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A watershed-scale assessment of a process soil CO₂ production and efflux model

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[1] Growing season soil CO₂ efflux is known to vary laterally by as much as seven fold within small subalpine watersheds (<5 km²), and such degree of variability has been strongly related to the landscape-imposed redistribution of soil water. Current empirical or process models offer low potential to simulate this variability or to simulate watershed-scale dynamics of soil CO₂ efflux. We modified an existing process soil CO₂ production and efflux model to include spatially variable soil moisture, and applied it to a well-studied and moderately complex watershed of the northern Rocky Mountains. We started at the point scale and progressively modeled processes up to the watershed scale. We corroborated model performance using an independent data set of soil CO₂ efflux measurements from 53 sites distributed across the 393 ha watershed. Our approach (1) simulated the seasonality of soil CO₂ efflux at riparian sites; (2) reproduced short-term (diel) dynamics of soil CO₂ concentration ([CO₂]) at riparian sites, particularly observed hysteresis patterns in the soil [CO₂]–soil temperature relationship; and (3) simulated growing season estimates of soil CO₂ efflux at dry sites across the landscape (98% of area). Model limitations included poor simulation of growing season (cumulative) soil CO₂ efflux at sites with a large drainage area, likely as a result of poorly modeled soil water content and challenges in parametrization of root and microbial activities. Our study provides important insight into coupling hydrological and biogeochemical models at landscape scales, and highlights the role of landscape structure and heterogeneity when modeling spatial variability of biogeochemical processes.


1. Introduction

[2] Growing season soil CO₂ efflux is known to vary laterally by as much as seven fold within small subalpine watersheds (<5 km²), and such degree of variability has been strongly related to the landscape-imposed redistribution of soil water [Riveros-Iregui and McGlynn, 2009]. Empirical models of soil CO₂ efflux abound based on derived relationships with soil temperature [e.g., Kucera and Kirkham, 1971; Ratkowsky et al., 1982; Winkler et al., 1996], soil water content [e.g., Orchard and Cook, 1983; Davidson et al., 2000; Liu et al., 2002; Yuste et al., 2003], substrate [e.g., Raich and Nadelhoffer, 1989; Ryan et al., 1996; Janssens et al., 2001; Reichstein et al., 2003], or morphologic variables such as upslope accumulated area (UAA) [Riveros-Iregui and McGlynn, 2009] and microtopography [Lee et al., 2011]. On the other hand, process models represent the mechanisms known to govern soil CO₂ efflux, and are derived from system examination and physical evidence [e.g., Parton et al., 1987; Rastetter et al., 1991; Potter et al., 1993; Suarez and Simunek, 1993; Rastetter et al., 1997; Fang and Moncireff, 1999; Welsch and Hornberger, 2004]. However, both empirical and process models to date offer low potential to simulate the observed, natural variability of soil CO₂ efflux across mountainous catchments.

[3] A common problem in current soil CO₂ efflux models, and in many catchment-scale biogeochemical models, is the omission of spatial and temporal variability of soil moisture. It has been recently demonstrated that soil water content can control the spatial [Pacific et al., 2008; Riveros-Iregui and McGlynn, 2009] and temporal [Riveros-Iregui et al., 2007; Riveros-Iregui et al., 2008; Pacific et al., 2009] variability of soil CO₂ efflux in subalpine systems of the western United States or in boreal forest systems of Alaska [Kane et al., 2006]. To date, a robust implementation of the lateral distribution of soil water into biogeochemical models is lacking. Understanding the effects of soil moisture heterogeneity on soil CO₂ efflux from diel to seasonal scales, and from the point to the ecosystem scale, will enhance process knowledge of the spatial variability of biogeochemical processes across many ecosystems.
We applied an existing process soil CO$_2$ production model [Fang and Moncrieff, 1999; Welsch and Hornberger, 2004] in combination with a recently developed CO$_2$ production and diffusion model [Riveros-Iregui et al., 2007], to a well-studied subalpine watershed of the northern Rocky Mountains. We implemented this model by progressively adding process understanding starting at the point scale and advancing to the watershed scale. Given our catchment-scale focus, we used a single-layer model because it is useful to examine the effects of laterally variable environmental gradients (e.g., soil moisture) on catchment scale biogeochemistry. We acknowledge that a multilayer model may yield different (and certainly more detailed) results across individual soil profiles. However, we were encouraged by the pragmatic approach of Rappach and Finnigan [1988], who highlight the usefulness of single-layer models in systems with a length scale much larger than that of the multilayered processes themselves (e.g., medium- or large-scale catchments). Our study takes advantage of a well-established and efficient hydrologic model that simulates the lateral variability of soil water content across the landscape, as well as the convergence and divergence of unsaturated flow. In this paper we seek (1) to critically assess the performance of a soil CO$_2$ process and efflux model applied across a moderately complex catchment; (2) to investigate the role of spatial and temporal variability of soil moisture on simulated soil CO$_2$ efflux; and (3) to corroborate model performance using an independent data set of CO$_2$ efflux measurements at distributed sites across the same watershed. We address two outstanding research questions: the role of hydrology as a spatial and temporal control of soil CO$_2$ efflux, and the role of model-data comparison in the development of biogeochemical models in mountainous watersheds.

