J., 2011. Persistent wind-induced enhancement of diffusive CO2 transport in a mountain forest snowpack. Journal of Geophysical Research: Biogeosciences, 116(G4): G04006.

Carbone, M.S. and Vargas, R., 2008. Automated soil respiration measurements: new information, opportunities and challenges. New Phytologist, 177(2): 295-297.

Davidson EA, Savage K, Verchot LV, Navarro R. 2002. Minimizing artifacts and biases in chamber-based measurements of soil respiration. Agricultural and Forest Meteorology 113(1-4):21-37.

Davidson, E., Verchot, L., Cattânio, H., Ackerman, I. L., & Carvalho, J. (2000). Effects of soil water content on soil respiration in forests and cattle pastures of eastern Amazonia. Biogeochemistry , 48, 53-69.

Davidson, E.A. and Janssens, I.A., 2006. Temperature sensitivity of soil carbon decomposition. Nature, 440: 165-173.

Davidson, E.A., Janssens, I.A. and Luo, Y., 2006a. On the variability of respiration in terrestrial ecosystems: moving beyond Q10. Global Change Biology, 12(2): 154-164.

Davidson, E.A., Savage, K.E., Trumbore, S.E. and Borken, W., 2006b. Vertical partitioning of CO2 production within a temperate forest soil. Global Change Biology, 12(6): 944-956.

Denman, K.L., et al., 2007. Couplings between changes in the climate system andbiogeochemistry. In: Solomon, S., et al. (Eds.), Climate change 2007: the physicalscience basis. Contribution of working group I to the fourth assessment reportof the Intergovernmental Panel on Climate Change. Cambridge University Press,Cambridge, UK; New York, NY, USA.

Doff sotta, E., et al. (2004). "Soil CO2 efflux in a tropical forest in the central Amazon." Global Change Biology 10(5): 601-617.

Ekblad, A. and Högberg, P., 2001. Natural abundance of 13C in CO2 respired from forest soils reveals speed of link between tree photosynthesis and root respiration. Oecologia, 127: 305-308.

Ekblad, A., Boström, B., Holm, A. and Comstedt, D., 2005. Forest soil respiration rate and δ13C is regulated by recent above ground weather conditions. Oecologia, 143(1): 136-142.

Epron, D., Farque, L., Lucot, E. and Badot, P.-M., 1999. Soil CO2 efflux in a beech forest: the contribution of root respiration. Annals of Forest Science, 56(4): 289-295.

Fang, C. and Moncrieff, J.B., 1999. A model for soil CO2 production and transport 1:: Model development. Agricultural and Forest Meteorology, 95(4): 225-236.

Fang, C. and Moncrieff, J.B., 2001. The dependence of soil CO2 efflux on temperature. Soil Biology and Biochemistry, 33(2): 155-165.

FAO, 2006. World Reference Base for Soil Resources 2006. World Soil ResourcesReport No 103, FAO, Rome.

Fassbinder, J.J., Griffis, T.J. and Baker, J.M., 2012. Interannual, seasonal, and diel variability in the carbon isotope composition of respiration in a C3/C4 agricultural ecosystem. Agricultural and Forest Meteorology, 153(0): 144-153.

Flechard, C.R. et al., 2007. Temporal changes in soil pore space CO2 concentration and storage under permanent grassland. Agricultural and Forest Meteorology, 142(1): 66-84.

Gamnitzer, U., Moyes, A.B., Bowling, D.R. and H., S., 2011. Measuring and modelling the isotopic composition of soil respiration: insight from a grassland tracer experiment. Biogeosciences, 8(5).

Gavrichkova, O. and Kuzyakov, Y., 2012. Direct phloem transport and pressure concentration waves in linking shoot and rhizosphere activity. Plant and Soil, 351(1-2): 23-30.

Goffin, S. et al., 2014. Characterization of the soil CO2 production and its carbon isotope composition in forest soil layers using the flux-gradient approach. Agricultural and Forest Meteorology, 188(0): 45-57.

Hirano, T., 2005. Seasonal and diurnal variations in topsoil and subsoil respiration under snowpack in a temperate deciduous forest. Global Biogeochemical Cycles, 19(2): n/a-n/a.

Hirano, T., Kim, H. and Tanaka, Y., 2003. Long-term half-hourly measurement of soil CO2 concentration and soil respiration in a temperate deciduous forest. Journal of Geophysical Research: Atmospheres, 108(D20): n/a-n/a.

Hirsch, A.I., Trumbore, S.E. and Goulden, M.L., 2004. The surface CO2 gradient and pore-space storage flux in a high-porosity litter layer. Tellus B, 56(4): 312-321.

