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Comparison of Models for Determining Soil-Surface Carbon Dioxide Effluxes in Different Agricultural Systems

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ABSTRACT

Models of instantaneous soil-surface CO_2 efflux (SCE_{ins}) are critical for understanding the potential drivers of soil C loss. Several simple SCE_{ins} models have been reported in the literature. Our objective was to compare and validate selected soil temperature (T_s)- and water content (θ_v)-based equations for modeling SCE_{ins} among a variety of cropping systems and land management practices. Soil-surface CO_2 effluxes were measured and modeled for grain-harvested corn (*Zea mays* L.)–soybean [*Glycine max* (L.) Merr.] rotations, grain- and stover-harvested continuous corn systems with and without a cover crop, and reconstructed prairies with and without N fertilization on soils with subsurface drainage. Soil-surface CO_2 effluxes, T_s, and θ_v were measured from 2008 to 2011. Models calibrated with weekly measured SCE_{ins}, T_s, and θ_v throughout the growing season produced lower root mean squared error (RMSE) than models calibrated with several weeks of hourly measured data. Model selection significantly affected SCE_{ins} estimations, with models that use only T_s parameters having lower RMSE than models that use both T_s and θ_v. However, the model that produced the lowest RMSE during validation estimated growing-season SCE that did not significantly differ from numerical integration of weekly measured SCE_{ins}. All models had similar residual errors with autocorrelated trends at monthly, weekly, and hourly scales. Autoregressive moving average functions were able to precisely describe the temporal errors. To accurately model SCE_{ins} and scale across time, improvement of temporal errors in T_s– and θ_v–based SCE_{ins} models is needed to obtain accurate and precise closure of C balances for managed and natural ecosystems.

Instantaneous soil-surface CO_2 efflux (SCE_{ins}) is a major pathway of C loss from soils (Lal, 2004). However, SCE_{ins} varies in time and space due to climatic, soil, and vegetative states (Daigh et al., 2014a; Blagodatsky and Smith, 2012; Vargas et al., 2011). To close managed- and natural-ecosystem C balances, as well as aid land-management decision support tools, precise and accurate estimations of SCE_{ins} and growing-season cumulative soil-surface CO_2 efflux (SCE_{cum}) across land management practices and ecosystems are needed (Vargas et al., 2011; Blagodatsky and Smith, 2012).

Soil-surface CO_2 efflux models can aid in filling measurement gaps and give insight into long-term and widespread land management impacts on soil health and C cycling. Among the most commonly used SCE_{ins} models are those by van't Hoff (1898) and Kirschbaum (1995), which are based on the sensitivity of soil respiration to soil temperature (T_s) through either stationary or dynamic exponential expressions. Some models have incorporated volumetric soil water content (θ_v) or water-filled pore space terms with the van't Hoff or Kirschbaum models (Pumpanen et al., 2003; Nielsen and Wendroth, 2003; Skopp et al., 1990; Doran et al., 1988). Pumpanen et al. (2003) used a multiplicative term that represents the limitations of O_2 diffusion to microbial sites as well as water-limited substrate motility (Skopp et al., 1990; Doran et al., 1988). Nielsen and Wendroth (2003) used an additive soil θ_v term in the exponential component of the van't Hoff model. To estimate SCE_{cum}, a simple numerical integration (SCE_{cum}–NI) was used in many studies when periodic SCE_{ins} measurements were obtained (Kaspar and Parkin, 2011; Guzman and Al-Kaisi, 2010; Parkin and Kaspar, 2004). The SCE_{cum}–NI method is appealing because a relatively low number of sampling dates are needed, but it is prone to errors as the sampling interval increases (Parkin and Kaspar, 2004). Additionally, the SCE_{cum}–NI method does not provide any further information for estimates of SCE_{ins} outside the observation period and does not provide any information for modeling present conditions or forward modeling in time.

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Abbreviations: ARIMA, autoregressive, differenced, moving average; CC, continuous corn without cover crop; CCW, continuous corn with winter rye cover crop; C-s, corn phase of the corn–soybean rotation; c-S, soybean phase of the corn–soybean rotation; Km, Kirschbaum model; M1m, van't Hoff model first modified approach; M2m, van't Hoff model second modified approach; NI, numerical integration; Pr, reconstructed mixed prairie without fertilization; PrF, reconstructed mixed prairie with fertilization; RMSE, root mean squared error; SCE_{cum}, growing-season cumulative soil-surface carbon dioxide efflux; SCE_{ins}, instantaneous soil-surface carbon dioxide efflux; VHm, van't Hoff model.

The heterogeneity of SCE_{ins}, in time and space, presents difficulties in precisely estimating soil C losses. Continuous or high-frequency temporal and spatial sampling protocols can be expensive and labor intensive, increasing the appeal of simple process-based estimation models. There are a variety of simple SCE_{ins} models reported in the scientific literature. Independent comparison and validation of such models has been reported in only a few studies (Richardson et al., 2006; Del Grosso et al., 2005; Falge et al., 2001). Falge et al. (2001) evaluated the exponential models of van't Hoff (1898), Arrhenius (1889), and Lloyd and Taylor (1994) but did not observe differences in residual errors. However, they only evaluated these models during nighttime periods, and they were validated with eddy covariance data, which measures the combined CO_2 fluxes of leafs, boles, and soil, providing no insight into individual component contributions. Del Grosso et al. (2005) evaluated six models, including linear, exponential, and a new arctangent model, for estimating SCE_{ins} among several natural and agroecosystems. In contrast to Falge et al. (2001), Del Grosso et al. (2005) used chamber-based measurements of SCE_{ins} and observed that some models provided a range of relative agreement during validation. However, the models evaluated had only 30 to 49% goodness-of-fit among the ecosystems examined (Del Grosso et al., 2005). Richardson et al. (2006) evaluated 18 simple models ranging from polynomials, exponentials, and Fourier regression to neural networks using 5.5 mo of data from a forest ecosystem in Maine. Tuomi et al. (2008) evaluated six models for their ability to accurately describe the sensitivity of soil respiration to T_s. Their evaluation suggested that the proposed arctangent model of Del Grosso et al. (2005) was overparameterized and that several exponential models had similar sums of squared residuals.