2. Study Site

The study site was the Tenderfoot Creek Experimental Forest (TCEF), a subalpine catchment located in the Little Belt Mountains of central Montana. This forest is representative of the subalpine ecosystems of the northern Rocky Mountains and is subject to a steady seasonal dry-down in soil moisture [Woods et al., 2006; Riveros-Iregui et al., 2007]. The 393 ha catchment of interest contains a second-order perennial stream, Stringer Creek that drains into Tenderfoot Creek, which ultimately drains into the Missouri River. At the TCEF, freezing temperatures and snow can occur any month of the year, and the mean annual temperature is 0°C [Farnes et al., 1995]. During the period of this study (21 June 21–2 September 2006), air temperature ranged from 28.8°C (30 July) to −2.1°C (2 September), with an average of 13.6°C. The growing season for the majority of the TCEF can extend from 45 to 90 days, decreasing in length toward the ridges. Cumulative precipitation during the period of this study was 42 mm with the highest daily precipitation falling on 29 June (9.2 mm), and monthly precipitation of 9.8 mm (21–30 June), 23.4 mm (July), and 8.9 mm (August). Mean annual precipitation is 880 mm with a majority (>70%) falling as snow [Farnes et al., 1995]. The Stringer Creek watershed ranges in elevation from 2090 to 2421 m and has a full range of slope, aspect, and topographic convergence and divergence.

Because this catchment has been the focus of several hydrologic and biogeochemical studies in the last few years [Riveros-Iregui et al., 2007; Pacific et al., 2008; Riveros-Iregui, 2008; Riveros-Iregui et al., 2008; Jenco et al., 2009], Stringer Creek watershed is an ideal site to assess the performance of a coupled hydrological-biogeochemical model at the landscape scale.

The two predominant ecosystems at Stringer Creek are riparian meadows (near the Stringer Creek channel) and upland forests. Vegetation cover at riparian meadows is dominated by *Calamagrostis canadensis* (bluejoint reedgrass), whereas vegetation in upland forests is dominated by *Pinus contorta* (lodgepole pine) and to a lesser extent *Abies lasiocarpa* (subalpine fir) and *Picea Engelmannii* (Engelmann spruce). *Vaccinium scoparium* (whortleberry) is the predominant understory species. Given its relatively simple and homogenous vegetation cover, Stringer Creek is a suitable site to implement a model focused on effects of soil water content on soil CO$_2$ efflux at the watershed scale.

3. Model

3.1. Soil Water Content Model

Recent studies in subalpine ecosystems have highlighted the importance of the lateral redistribution of soil water as a control of soil CO$_2$ production and efflux, both temporally [Riveros-Iregui et al., 2007] and spatially [Riveros-Iregui and McGlynn, 2009]. To model soil water content at the catchment scale, we applied TOPMODEL [Beven and Kirkby, 1979] for its ability to describe flow and connectivity within a catchment on the basis of topographic similarity among grid cells of a digital elevation model. We employed a version of TOPMODEL modified by Scanlon et al. [2005] that estimates shallow, unsaturated flow (i.e., lateral soil water flux $q_l$) in addition to saturated, groundwater flow and overland flow for each grid cell. This version of TOPMODEL also included a calibrated parameter to estimate groundwater recharge (i.e., vertical soil water flux $q_v$), and a mechanistic model of vertical flow through the soil-plant-atmosphere continuum [Emanuel et al., 2010] to develop a soil water balance for each grid cell (5 m) of the watershed,

\[
\frac{d\theta}{dt} = \frac{1}{z_c} (I - ET - q_v - q_l),
\]

where $\theta$ is volumetric soil moisture, $q_v$ is vertical soil water flux, $q_l$ is lateral soil water flux, $z_c$ is the depth of the root zone, $I$ is infiltration, and $ET$ is evapotranspiration (See Table 1). Infiltration and $ET$ were modeled from lidar-derived vegetation characteristics within each grid cell and prescribed meteorological conditions interpolated from seven meteorological stations within the watershed following Jolley et al. [2005] and Emanuel et al. [2010]. Because topography, vegetation, and meteorological conditions vary across the watershed, the soil water balance (2-D; vertical and along the hillslope) was solved separately for each grid cell of the watershed for each half-hour of the 2006 growing season (21 June through 2 September 2006). The model was recently applied to the Stringer Creek watershed, demonstrating its ability to simulate water-controlling processes at the catchment scale [Emanuel et al., 2010]. Model output was compared to runoff measured by the US Forest Service.
at the catchment outlet and to total ET measured by an eddy covariance tower [Emanuel et al., 2010], validating the use of the model to accurately simulate seasonal hydrologic balance of Stringer Creek catchment. Despite differences in absolute magnitude in particular toward the dry end of the soil water content range (see auxiliary material), seasonal trends of simulated soil water content replicated our observations very closely ($r^2 = 0.97$).

[1] Soil $\text{CO}_2$ production is typically calculated as a function of water stress on plant and microbial activities [Simunek and Suarez, 1993; Welsch and Hornberger, 2004]; thus we calculated soil water matric potential or soil tension ($h$) as a surrogate for water stress by solving a widely applied soil moisture–soil tension relationship [van Genuchten, 1980]

$$h = \left(\frac{(\theta_s - \theta_r)}{(\theta_s - \theta_r)} \right)^\frac{1}{\alpha}, \tag{1}$$

where $\theta_s$ is the saturated water content, $\theta_r$ is the residual water content, $\alpha$ is a fitting parameter for tension at air entry, $m$ is given by $m = 1 - (1/n)$, and $n$ is a fitting parameter estimated from observed data. The van Genuchten relationship has been widely applied and deemed accurate when simulating diffusion as a function of air–filled porosity across multiple soil types and porosities [Moldrup et al., 2005a, 2005b].