Högberg, P. and Read, D.J., 2006. Towards a more plant physiological perspective on soil ecology. Trends in Ecology & Evolution, 21(10): 548-554.

Holst, J. et al., 2008. Impacts of summer water limitation on the carbon balance of a Scots pine forest in the southern upper Rhine plain. Agricultural and Forest Meteorology, 148(11): 1815-1826.

Janssens, I.A. and Pilegaard, K., 2003. Large seasonal changes in Q10 of soil respiration in a beech forest. Global Change Biology, 9(6): 911-918.

Jassal, R.S. et al., 2004. A model of the production and transport of CO2 in soil: predicting soil CO2 concentrations and CO2 efflux from a forest floor. Agricultural and Forest Meteorology, 124(3–4): 219-236.

Kätterer, T., Reichstein, M., Andrén, O. and Lomander, A., 1998. Temperature dependence of organic matter decomposition: a critical review using literature data analyzed with different models. Biol Fertil Soils, 27(3): 258-262.

Kuzyakov, Y. and Gavrichkova, O., 2010. REVIEW: Time lag between photosynthesis and carbon dioxide efflux from soil: a review of mechanisms and controls. Global Change Biology, 16(12): 3386-3406.

Lehmann, B.E., Lehmann, M., Neftel, A. and Tarakanov, S.V., 2000. Radon-222 monitoring of soil diffusivity. Geophysical Research Letters, 27(23): 3917-3920.

Lloyed, J. and Taylor, J.A., 1994. On the Temperature Dependence of Soil Respiration. Functional Ecology, 8: 315-323.

Longdoz B, Yernaux M, Aubinet M (2000) Soil CO_2 efflux measurements in a mixed forest: impact of chamber disturbances, spatial variability and seasonal evolution. Glob Change Biol 6:907–917.

Luo, Y. and Zhou, X., 2006. Preface, Soil Respiration and the Environment. Academic Press, Burlington, pp. ix-xi.

Maier, M. and Schack-Kirchner, H., 2014. Using the gradient method to determine soil gas flux: A review. Agricultural and Forest Meteorology, 192–193(0): 78-95.

Maier, M. et al., 2012. Turbulence Effect on Gas Transport in Three Contrasting Forest Soils. Soil Sci. Soc. Am. J., 76(5): 1518-1528.

This is the preprint version of a manuscript that has been published in Plant and Soil 2015
DOI: 10.1007/s11104-015-2381-0

Maier, M., Schack-Kirchner, H., Hildebrand, E.E. and Holst, J., 2010. Pore-space CO2 dynamics in a deep, well-aerated soil. European Journal of Soil Science, 61(6): 877-887.

Marron, N., Plain, C., Longdoz, B. and Epron, D., 2009. Seasonal and daily time course of the 13C composition in soil CO2 efflux recorded with a tunable diode laser spectrophotometer (TDLS). Plant and Soil, 318(1-2): 137-151.

Mencuccini, M. and Holtta, T., 2009. The significance of phloem transport for the speed with which canopy photosynthesis and belowground respiration are linked. New Phytologist, 185, 189–203.

Moyes, A.B., Gaines, S.J., Siegwolf, R.T.W. and Bowling, D.R., 2010. Diffusive fractionation complicates isotopic partitioning of autotrophic and heterotrophic sources of soil respiration. Plant, Cell & Environment, 33(11): 1804-1819.

Phillips, C.L. et al., 2010. Soil moisture effects on the carbon isotope composition of soil respiration. Rapid Communications in Mass Spectrometry, 24(9): 1271-1280.

Plain, C. et al., 2009. Tracing of recently assimilated carbon in respiration at high temporal resolution in the field with a tuneable diode laser absorption spectrometer after in situ 13CO2 pulse labelling of 20-year-old beech trees. Tree Physiology, 29(11): 1433-1445.

Pumpanen, J., Bernard Longdoz, and Kutsch., W.L., 2010. Field measurements of soil respiration: principles and constraints, potentials and limitations of different methods. Soil Carbon Dynamics. Cambridge University Press.

Pumpanen, J. et al., 2008. Respiration in Boreal Forest Soil as Determined from Carbon Dioxide Concentration Profile. Soil Science Society of America Journal, 72(5): 1187.

Rayment MB, Jarvis PG (1997) An improved open chamber system for measuring soil CO2 effluxes of a Boreal black spruce forest. J Geophys Res 102:28779–28784.

Risk, D., Kellman, L. and Beltrami, H., 2002. Carbon dioxide in soil profiles: Production and temperature dependence. Geophysical Research Letters, 29(6): 11-1-11-4.