To our knowledge, no studies have evaluated the following: (i) the influence of model calibrations done with weekly vs. hourly measured SCE_{ins}, T_s, and θ_v, (ii) how well models compare to a simple numerical integration of weekly measured effluxes when estimating SCE_{cum}, (iii) the behavior of data collected in grain- and bioenergy-based cropping systems in mineral soils under drainage management, and (iv) the correlations in the model residual errors using time-series analyses. Therefore, our objective was to address each of these four items by comparing and validating selected soil T_s– and θ_v–based SCE_{ins} models among several corn and soybean systems and mixed reconstructed prairies and to evaluate model residual error covariate structures.

METHODS AND MATERIALS

Site Description and Experimental Design

Soil-surface CO_2 effluxes, T_s, and θ_v were measured from 2008 through 2011 at the Iowa State University's Comparison of Biofuel Cropping Systems research site near Ames. Experimental plots (n = 24) were 61 by 27 m on Webster (fine-loamy, mixed, superactive, mesic Typic Endoaquoll) and Nicollet (fine-loamy, mixed, superactive, mesic Aquic Hapludoll) soils. These plots were historically managed with subsurface drainage under corn and soybean rotations. The 30-yr (1981–2010) mean annual precipitation and air temperature are 935 mm and 8.9°C, respectively (NOAA, 2012).

Cropping systems used for evaluating SCE_{ins} models consisted of corn–soybean rotations with each crop grown each year, continuous corn with and without winter rye (*Secale cereale* L.) cover crop (CC and CCW, respectively), and reconstructed mixed prairie systems with and without fertilization (PrF and Pr, respectively). Corn and soybean phases of the corn–soybean rotations are referred to as C-s and c-S, respectively. Among the row crop systems, C-s and c-S were harvested only for grain, whereas CC and CCW were harvested for both grain and approximately 50% of the produced corn stover. Within the row crop systems, intra-crop management zones were identified as potential sources of spatial variability and were included in the SCE_{ins}, T_s, and θ_v sampling protocol (Daigh et al., 2014a). These zones included the plant row (Row; in C-s, s-C, CC, and CCW), interplant row with sidedress N injected (Fert; in C-s, CC, and CCW), interplant row with tractor tire traffic (Traf; in C-s, CC, and CCW), and interplant row without sidedress N injection or tire traffic (Btw; in C-s, s-C, CC, and CCW). All cropping systems were replicated four times in a randomized complete block design. Further details of soil and agronomic management of these plots were provided by Daigh et al. (2014a, 2014b).

Soil-Surface Carbon Dioxide Efflux, Temperature, and Water Content Sampling

Soil-surface CO_2 effluxes were measured between the annual planting of seed and harvest on 64 dates between June 2008 through September 2011 at weekly intervals using LI-COR 8100-103 and -104 infrared gas analyzer systems with a LI-8150 multiplexer (LI-COR Bioscience). To encourage vertical gas transport and to provide a base for the LI-COR 8100 systems, 20-cm-diameter by 12-cm-tall polyvinyl chloride (PVC) collars (n = 72) were installed near the beginning of the growing season and left in place until harvest except when large crop production equipment required temporary removal of the collars. Experimental plots contained either two or four sample locations depending on crop type. Vegetation was not allowed to grow inside the PVC collars throughout the growing season. Although no live aboveground plant tissues were included in the SCE_{ins} measurement, these agricultural crops have large fibrous root systems that could easily enter the soil below the measurement area due to the shallow installation depth (9 cm) of the collars. Details of SCE_{ins} measurement were also described by Daigh et al. (2014a). In addition to the weekly measurements, hourly SCE_{ins} measurements were periodically taken during 1 to 4 wk in selected plots during 2010 and 2011. Volumetric soil water content and T_s measurements were taken to a 6-cm depth at the time of weekly and hourly SCE_{ins} measurements. An additional set of year-round soil θ_v and T_s measurements were taken in all plots at a 5-cm depth at 30-min intervals for the planting-to-harvest period and at 120-min intervals for the harvest-to-planting period from June 2008 to November 2011 in the Fert intra-crop management zone for C-s, CC, and CCW and in the Btw intra-crop management zone for c-S using Decagon Devices 5TE ECH_2O sensors and EM50 dataloggers (Fig. 1). The year-round soil θ_v ranged from near saturation during spring and sometimes fall precipitation events to values <0.1 $cm^3\ cm^{-3}$ during much of the winter months (Fig. 1). However, soil water contents were determined indirectly by measuring the soil's dielectric permittivity. Soil water that transforms to ice during winter months has a lower dielectric permittivity than liquid water. Thus, soil water contents during winter months when soil ice is present results in an underestimation of total soil water content (i.e., liquid and solid water). Additionally, the frequency and intensity of precipitation events throughout 2010 and early 2011 were greater than that observed during 2008 and 2009 and often had approximately 150 to 300% greater precipitation than the 30-yr monthly means (Daigh et al., 2014a, 2014b). The year-round soil T_s ranged from 15 to 35°C during peak summer months annually and from −10 to 5°C during the winter months annually (Fig. 1).