### 3.2 Soil Temperature Model

[1] Soil temperature controls soil $\text{CO}_2$ production and efflux at short- and long-time scales [e.g., Lloyd and Taylor, 1994; Winkler et al., 1996]. To model soil temperature for the entire catchment, we used interpolated, distributed air temperature at 10 m grid resolution derived from the Spatial Observation Gridding System (SOGS) [Jolly et al., 2005] for the period between 21 June and 2 September 2006, at half-hour intervals. This scale-independent system is known to yield a mean absolute error smaller than 2°C [Jolly et al., 2005]. We then used the approximation of Kang et al. [2000] (developed to simulate spatiotemporal variability of soil temperature in forested soils) to calculate soil temperature at half-hour intervals. This relationship assumes that soil temperature can be estimated at any depth ($z$) as follows: when $A_j > T_{S-j-1}$,

$$T_{S,j}(z) = T_{S,j-1}(z) + [A_j - T_{S,j-1}(z)] \exp \left[ -z \left( \frac{\pi}{k A} \right)^2 \right] \tag{2}$$

and when $A_j \leq T_{S-j-1}$,

$$T_{S,j}(z) = T_{S,j-1}(z) + [A_j - T_{S,j-1}(z)] \exp \left[ -z \left( \frac{\pi}{k A} \right)^2 \right] \tag{3}$$

where $A_j$ is air temperature at the time $j$, $T_S$ is soil temperature, $k$ is the soil thermal diffusivity ($1.54 \times 10^{-3}$ cm$^2$/s), $p$ is the period of diurnal temperature variation (86,400 s), and $k$ is the extinction coefficient from the Beer-Lambert Law for radiation through canopy as a function of leaf area index (LAI) and ground litter LAI equivalent. Measured LAI in the forest (98% of watershed area) ranged from 1.1 to 1.35, whereas measured LAI in riparian areas (2% of watershed area) ranged from 0.8 or less at the beginning of the season, to a high of 2.0 in the middle of the growing season, rapidly decreasing by late summer with grass senescence (unpublished data). Thus for simplicity in the soil temperature model, we used a LAI value of 1.2 m$^2$ and for both vegetation covers, as well as ground litter value of 1.5 m$^2$ m$^{-2}$, throughout the growing season. While we acknowledge potential inaccuracies introduced by this assumption especially in riparian areas, such inaccuracies were typically small (~0.8°C error in $T_S$ for every change of 0.5 m$^2$ m$^{-2}$ in LAI at $T_S = 18^\circ$C, and smaller at lower temperatures) and the model was a good predictor of the seasonality of soil temperature. Based on calibration with measured soil temperature at two sites, the estimated mean absolute error for

### Table 1. Variables Included in Models of Soil Water Content, Soil Temperature, and Soil $\text{CO}_2$ Production and Efflux, as well as in the Terrain Analysis

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau$</td>
<td>Depth to root zone</td>
<td>m</td>
</tr>
<tr>
<td>$\iota$</td>
<td>Infiltration</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$\psi_T$</td>
<td>Evapotranspiration</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$q_v$</td>
<td>Vertical water flux</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$q_l$</td>
<td>Lateral water flux</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Fitting parameter for tension</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$m$</td>
<td>Fitting parameter</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$h$</td>
<td>Soil tension</td>
<td>m</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Soil water content</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_r$</td>
<td>Residual soil water content</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_s$</td>
<td>Saturated soil water content</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Air temperature</td>
<td>°C</td>
</tr>
<tr>
<td>$T_S$</td>
<td>Soil temperature</td>
<td>°C</td>
</tr>
<tr>
<td>$k_S$</td>
<td>Soil thermal diffusivity</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$Z$</td>
<td>Soil depth</td>
<td>m</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Period of diurnal temperature variation</td>
<td>s</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Extinction coefficient</td>
<td>m$^2$ m$^{-2}$</td>
</tr>
<tr>
<td>LAI</td>
<td>Leaf area index</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$f_A$</td>
<td>Air-filled porosity</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$\gamma_a$</td>
<td>Autotrophic respiration rate</td>
<td>g CO$_2$ m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\gamma_H$</td>
<td>Heterotrophic respiration rate</td>
<td>g CO$_2$ m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>PAR</td>
<td>Photosynthetically active radiation</td>
<td>mmol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$R_b$</td>
<td>Root fraction</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>$S_o$</td>
<td>Soil organic content</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>$S_{c}$</td>
<td>Soil tension when CO$_2$ production stops, soil too wet</td>
<td>m</td>
</tr>
<tr>
<td>$S_{t}$</td>
<td>Soil tension when CO$_2$ production is optimal</td>
<td>m</td>
</tr>
<tr>
<td>$UAA$</td>
<td>Upslope accumulated area</td>
<td>m$^2$</td>
</tr>
</tbody>
</table>

$^1$Auxiliary materials are available in the HTML. doi:10.1029/2010WR009941.
soil temperature was lower than 1.5°C across the 74 days of the simulation and across a seasonal range of ~20°C (see auxiliary material).