Risk, D., Kellman, L. and Beltrami, H., 2008. A new method for in situ soil gas diffusivity measurement and applications in the monitoring of subsurface CO2 production. Journal of Geophysical Research: Biogeosciences, 113(G2): G02018.

Risk, D., Nickerson, N., Phillips, C.L., Kellman, L. and Moroni, M., 2012. Drought alters respired δ13CO2 from autotrophic, but not heterotrophic soil respiration. Soil Biology and Biochemistry, 50(0): 26-32.

Riveros-Iregui, D.A., McGlynn, B.L., Epstein, H.E. and Welsch, D.L., 2008. Interpretation and evaluation of combined measurement techniques for soil CO2 efflux: Discrete surface chambers and continuous soil CO2 concentration probes. Journal of Geophysical Research: Biogeosciences, 113(G4): G04027.

Ryan, M.G. and Law, B.E., 2005. Interpreting, measuring, and modeling soil respiration. Biogeochemistry, 73(1): 3-27.

Savage KE, Davidson EA. 2003. A comparison of manual and automated systems for soil CO2 flux measurements: trade-offs between spatial and temporal resolution. Journal of Experimental Botany 54(384):891-899.

Schwen, A. et al., 2011. A Modified Method for the In Situ Measurement of Soil Gas Diffusivity. Soil Sci. Soc. Am. J., 75(3): 813-821.

Seok, B. et al., 2009. An automated system for continuous measurements of trace gas fluxes through snow: an evaluation of the gas diffusion method at a subalpine forest site, Niwot Ridge, Colorado. Biogeochemistry, 95(1): 95-113.

Subke, J.-A., Reichstein, M. and Tenhunen, J.D., 2003. Explaining temporal variation in soil CO2 efflux in a mature spruce forest in Southern Germany. Soil Biology and Biochemistry, 35(11): 1467-1483.

Takle, E.S. et al., 2003. High-frequency pressure variations in the vicinity of a surface CO< sub> 2</sub> flux chamber. Agricultural and forest meteorology, 114(3): 245-250.

Takle, E.S. et al., 2004. Influence of high-frequency ambient pressure pumping on carbon dioxide efflux from soil. Agricultural and Forest Meteorology, 124(3–4): 193-206.

Tang, J., Baldocchi, D.D., Qi, Y. and Xu, L., 2003. Assessing soil CO2 efflux using continuous measurements of CO2 profiles in soils with small solid-state sensors. Agricultural and Forest Meteorology, 118(3–4): 207-220.

Tang, J., Misson, L., Gershenson, A., Cheng, W. and Goldstein, A.H., 2005. Continuous measurements of soil respiration with and without roots in a ponderosa pine plantation in the Sierra Nevada Mountains. Agricultural and Forest Meteorology, 132: 212-227.

Thompson MV, Holbrook NM (2003) Scaling phloem transport: water potential equilibrium and osmoregulatory flow. Plant, Cell and Environment, 26, 1561–1577.

Turcu, V.E., Jones, S.B. and Or, D., 2005. Continuous Soil Carbon Dioxide and Oxygen Measurements and Estimation of Gradient-Based Gaseous Flux. Vadose Zone J., 4(4): 1161-1169.

Van Bochove, E., Bertrand, N. and Caron, J., 1998. In Situ Estimation of the Gaseous Nitrous Oxide Diffusion Coefficient in a Sandy Loam Soil. Soil Sci. Soc. Am. J., 62(5): 1178-1184.

Vargas, R., Carbone, M., Reichstein, M. and Baldocchi, D., 2011. Frontiers and challenges in soil respiration research: from measurements to model-data integration. Biogeochemistry, 102(1-3): 1-13.

Wan, S. and Luo, Y., 2003. Substrate regulation of soil respiration in a tallgrass prairie: Results of a clipping and shading experiment. Global Biogeochemical Cycles, 17(2): 1054.

Wingate, L. et al., 2010. Photosynthetic carbon isotope discrimination and its relationship to the carbon isotope signals of stem, soil and ecosystem respiration. New Phytologist, 188: 576–589.

Xu, M., & Qi, Y. (2001). Soil-surface CO2 efflux and its spatial and temporal variations in a young ponderosa pine plantation in nothern California. Global Change Biology , 7, 667-677.

Xu, L., Baldocchi, D.D. and Tang, J., 2004. How soil moisture, rain pulses, and growth alter the response of ecosystem respiration to temperature. Global Biogeochemical Cycles, 18(4): n/a-n/a.

Yuste, J.C., Janssens, I.A. and Ceulemans, R., 2005. Calibration and validation of an empirical approach to model soil CO2 efflux in a deciduous forest. Biogeochemistry, 73(1): 209-230