Regression equations were developed between the weekly measured soil θ_v and T_s in all intra-crop management positions for all crops and the year-round soil θ_v and T_s measured in all corresponding cropping systems from 2009 through 2011 (Table 1). Curve fitting was done using least squares for soil θ_v and T_s in one experimental block from 2009 through 2011, and then soil T_s and θ_v were simulated for all other plots across all years. The simulated year-round T_s and θ_v were then validated using the measured soil θ_v and T_s from the remaining three experimental blocks (Table 1). For C-s and c-S, each crop year is considered as starting at planting of seed through the next annual planting of seed. Daigh et al. (2014a) observed that weekly measured soil θ_v, to a 6-cm depth, differed among intra-crop management zones but did not significantly differ among cropping systems at this site. Therefore, when soil θ_v data were not available for an intra-crop management zone, the regression equation from the next similar crop was used (Table 1). The year-round soil θ_v and T_s measurements made with the ECH$_2$O sensors in the Fert and Btw intra-crop management zones for C-s and c-S were not used as input for the SCE$_{ins}$ models. Instead, simulated soil θ_v and T_s for the Fert and Btw intra-crop management zones were done by regression equations, similar to how it was done for the Row and Traf intra-crop management zones. This was to prevent unknown errors associated with spatial variability between where the weekly soil θ_v and T_s measurements were obtained (i.e., <20-cm distance from the SCE$_{ins}$ measurements) and where the year-round soil θ_v and T_s measurements were obtained by the ECH$_2$O sensors (i.e., approximately 200 cm away from the SCE$_{ins}$ measurements).

Soil-Surface Carbon Dioxide Efflux Prediction

The SCE$_{ins}$ and SCE$_{cum}$ were modeled for each cropping system's intra-crop management zones. The SCE$_{ins}$ and SCE$_{cum}$ were then weighted based on each intra-crop management zone's proportional area. Daigh et al. (2014a) reported that SCE$_{ins}$ values periodically differ among intra-crop management zones of continuous corn with stover removal and that the use of a cover crop reduced how often these differences occurred. In contrast, they observed that SCE$_{ins}$ in the C-s and c-S rotations did not differ among intra-crop management zones. Therefore, a weighting of SCE$_{ins}$ across a crop's intra-crop management zones is necessary to account for these fine-spatial-scale differences. Soil-surface CO_2 efflux modeling approaches included numerical integration (SCE$_{cum}$–NI) and simple T_s– and θ_v–based models with parameter estimation first done using weekly measurements across all growing seasons and then using hourly measurements during 1 to 4 wk

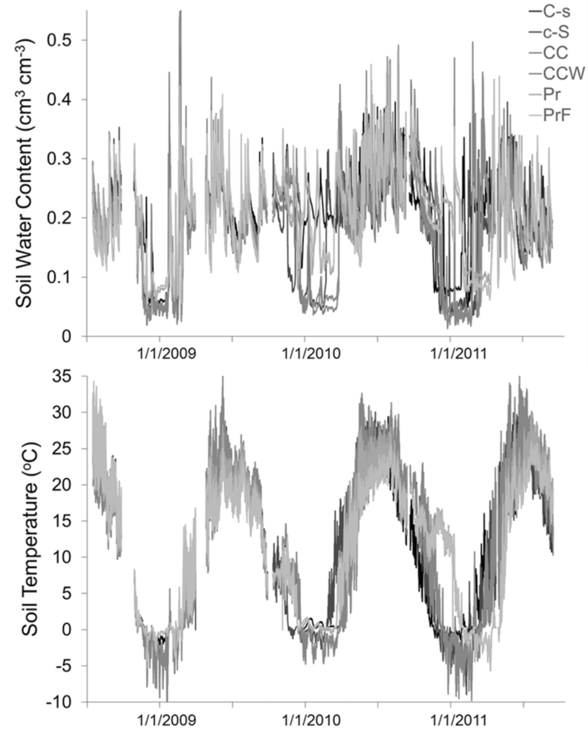

Fig. 1. Measured soil water content and soil temperature for the corn (C-s) and soybean (c-S) phases of a corn–soybean rotation, continuous corn with no cover crop (CC), continuous corn with a winter rye cover crop (CCW), unfertilized prairie (Pr) and fertilized prairie (PrF) cropping systems from June 2008 to November 2011. Values are the means of four experimental blocks. Note that soil water contents were determined by measuring the soil's dielectric permittivity. Soil water that transforms to ice during winter months has a lower dielectric permittivity than liquid water. Thus, soil water contents during winter months when soil ice is present results in an underestimation of total soil water content (i.e., liquid and solid water).

during the summers of 2010 and 2011 (Table 2). Similar to the simulated T_s and θ_v, parameter estimation was done for each cropping system intra-crop management zone using measurements from one experimental block and then validated with measurements from the remaining three experimental blocks.

The SCE$_{cum}$–NI was determined by

$$\mathrm{SCE_{cum}} = \sum_{i}^{n} \frac{X_i + X_{i+1}}{2}\left(t_{i+1} - t_i\right) \quad [1]$$

where X_i and X_{i+1} are the SCE$_{ins}$ measured at times t_i and t_{i+1}, respectively (Kaspar and Parkin, 2011; Guzman and Al-Kaisi, 2010; Parkin and Kaspar, 2004).