3.3. Soil CO₂ Production and Efflux Model

[10] The dynamics of CO₂ in soil air can be explained by the following mass balance equation [Riveros-Iregui et al., 2007]:

\[
f_a \frac{\partial [CO_2]}{\partial t} = -D \frac{\partial^2 [CO_2]}{\partial z^2} + \gamma_A (B, PAR, \theta) + \gamma_H (M, T_S, \theta),
\]  

where \(f_a\) is the air-filled porosity, \(D\) is the diffusion coefficient of CO₂ in the air-filled pore space, \(\gamma_A\) and \(\gamma_H\) are the rates of CO₂ production from autotrophic and heterotrophic activities, respectively, \(B\) is root biomass, \(PAR\) is photosynthetically active radiation, and \(M\) is soil organic matter. It is important to note that \(PAR\) and \(T_S\) vary in time on a diel basis, whereas \(\theta\) varies in time on a seasonal basis. As a result, there is asynchronism in the timing and effect of each variable on the resulting soil CO₂ concentration ([CO₂]). While equation (5) presents the dynamics of [CO₂] at any given depth \(z\), the right-hand side of equation (5) is divided into two components: a “production” component \((\gamma_A + \gamma_H)\) and a “diffusion” component \(D \frac{\partial^2 [CO_2]}{\partial z^2}\).

To implement the production component, we adapted the soil CO₂ production component of a previously developed model [Fang and Moncrieff, 1999; Welsch and Hornberger, 2004, and in it, B and M were based on field observations [Riveros-Iregui and McGlynn, 2009] and kept constant across the catchment (\(B = 7.6\) kg m⁻³ and \(M = 16.5\) kg C m⁻³). \(PAR\) was scaled between 0 and 1 across the season. The model has been used across different forested ecosystems [Moncrieff and Fang, 1999; Welsch and Hornberger, 2004; Saiz et al., 2007] because it includes the main effects of environmental factors (i.e., soil temperature, soil moisture, soil [O₂]) on the generation of soil CO₂ from plant and microbial activities. Rates of autotrophic and heterotrophic activities were calibrated based on optimal rates for \(\theta\) and \(T_S\) found in the literature [Fang and Moncrieff, 1999; Hamman et al., 2008] and corroborated with soil CO₂ efflux rates at the site [Riveros-Iregui and McGlynn, 2009].

[11] As presented in equation (5), production and diffusion components have opposite signs, so the diffusion component provides diffusion-limited feedback to the model at low values of \(f_a\) [see Riveros-Iregui et al., 2007]. Specifically, variably in \(\theta\) controls the transition from a diffusion-limited system to a production-limited system [Riveros-Iregui et al., 2007]. Once CO₂ production was modeled we added the diffusion component of equation (5) to modeled production. We assumed a homogenous diffusion coefficient \(D\) across the watershed, based on several calculated values of \(D\) as a function of total porosity \((\Phi)\) and \(f_a\), and using the model proposed by Moldrup et al. [1999]:

\[
\frac{D}{D_0} = \Phi^2 \left( \frac{f_a}{\Phi} \right)^{2/3},
\]

where \(D_0\) is the gas diffusion coefficient in free air, \(b\) is the Campbell [1974] pore size distribution parameter, \(\Phi\) is total soil porosity, and \(f_a\) is calculated as \(\Phi\) minus \(\theta\). The \(b\) parameter was derived from the following relationship with clay fraction content \((CF)\) \((r^2 = 0.96)\) [Clapp and Hornberger, 1978; Olesen et al., 1996; Rolston and Moldrup, 2002]:

\[
b = 13.6CF + 3.5.
\]  

[12] This method is widely applied and it has been amply tested to model \(D\) across a range of soil types and water contents [Baldocchi et al., 2006; Kawamoto et al., 2006; Resurreccion et al., 2007]. Solubility of CO₂ in the gas phase as well as the vertical advection by soil water were assumed negligible, given that CO₂ diffusion in the gas phase is several orders of magnitude higher than in the liquid phase [Simunek and Suarez, 1993; Welsch and Hornberger, 2004].

[13] We estimated the effects of soil tension in controlling rates of autotrophic and heterotrophic respiration \((\gamma_A\) and \(\gamma_H\); equation (5)). According to Simunek and Suarez [1993] and Welsch and Hornberger [2004], the CO₂ reduction coefficient \(f_s(h)\) is a function of soil tension as illustrated by the following relationships:

\[
f_s(h) = \frac{\log[h] - \log[h_0]}{\log[h] - \log[h_0]}, \quad h \in (h_0, h_1),
\]

\[
f_s(h) = \frac{\log[h] - \log[h_1]}{\log[h] - \log[h_1]}, \quad h \in (h_1, h_2),
\]

\[
f_s(h) = 0, \quad h \in (\infty, h_1) \cup (h_2, \infty),
\]

where \(h_0\) is the tension when CO₂ production is optimal, and \(h_1\) and \(h_2\) are soil tension values when respiration ceases because conditions are too wet or too dry, respectively.

3.4. Field Observations and Landscape Analysis

[14] At one riparian meadow site and one upland forest site (Figure 1), we measured volumetric soil water content (CSI model 616, Campbell Scientific Inc., Logan, UT) and soil temperature (CSI model 107, Campbell Scientific Inc., Logan, UT) 20 cm below the soil surface. At the same two sites, continuous measurements of soil [CO₂] were collected with solid-state CO₂ probes (GMP221 with transmitter, Vaisala, Helsinki, Finland) installed 20 cm below the soil surface on 7 June 2006. All data were logged at 20 min intervals with a data logger (model CR10x, Campbell Scientific Inc., Logan, UT). Further details on field measurements have been described in a field-based study [Riveros-Iregui et al., 2008].

[15] To validate modeled soil CO₂ efflux, we used independent measurements at 53 sites distributed across the watershed (Figure 1) collected during the 2006 growing season and reported in a previous study [Riveros-Iregui and McGlynn, 2009]. Although the previous study reported measurements from 62 sites, an incongruity in boundaries between the lidar-derived digital elevation imagery and actual watershed area resulted in nine fewer sites for this study. Measurements of soil CO₂ efflux were made according to procedures described by Pacific et al. [2008] and Riveros-Iregui et al. [2008]. Measurements were collected
in triplicate every 2–7 days, using a soil respiration chamber model SRC-1 (PP Systems, Massachusetts, USA) equipped with an infrared gas analyzer (IRGA; EGM-4, PP Systems, Massachusetts, USA).

[16] To estimate relative wetness potential at each site, we calculated upslope accumulated area (UAA (m²)) for each 3 m pixel of a digital elevation model (DEM) of the watershed (Figure 1), based on the triangular multiple flow direction algorithm [Seibert and McGlynn, 2007]. UAA represents the amount of area draining to a specific location in the landscape [Beven and Kirkby, 1979; McGlynn and Seibert, 2003] and serves as a metric for patterns of water flow and comparison among sites of the same watershed [Western and Grayson, 1998; Grayson and Western, 2001].

3.5. Modeling Approach

[17] The modeling approach can be divided into three steps. First, soil CO₂ production (or \( \gamma_A + \gamma_H \) in equation (5)) was modeled at 30 min intervals at 20 cm depth for the riparian and upland sites (Figure 1). Model calibration was performed using these two sites given the good temporal coverage of observations of soil water content, soil temperature, and soil [CO₂] [Riveros-Iregui et al., 2008], and using Monte Carlo analysis. This analysis has been used in parametrization of hydrological models [Freer et al., 1996; Campbell et al., 1999] and more recently in parametrization of ecosystem respiration models [Knohl et al., 2008; Ricciuto et al., 2008]. Six parameters, \( \gamma_A \), \( \gamma_H \), \( h_a \), \( h_b \), \( h_c \), and \( n \), were sampled randomly from uniform distributions based on the range of known variability of these parameters found in the literature [Fang and Moncrieff, 1999]. The process was repeated 25,000 times and in each step the parameters were used to estimate the Nash-Sutcliffe coefficient \([Nash and Sutcliffe, 1970]\) of model efficiency (\( E \)). Selected values were chosen based on the set of parameters that yielded the highest \( E \).

[18] Second, once \( E \) did not improve any further, we applied the diffusion term of equation (5), or \( \frac{D \partial [CO_2]}{\partial z} \), to modeled soil CO₂ production. In doing so, we assumed only one soil layer and modeled diffusion (efflux) from a 20 cm depth to the soil surface \((z = 0 \text{ cm})\), where [CO₂] was set constant at 450 ppm. Previous studies have used similar assumptions at the soil surface [Tang et al., 2005; Riveros-Iregui et al., 2008] and demonstrated that these assumed values do not compromise calculation of soil CO₂ efflux, as the diel variability of [CO₂] at depth is much greater than the diel variability of [CO₂] above the soil surface given the atmospheric buffer (see Riveros-Iregui et al. [2008] for a sensitivity analysis of this assumption). Applied this way (step 1, step 2), we used our modeling approach to test sites of the landscape that were production limited (i.e., where autotrophic and heterotrophic respirations were limited by low soil moisture) and sites of the landscape that were diffusion limited (i.e., where soil CO₂ diffusion and efflux was limited by high soil moisture). This approach also allowed us to investigate whether diffusion (modified entirely by the spatiotemporal variability of \( \theta \)) played a larger role in some landscape areas than others. To date, the fundamental balance between production and diffusion has not been simultaneously implemented into soil respiration models, yet the diffusion-limited feedback emerging during high moisture can be significant in wet soils during some times of the year [Riveros-Iregui et al., 2007; Pacific et al., 2008, 2009].

[19] Third, once the model was parametrized and calibrated to simulate production and diffusion at the riparian meadow and upland forest sites, we applied it to the entire watershed via a 10 m digital elevation model (DEM). Results were validated using independent measurements of soil CO₂ efflux (or the resulting \( D \frac{\partial [CO_2]}{\partial z} \) at the soil surface) at 53 sites distributed across the watershed [Riveros-Iregui and McGlynn, 2009]. We assumed a homogenous soil type (sandy loam) and depth across the entire watershed. Model performance was evaluated based on the mean absolute error (MAE) of observed and modeled efflux across the 53 sites.