The simple T_s– and θ_v–based equations used in this study included those based on known empirical relationships among SCE$_{ins}$ and soil physical states including T_s and θ_v (Parkin and Kaspar, 2003; Fang and Moncrieff, 2001; Skopp et al., 1990). The simplest models consist of the widely used Q_{10} approach and the van't Hoff model (SCE$_{ins}$–VHm), relating soil CO_2 production to T_s as

$$\mathrm{SCE_{ins}} = \alpha \exp\left(\beta T_s\right) \quad [2]$$

where α and β are fitted parameters (van't Hoff, 1898), and the Kirschbaum model (SCE$_{ins}$–Km):

$$SCE_{ins} = \alpha \exp\left[a\left(\frac{T_s - b}{T_s + c}\right)\right] \quad [3]$$

where α is a fitted parameter and a, b, and c are constants with values of 3.36, 40, and 31.79, respectively, as given by Kirschbaum (1995, 2000) and Paul (2001). The SCE_{ins}–Km is the same as the Lloyd and Taylor (1994) function but has been modified for a wider range of soils (Paul, 2001; Kirschbaum 1995, 2000). The SCE_{ins}–VHm and SCE_{ins}–Km were then modified to produce two more approaches that include soil θv terms. The first modified approach (SCE_{ins}–M1m) uses a multiplicative water-filled pore space term that accounts for limitations of O_2 diffusion to microbial sites when soil θv is large and limitations for available water for substrate motility when soil θv is small (Skopp et al., 1990; Doran et al., 1988):

$$SCE_{ins} = \left[\alpha \exp\left(\beta T_s\right)\right]\left\{\min\left[d\theta_v^f, e\left(E_o - \theta_v\right)^g, 1\right]\right\} \quad [4]$$

where α and β are fitted parameters, E_o is soil total porosity, and empirical constants *d*, *e*, *f*, and *g* are 3.83, 4.43, 1.25, and 0.854, respectively, as given by Skopp et al. (1990). The second modified approach (SCE_{ins}–M2m) uses an additive θ_v term in the exponential component of the SCE_{ins}–VHm (Nielsen and Wendroth, 2003):

$$SCE_{ins} = \chi_o \exp\left(\alpha T_s + \beta\theta_v\right) \quad [5]$$

where χ_o, α, and β are fitted parameters.

Modeled SCE_{ins} as described in Eq. [2–5] are appealing due to known empirical relationships that SCE_{ins} has with T_s and θ_v. However, these models do not take into account specific mechanisms but averages across many soil processes. Due to this fact, there is the potential for site-specific temporal correlation structures when modeling SCE_{ins}. Therefore, autoregressive, differenced, moving average (ARIMA) models were

Table 1. Soil temperature and water content fitted equations and RMSE of simulated data.

Crop†	MZ‡	Fitted equation§	RMSE	Bias
			—— °C or m^3 m^{-3} ——	
		Temperature		
C-s	Btw	$x^{1.040}$	2.68	0.02
	Fert	$x^{1.034}$	2.40	–0.22
	Traf	$x^{1.036}$	2.14	0.23
	Row	$x^{1.042}$	2.43	0.21
c-S	Btw	1.147*x* + 0.15	9.43	–1.43
	Row	$7.362x^{0.364}$	4.28	–0.64
CC	Btw	$2.045x^{0.798}$	4.49	–0.96
	Fert	$x^{1.019}$	12.35	6.61
	Traf	$x^{1.017}$	4.74	–1.59
	Row	$8.564x^{0.318}$	4.27	–0.07
CCW	Btw	$3.716x^{0.584}$	3.66	–0.37
	Fert	$1.707x^{0.836}$	4.12	–0.50
	Traf	$2.044x^{0.792}$	4.03	0.44
	Row	$2.047x^{0.783}$	3.87	–0.40
Pr		1.167*x* + 0.155	7.24	2.27
PrF		$2.06x^{0.787}$	5.21	–0.94
Overall			4.43	–0.06
		Volumetric soil water content		
C-s	Btw	0.951*x* + 0.068	0.048	<0.001
	Fert	0.831*x* + 0.108	0.052	<0.001
	Traf	0.677*x* + 0.174	0.038	–0.001
	Row	0.822*x* + 0.093	0.053	–0.007
c-S	Btw	0.696*x* + 0.094	0.101	0.016
	Row	0.849*x* + 0.061	0.061	<0.001
CC	Btw	0.849*x* + 0.061	0.068	–0.017
	Fert	1.263*x* + 0.031	0.093	0.038
	Traf	1.636*x*	0.126	0.052
	Row	0.440*x* + 0.166	0.048	<0.001
CCW	Btw	1.067*x* + 0.014	0.064	<0.001
	Fert	1.200*x* + 0.030	0.068	–0.006
	Traf	1.053*x* + 0.086	0.068	–0.001
	Row	0.765*x* + 0.107	0.066	–0.005
Pr		0.662*x* + 0.083	0.073	<0.001
PrF		0.708*x* + 0.152	0.072	0.009
Overall			0.064	–0.001

† C-s, corn phase of corn–soybean rotation; c-S, soybean phase of corn–soybean rotation; CC, continuous corn; CCW, continuous corn with winter cover crop; Pr, prairie; PrF, fertilized prairie.

‡ MZ, intra-crop management zone; Btw, interrow; Fert, interrow with sidedress N application; Traf, interrow with wheel traffic; Row, in plant row.

§ Variable x is the measured soil temperature (°C) or measured volumetric soil water content (cm^3 cm^{-3}).

Table 2. Validation of modeled, intra-crop management zone weighted soil-surface CO2 effluxes for cropping systems calibrated with weekly measured data.

Model†	Crop‡	RMSE	Bias
		—— µmol CO_2 m^{-2} s^{-1} ——	
VHm	C-s	1.29	0.17
	c-S	1.28	–0.15
	CC	1.41	–0.38
	CCW	1.24	0.19
	Pr	1.71	0.18
	PrF	1.73	–1.26
	Mean	1.44	–0.21
Km	C-s	1.88	0.41
	c-S	1.50	0.06
	CC	1.38	–0.08
	CCW	1.24	0.27
	Pr	1.34	–0.54
	PrF	1.23	–0.47
	Mean	1.43	–0.35
M1m	C-s	1.93	–1.40
	c-S	1.79	–1.14
	CC	2.16	–1.58
	CCW	1.91	–1.36
	Pr	2.21	–1.52
	PrF	2.38	–2.01
	Mean	2.06	–1.52
M2m	C-s	1.37	0.10
	c-S	1.29	0.35
	CC	1.61	–0.45
	CCW	1.30	0.20
	Pr	2.54	–0.77
	PrF	1.56	–0.84
	Mean	1.61	–1.41

† VHm, van't Hoff model; Km, Kirschbaum model; M1m, first modified van't Hoff model; M2m, second modified van't Hoff model.

‡ C-s, corn phase of corn–soybean rotation; c-S, soybean phase of corn–soybean rotation; CC, continuous corn; CCW, continuous corn with winter cover crop; Pr, prairie; PrF, fertilized prairie.

determined using model residual errors of the hourly measured SCE_{ins} in 2011. The autocorrelation function (ACF) length of model residual errors were used for determining the autoregressive (AR) order, partial autocorrelation function (PACF) length for the moving average (MA) order, and a first-order differencing to obtain stationary means. The order (p) of the AR and MA components were selected using the Akaike information criterion (AIC). The ACF, PACF coefficients (ϕ), and AIC were determined by

$$\mathrm{ACF} = \frac{\mathrm{cov}\left[A_i(t),\, A_i(t+h)\right]}{\sqrt{\mathrm{var}\left[A_i(t)\right]}\sqrt{\mathrm{var}\left[A_i(t+h)\right]}} \quad [6]$$

$$\mathrm{PACF}\ \phi_{i+1,i+1} = \frac{r(i+1) - \sum_{j=1}^{i}\left[\left(\phi_{p,j}\right)\mathrm{ACF}(i+1-j)\right]}{1 - \sum_{j=1}^{i}\left[\left(\phi_{i,j}\right)\mathrm{ACF}(j)\right]} \quad [7]$$

$$\mathrm{AIC} = \ln\left(\mathrm{RSS_{avg}}\right) + \frac{2k}{N} \quad [8]$$

$$\mathrm{RSS_{avg}} = \frac{1}{N}\sum_{i=1}^{N}\left[A_i - A_i^{*}\right]^2 \quad [9]$$

where cov and var are the covariance and variance, respectively, A_i is the measured SCE_{ins} at a 1-h interval, t is the point in time of A_i, h is the time lag (in h) for determining the PACF, $\phi_{i+1,j}$ is $\phi_{i,j}$ minus the product of $\phi_{i+1,i+1}$ and $\phi_{i,i-j+1}$, where j is 1, 2, ..., i, and i is 1, 2, ..., p; when $i > p$, then PACF is zero; RSS_{avg} is the average residual sum of squares, k is the number of regression coefficients, N is the number of observations, and A_i^{*} is the modeled SCE_{ins}.

Once all models were calibrated using the weekly and then hourly measured SCE_{ins}, the models were validated using the weekly measured and spatially weighted SCE_{ins} for all cropping systems. To compare model performances, the root mean squared error (RMSE) and bias were used to determine which models performed best:

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(A_i - A_i^{*}\right)^2} \quad [10]$$

$$\mathrm{Bias} = \frac{1}{N}\sum_{i=1}^{N}\left(A_i - A_i^{*}\right) \quad [11]$$

For statistical comparisons among Eq. [2–5], the modeled SCE_{ins} were accumulated with time for each growing season using the same dates as used in the SCE_{cum}–NI method. A general linear model analysis of variance was performed to determine the effect of model, cropping system, year, and their interactions on SCE_{cum} weighted across intra-crop management zones. When appropriate, means were separated using Tukey's test at the 0.05 level. Statistical analyses were conducted using SAS (Version 9.2, SAS Institute).

RESULTS AND DISCUSSION

Soil Temperature and Water Content Assimilation and Model Calibrations

Simulated T_s and θ_v for intra-crop management zones across all years using the least squares fitted regression equations produced reasonable results during validation (Table 1). The RMSEs for T_s and θ_v were 4.4°C and 0.06 $cm^3\ cm^{-3}$, respectively, and are slightly larger or similar to errors reported in methodology studies for advanced modeling of T_s and θ_v (Pan et al., 2012; Tabari et al., 2011; Gribb et al., 2009; Grant et al., 1993; Table 1). Such studies reported that the use of pedotransfer functions in an ensemble Kalman filter, the use of soil profile θ_v and water potential gradients in modeling soil water redistribution, or the use of multivariate linear regressions incorporating atmospheric relative humidity and precipitation can reduce the RMSEs of simulated T_s and θ_v by 50%. However, we considered the simulated soil θ_v and T_s in this study to be reasonable because the simulated data (i) described well the dynamic trends with time, and (ii) provided a robust set of T_s and θ_v inputs to allow a fair comparison among SCE_{ins} models (Table 1; Fig. 2).