4. Results

4.1. Model Parametrization

[20] The selected set of parameters based on the Monte Carlo analysis is shown in Figure 2. Each sampled model parameter is plotted against the Nash-Sutcliffe coefficient of model efficiency. This plot shows the sensitivity of individual model parameters where a strong change in the model efficiency is observed over some range of the parameter [Freer et al., 1996]. Based on these plots we selected optimal values of \( \gamma_A \), \( \gamma_H \), \( h_a \), \( h_b \), \( h_c \), and \( n \) parameters for the model (Table 2). These parameters yielded a combined Nash-Sutcliffe coefficient of model efficiency (\( E \)) of 0.0881 at the riparian site and −4.71 at the upland site. In selecting these parameters, we assumed they were constant throughout the watershed.

4.2. Long-Term (Seasonal) Dynamics

[21] The seasonal dynamics of soil [CO₂] are presented in Figure 3. At the riparian site, observed soil [CO₂] varied

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**Figure 1.** Location of riparian and upland calibration sites (crosses) and 53 independent measurement (validation) sites (circles). Shading represents the calculated 3 m upslope accumulated area (UAA), a metric for relative wetness potential among sites of the same watershed. See section 3 for additional details.
from over 12,000 ppm at the beginning of the growing season to about 2000 ppm by the end of the summer (Figure 3). Applying only the production component of the model (i.e., not accounting for diffusion), modeled soil [CO₂] varied from around 5000 ppm at the beginning of the growing season to about 2000 ppm by the end of the summer (Figure 5). An additional strength of the model was its ability to simulate observed hysteresis in the soil [CO₂]-soil temperature relationships throughout the growing season (Figures 5 and 6). The diel range of soil [CO₂] was not simulated as well at the upland site. While the diel range of observed soil [CO₂] was low (little or no hysteresis; Figure 6), modeled [CO₂] exaggerated hysteresis (i.e., the model overpredicted [CO₂]) at the dry site. Given that continuous measurements were made only at two sites with contrasting soil moisture, this feature of the model could not be further explored at other sites (e.g., intermediate sites).

5. Discussion

The seasonality of soil [CO₂] was well simulated at the riparian site (Figure 3), especially when accounting for soil CO₂ diffusion. Despite the low soil [CO₂] after 30 July (Figure 3b), E improved from to 0.0881 to 0.708 at the riparian site. Similar analysis at the upland site demonstrated that E did not improve after accounting for diffusion at this site (Figure 4), likely because of much lower soil water content at this site (average ~0.13 m⁻³).

4.3. Short-Term (Diel) Dynamics

The magnitude of the short-term (diel) variability in soil [CO₂] was well simulated by the model at the riparian site, suggesting appropriate parametrization and incorporation of soil temperature and PAR into model structure. Observed diel range in soil [CO₂] varied from ~5000 ppm on 13 June, to 2000 ppm on 23 June, to near zero by the end of July (Figure 5). An additional strength of the model was its ability to simulate observed hysteresis in the soil [CO₂]-soil temperature relationships throughout the growing season (Figures 5 and 6). The diel range of soil [CO₂] was not simulated as well at the upland site. While the diel range of observed soil [CO₂] was low (little or no hysteresis; Figure 6), modeled [CO₂] exaggerated hysteresis (i.e., the model overpredicted [CO₂]) at the dry site. Given that continuous measurements were made only at two sites with contrasting soil moisture, this feature of the model could not be further explored at other sites (e.g., intermediate sites).

4.4. Spatial Variability of Modeled Efflux

Across the entire catchment, modeled soil CO₂ efflux varied from 4.6 to 26.4 mol CO₂ m⁻² over 71 days, with a mean efflux of 11.1 mol CO₂ m⁻² over the same period. Compared against the 53 sites, the model performed better at those locations with small drainage area (Figure 7), where despite a modest overprediction the model simulated the magnitude of seasonal fluxes well. At sites with large drainage area, however, model performance progressively declined and modeled CO₂ fluxes were increasingly underestimated (Figure 8). Lateral differences in CO₂ production and CO₂ diffusion resulted in different spatial patterns of soil CO₂ efflux at different times of the year. For example, early in the growing season (24 June) efflux range across the catchment was low (less than 2 μmol CO₂ m⁻² s⁻¹; Figure 9). By the peak of the growing season (23 July), the range across the catchment was the largest (~8 μmol CO₂ m⁻² s⁻¹), whereas by late August the range of catchment efflux decreased although the spatial differences remained more pronounced than during early summer.

Table 2. Selected Soil CO₂ Production Model Parameters Based on Monte Carlo Analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Range (min: max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma_H$</td>
<td>0.8388</td>
<td>(0.23: 1.64)</td>
</tr>
<tr>
<td>$\gamma_A$</td>
<td>0.3283</td>
<td>(0.04: 2.96)</td>
</tr>
<tr>
<td>$h_1$</td>
<td>9.1137</td>
<td>(5.01: 9.94)</td>
</tr>
<tr>
<td>$h_2$</td>
<td>30.2073</td>
<td>(30.1: 134.4)</td>
</tr>
<tr>
<td>$h_3$</td>
<td>9536.3</td>
<td>(8005: 14,971)</td>
</tr>
<tr>
<td>$n$</td>
<td>1.743</td>
<td>(1.60: 2.49)</td>
</tr>
</tbody>
</table>

*Parameter range corresponds to range for the top 5% values of E.*
time scales [Riveros-Iregui et al., 2007; Pacific et al., 2008, 2011]. At the upland site E did not improve after accounting for diffusion, perhaps because of significantly lower soil moisture relative to the riparian site. In fact, E decreased and MAE increased, suggesting that in dry soils diffusion does not limit soil CO$_2$ efflux (i.e., all CO$_2$ that is produced leaves as efflux). An issue that emerged when accounting for diffusion at low soil water content values (i.e., after 30 July in Figure 3b; or Figure 4b) was the decrease in model performance. This decrease is an artifact caused by the application of cost functions (such as E, MAE) across the full range of soil [CO$_2$]. These cost functions are more sensitive to large discrepancies, because minimizing a large error has a larger impact on MAE and E than minimizing a small error. It has been established that both “wet” and “dry” catchment behavior cannot always be accurately represented with a single set of parameters [Wagener, 2003]; thus, our findings suggest that when applying biogeochemical models at the watershed scale, caution should be taken and model parametrization and assessment should reflect, at least to a first degree, the lateral variability of soil water (wet versus dry sites) as well as its seasonality (wet versus dry times of the year).

[25] Implementing a PAR-dependent variable (equation (5)) as a temporal control on autotrophic activity improved the simulation of hysteresis patterns in the soil [CO$_2$]–soil temperature relationship at the riparian site (Figure 5). As recently demonstrated, there is a temperature independent component in soil [CO$_2$] that can be explained by the variability of PAR [Liu et al., 2006; Riveros-Iregui et al., 2007; Vargas and Allen, 2008]. However, similar analysis at the upland site showed that the model overestimated hysteresis at this site (e.g., 23 July; Figure 6), likely because the effects of PAR on soil CO$_2$ efflux are different between sites. This suggests that the parametrization of PAR on soil CO$_2$ efflux at the catchment scale is useful but it needs to be further explored in combination with variable vegetation cover and dynamic soil moisture conditions.

[26] The model simulated cumulative rates of efflux at those areas with low UAA better than at areas with high UAA. In fact, MAE was 6.6 mol CO$_2$ m$^{-2}$ for 71 days across the 53 sites, but it was only 1.75 mol CO$_2$ m$^{-2}$ for the same period at those sites with UAA below ~1600 m$^2$ (32 sites total; Figure 7). At sites with large UAA, the model did not perform well because of poorly modeled soil water content. Similar deficiencies had been observed while using the model across gradients of soil moisture in other ecosystems [Moncrieff and Fang, 1999; Welsch and Hornberger, 2004; Saiz et al., 2007]. Because modeling the spatial variability of soil water content remains an ample area of research, it is anticipated that improving catchment scale biogeochemical models will remain dependent upon uncertainties of models of soil water content. A second deficiency in our modeling approach lies in our understanding of catchment scale microbial processes and in the observed sensitivity of the model to microbial respiration rates. Figure 2 demonstrates that the model appears

Figure 3. Seasonal soil [CO$_2$] at 20 cm of the riparian site applying (a) only the soil CO$_2$ production component of the model; and (b) the production and efflux components of the model. Model ability to simulate soil [CO$_2$] considerably increased when efflux component (diffusion limitation feedback) was introduced into the model.

Figure 4. Seasonal soil [CO$_2$] at 20 cm of the upland site applying (a) only the soil CO$_2$ production component of the model; and (b) the production and efflux components of the model.
more sensitive to $\gamma_H$ and $h_b$ than to any other individual parameter as indicated by a steeper gradient in the highest model efficiencies. Figure 2 additionally indicates that there is asymmetry in the distribution of the sensitivity, depending on whether soil moisture is increasing or decreasing. The parameter $h_b$ shows some degree of threshold behavior whereby model simulations appear highly sensitive to values of $h_b$ below 50 cm, even though higher values are still feasible. While these plots do not include parameter interactions, they help inform which model parameters best constrain overall model uncertainty. Microbial communities have been found to be quite heterogeneous in space [Fierer et al., 2003] and time [Lipson and Schmidt, 2004] as a function of soil temperature [Zogg et al., 1997] and soil moisture [Kieft et al., 1993; Lundquist et al., 1999; Schimel et al., 1999]. In addition, Fierer and Jackson [2006] demonstrated that soil pH was correlated to the diversity of soil microbial communities at large scales. We measured vadose zone soil water pH from a subset of lower hillslope and riparian landscape positions and did not observe strong variability (pH ≤7.5; unpublished data). Nonetheless, soil pH could be an important variable and in some locations should be considered when modeling biogeochemical processes at the catchment scale. Additional ways to parametrize the variability of microbial activity, the lateral mobilization of soil organic matter and litter, and the effects of small precipitation events, will also be needed as catchment scale biogeochemical models are further developed.

[27] Modeling the subsurface as a single layer is a simplification of reality, but by doing so we could evaluate effects of patterns of seasonal soil moisture on biogeochemical processes across the entire watershed (Figure 9). We acknowledge that a multilayer model may yield different and certainly more detailed results across individual soil profiles; however, a single-layer model was useful to examine the effects of laterally variable environmental gradients on catchment scale soil CO$_2$ efflux. TOPMODEL is commonly configured with a single subsurface layer [e.g., Scanlon et al., 2005] that still facilitates vertical and lateral soil moisture dynamics while it avoids additional uncertainties and potential equifinality associated with multiple soil layers. The result is that while the soil vertical structure is simplified, the model simulates the observations of soil CO$_2$ efflux across a large portion of the landscape. Our results suggest that the model has the ability to reproduce soil CO$_2$ generating processes (autotrophic and heterotrophic) in addition to diffusion-related feedbacks at diel time scales. These are important improvements from traditional power-based models [Lloyd and Taylor, 1994] or empirical relationships that are applied uniformly across the catchment [e.g., Riveros-Iregui and McGlynn, 2009].