To determine an optimum calibration method for the SCE_{ins} models, each model was first calibrated using hourly measured SCE_{ins}, T_s, and θ_v during 1 to 4 wk in the summer of 2010 and 2011, and then a second calibration, independent of the first, was obtained using weekly measured SCE_{ins}, T_s, and θ_v during the growing seasons across all years. During model validation, the RMSE for SCE_{ins}–VHm and SCE_{ins}–Km did not substantially differ when calibrated with either weekly or hourly measured data when averaged across all cropping systems (i.e., <1% difference in RMSE). In contrast, the RMSE for SCE_{ins}–M1m and SCE_{ins}–M2m were 12 and 5% lower, respectively, when calibrated with weekly measured data compared with hourly measured data. The range of RMSE change

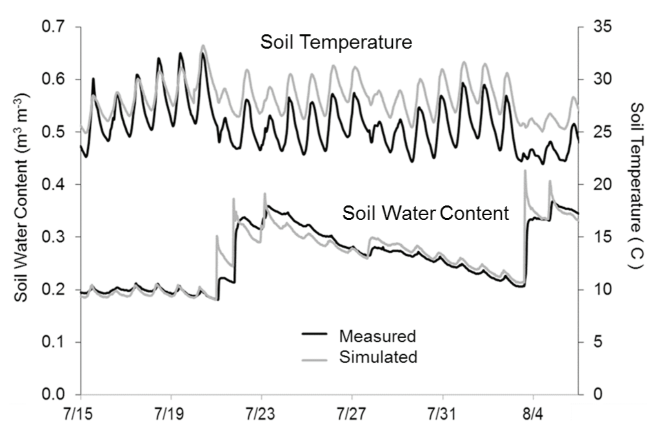

Fig. 2. Examples of measured and simulated soil water contents and soil temperatures. Data are from the N fertilizer intra-crop management zone in the corn phase of the corn–soybean cropping system in 2011. The hourly soil water content and soil temperature were measured within 20 cm of the soil-surface CO_2 efflux collars. Simulated soil water content and soil temperature were based on least squares fitted regression of hourly data from ECH_2O sensors (approximately 200 cm from the CO_2 efflux collars) to weekly measured data sampled within 20 cm of the CO_2 efflux collars and across 2009 to 2011. The hourly measured data shown, the weekly measured soil water contents, and the hourly measured data used in the fitted regression analysis were all obtained from different sensors.

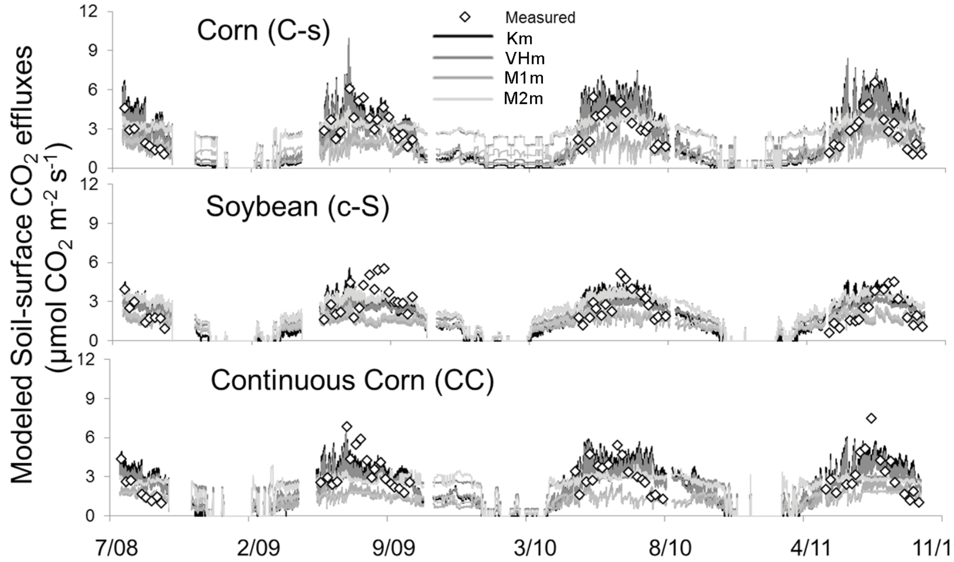

Fig. 3. Soil-surface CO_2 effluxes modeled using the Kirschbaum (Km), van't Hoff (VHm), first modified van't Hoff (M1m) and second modified van't Hoff (M2m) models and measured for corn, soybean, and continuous corn systems from June 2008 to November 2011.

for SCE_{ins}–M1m and SCE_{ins}–M2m were 6 to 20% and –5 to 21%, respectively, among cropping systems when calibrated with weekly measured data compared with hourly measured data. Across all models and cropping systems, RMSEs of SCE_{ins} models during validation were 1.86 and 1.64 µmol CO_2 m^{-2} s^{-1} when calibrated with hourly and weekly measured data, respectively.

The lower RMSEs of SCE_{ins} models calibrated with weekly measured data across all growing seasons suggest that these models are better at describing seasonal dynamics than diurnal cycles and weekly trends for our data set. Model calibrations with hourly data from the summer of 2010 and 2011 were expected to have a better fit with diurnal cycles and weekly trends associated with precipitation events because these measured data precisely describe daytime and nighttime SCE_{ins} as well as SCE_{ins} during and following precipitation events. In contrast, models calibrated with weekly measured data across all growing seasons are expected to more precisely describe seasonal dynamics because they represent a much longer period of SCE_{ins}. Based on these results, SCE_{ins} models calibrated with weekly measured SCE_{ins}, θ_v, and T_s were used for further model comparisons due to the overall lower RMSEs during validation (Table 2).

Comparison of Models

Models calibrated with weekly measured SCE_{ins}, θ_v, and T_s were used for comparisons. Soil-surface CO_2 effluxes varied substantially among models for all cropping systems and years (Fig. 3 and 4). Standard deviations among experimental blocks were typically lower than standard deviations among models. During the summer months of each year, SCE_{ins}–Km, SCE_{ins}–VHm, and SCE_{ins}–M2m produced greater SCE_{ins} and lower experimental-block standard deviations in all crops than SCE_{ins}–M1m. However, the models produced relatively similar effluxes during early spring after soil thaw and late fall before soil freezing.

Modeled SCE_{ins} typically ranged from 0 to 8 µmol CO_2 m^{-2} s^{-1} in all cropping systems with the exception of the SCE_{ins}–M2m estimates for Pr, which were as large as 12 µmol CO_2 m^{-2} s^{-1} during the summer months of 2011. Modeled SCE_{ins} for Pr and PrF tended to be larger than the row crops during the winter months. Although winter effluxes could not be validated in the current study, such effluxes are attributed to larger winter T_s in the prairies than in the row crops (Ewing and Horton, 2012). The ability to capture this trend was expected and demonstrates the potential of these models to estimate winter effluxes provided that winter T_s and θ_v data are available and that winter SCE_{ins} data are available for model calibration and validation.

When modeled SCE_{ins} were accumulated during the growing season, the effluxes differed significantly among models (Table 3). The differences among models accounted for 2.4 times as much variability as did differences among cropping systems (Table 3). Estimated SCE_{cum} were in the order of Km > NI > VHm > M2m > M1m when averaged across cropping systems and years (Table 3). However, SCE_{cum}–Km and SCE_{cum}–NI produced statistically similar SCE_{cum} values and had the largest effluxes of the models. In contrast, M1m produced the lowest average SCE_{cum} value and

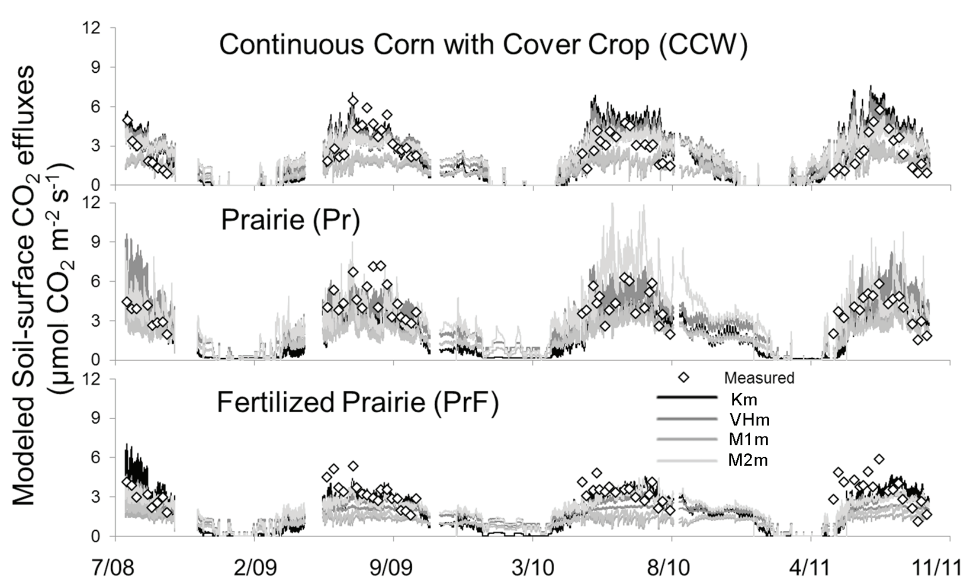

Fig. 4. Soil-surface CO_2 effluxes modeled using the Kirschbaum (Km), van't Hoff (VHm), first modified van't Hoff (M1m) and second modified van't Hoff (M2m) models and measured for continuous corn with cover crop, prairie, and fertilized prairie systems from June 2008 to November 2011.

was significantly different from all other models. These results emphasize the importance of model selection when attempting to model SCE_{cum} (Richardson et al., 2006).

The analysis of variance also revealed a significant year effect, which was expected due to weather variability and because data collection began midway through the 2008 growing season (Table 3). Modeled SCE_{cum} values were in the order of Pr > C-s > CCW > CC > c-S > PrF when averaged across models and years (Table 3). The low effluxes for PrF relative to all other cropping systems was due to greater crop canopy cover resulting in lower T_s during the growing season months (Daigh et al., 2014a; Jarchow and Liebman, 2013; Jarchow et al., 2012). However, the high effluxes for Pr relative to all other cropping systems are attributed to a root biomass 2.5 and 9.0 times greater than those of PrF and row crops, respectively (Dietzel et al., 2012). Although each main effect and their interactions were significant, the main effects (i.e., year, cropping system, and model) accounted for 89% of the total variability. Interaction effects were typically due to whether a model produced SCE_{cum} values for Pr that were either significantly different or similar to the other cropping systems. Each interaction effect accounted for only 1.7 to 4.1% of the total variability.

Table 3. Analysis of variance summary of cumulative intra-crop management zone weighted soil-surface CO_2 efflux per growing season among years, crops, models, and their interactions.

Variation source	*p* value	Contributed variance
		%
Year	<0.0001	45.5
Crop	<0.0001	12.6
Model	<0.0001	30.4
Crop ´ model	<0.0001	3.6
Year ´ model	<0.0001	4.1
Year ´ crop	<0.0001	2.0
Year ´ crop ´ model	<0.0001	1.7
	Growing season mean, Mg CO_2–C m^{-2}	
Year		
2011	4.16 a†	
2010	4.07 a	
2009	3.83 b	
2008	1.72 c	
Crop‡		
Pr	4.48 a	
C-s	3.58 b	
CCW	3.54 b	
CC	3.13 c	
c-S	3.11 c	
PrF	2.86 d	
Model§		
Km	4.10 a	
NI	4.09 a	
VHm	3.92 b	
M2m	3.88 b	
M1m	2.11 c	

† Means followed by different letters are significantly different at the 0.05 level.