Figure 5. Observed and simulated diel variation of soil [CO$_2$] at 20 cm of the riparian site. Clockwise hysteresis (as indicated by the arrow) was observed in all measured and modeled [CO$_2$].

Figure 6. Observed and simulated diel variation of soil [CO$_2$] at 20 cm of the upland site. Clockwise hysteresis (as indicated by the arrow) was observed in all measured and modeled [CO$_2$]. Note the different scale in the y axis compared to Figure 5.
A current issue in modeling biogeochemical processes at the watershed scale is validation against independent observations. Many models that do not appear to suffer from limitations lack assessment against observations that represent the system for which the model is intended (although see Richardson et al. [2006] for a study where such assessments have been made). Assessment for the entire catchment revealed that modeled efflux was on average $11.1 \text{ mol CO}_2 \text{ m}^{-2} \text{ 71 days}^{-1}$, which were below empirically modeled catchment efflux ($15.3 \text{ mol CO}_2 \text{ m}^{-2} \text{ 71 days}^{-1}$ [Riveros-Iregui and McGlynn, 2009]), but comparable to nighttime ecosystem respiration from an eddy covariance system installed over the forest ($11.9 \text{ mol CO}_2 \text{ m}^{-2} \text{ over the same period}$ [Riveros-Iregui et al., 2008]). However, assessment selecting only sites with large drainage area (e.g., riparian meadows) indicated that the agreement between observed versus modeled efflux was considerably lower at these sites (i.e., observed efflux was almost twice as high as modeled efflux; Figure 8). As demonstrated in previous studies for this catchment [Jencso et al., 2009; Riveros-Iregui and McGlynn, 2009], riparian meadows account for 2% of total catchment area, thus model performance at these sites has low impact on overall catchment flux. The spatial patterns in catchment efflux at different times of the year (Figure 9) confirmed field observations of differential timing for peaks in CO$_2$ production and CO$_2$ diffusion, and are in agreement with the hypothesis of spatially variable optimality of efflux [Pacific et al., 2008, 2009, 2011]. Taken together, these results show that our modeling approach simulates lateral differences in CO$_2$ production and CO$_2$ diffusion across different times of the year, and it is a much more realistic approach than lumped models at the catchment scale that cannot simulate this fundamental, distributed behavior of heterogeneous landscapes.

Our study demonstrates that the synergistic nature of full model-data integration can provide bidirectional feedback, as process models benefit from field knowledge, and new empirical data, new field observations, and new field experiments can be further designed and expanded based upon modeling results. We as a community are at a stage in which field observations are becoming increasingly available; thus generating models that realistically simulate the coupling of hydrological and biogeochemical processes, and at the same time make use of spatiotemporal data, is a way to move watershed science forward. It is anticipated that the spatiotemporal interdependencies of variables will remain difficult to measure, synthesize into conceptual frameworks, represent mathematically, and parametrize. Even with adequate conceptualization and model structure, watershed process parametrization will be problematic. This study provides important insight into coupling hydrological and biogeochemical models at landscape scales, and highlights the role of landscape structure and heterogeneity when modeling spatial variability of biogeochemical processes.

6. Conclusions

We modified and applied an existing process soil CO$_2$ production and efflux model to a well-studied, topographically complex watershed of the northern Rocky Mountains. The model performed well in three areas. (1) It simulated the seasonality of soil [CO$_2$] at a riparian site,
especially after implementation of a diffusion-limited component; (2) it reproduced short-term (diel) dynamics of soil \([\text{CO}_2]\), particularly hysteresis patterns in the soil \([\text{CO}_2]\)--soil temperature relationship; and (3) it simulated seasonal estimates of soil \([\text{CO}_2]\) efflux at dry sites of the landscape. The model performed poorly when simulating seasonal (cumulative) soil \([\text{CO}_2]\) efflux at sites with large drainage area, likely as a result of poorly modeled soil water content at these sites and poorly parametrized microbial activity. We suggest that future watershed-scale biogeochemical models focus on improving spatial characterization of soil moisture and root and microbial respiration rates. Enhanced parametrization of the variability of these factors will improve our understanding of biogeochemical processes governing land-atmosphere exchange of \([\text{CO}_2]\).

This study clearly demonstrated that if only modeled estimates of seasonal estimates of soil \([\text{CO}_2]\) efflux at dry sites were taken into account, these estimates would compare well with independent estimates of measured soil \([\text{CO}_2]\) efflux and independent eddy-covariance estimates of nighttime ecosystem respiration. However, our results also unveiled potential deficiencies when existing biogeochemical models are applied across strong soil moisture gradients in the landscape, and highlight the role of model assessment, experimental design, and the need for new observations that couple hydrological and biogeochemical understanding at the watershed scale, particularly in areas of pronounced topography.

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