‡ C-s, corn phase of corn–soybean rotation; c-S, soybean phase of corn–soybean rotation; CC, continuous corn; CCW, continuous corn with winter cover crop; Pr, prairie; PrF, fertilized prairie.

§ VHm, van't Hoff model; Km, Kirschbaum model; M1m, first modified van't Hoff model; M2m, second modified van't Hoff model.

Model Error Structures

Validation of modeled to measured SCE_{ins} revealed similar problematic issues among all models, crops, years, and experimental blocks (Fig. 3 and 4). In general, all models tended to overestimate SCE_{ins} early and late in the growing season while largely underestimating SCE_{ins} during the summer months (Fig. 3 and 4). The SCE_{ins}–M1m had the lowest absolute residual errors of all the models in the early and late stages of the growing season. However, the SCE_{ins}–M1m had the greatest absolute residual errors of all the models in the midsummer months. The SCE_{ins}–Km, SCE_{ins}–VHm, and SCE_{ins}–M2m tended to overestimate SCE_{ins} early in the growing season, followed by transitioning to underestimations during midsummer, followed by transitioning back to overestimations late in the growing season (Fig. 3 and 4). Among all models, the standardized residual errors typically ranged from 2 to –4 µmol CO_2 m^{-2} s^{-1}, with 48 and 72% of residuals ranging from 1 to –1 and 2 to –2 µmol CO_2 m^{-2} s^{-1}, respectively (Fig. 3 and 4). This range of residual errors is similar to those reported by Bauer et al. (2008) and Lloyd and Taylor (1994).

These trends of over- and underestimations of SCE_{ins} within each year may allow somewhat reliable estimations of SCE_{cum} or perhaps SCE_{cum} extended across an entire year. However, these models lack the temporal robustness needed for downscaling with time and may cause significant errors when estimating seasonal or daily soil C dynamics. The standardized residual errors are clearly autocorrelated with time and have large errors at the seasonal scale (Fig. 5). This was somewhat expected because Q_{10} values have been reported to shift seasonally (Yu et al., 2011). However,

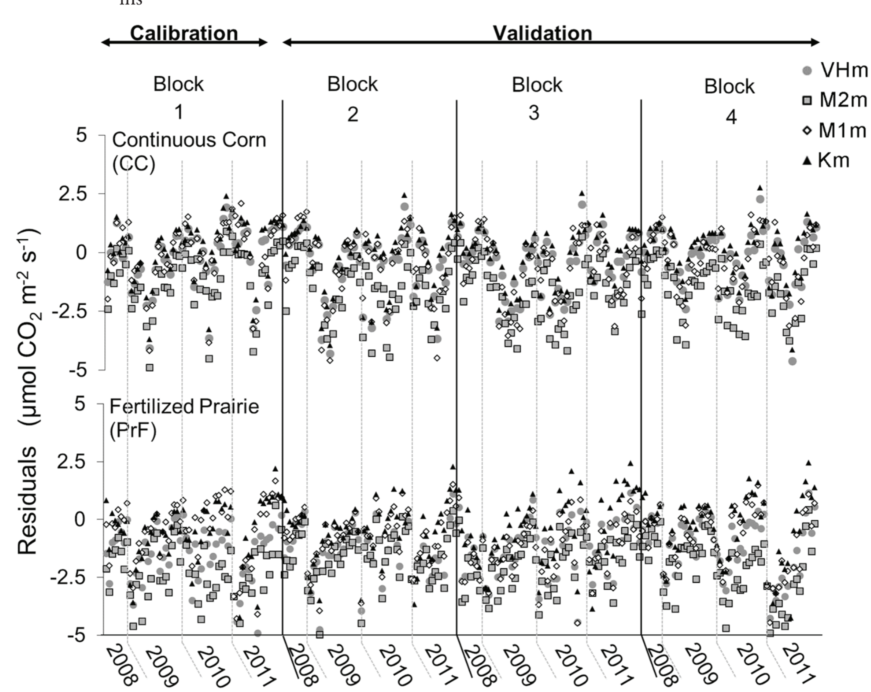

Fig. 5. Examples of residual errors by experimental block and year for the corn phase of the corn–soybean rotation (C-s), continuous corn with cover crop (CCW), and fertilized prairie (PrF) cropping systems using the Kirschbaum (Km), van't Hoff (VHm), first modified van't Hoff (M1m) and second modified van't Hoff (M2m) models. Data from Block 1 (noted as Calibration) were used for calibrating the models; data from Blocks 2, 3, and 4 were used for validation of the models.

this was not expected for SCE$_{ins}$–Km, which allows for the adjustment of the sensitivity of soil CO_2 production to changes in T_s (Paul, 2001; Kirschbaum, 2000, 1995). Overall, RMSEs of the modeled SCE$_{ins}$ across all years, blocks, and cropping systems were lowest for SCE$_{ins}$–Km and SCE$_{ins}$–VHm, with similar RMSEs of 1.43 and 1.44 μmol CO_2 m^{-2} s^{-1}, respectively, compared with SCE$_{ins}$–M1m and SCE$_{ins}$–M2m with RMSEs of 2.06 and 1.61 μmol CO_2 m^{-2} s^{-1}, respectively (Table 2).

Pumpanen et al. (2003) reported similar seasonal errors in modeled SCE$_{ins}$ for a forest ecosystem when using a model analogous to SCE$_{ins}$–M1m in the current study. However, their observed seasonal errors were inversely related to those observed in the current study, with underestimated SCE$_{ins}$ early and late in the year and either well-fitted or overestimated SCE$_{ins}$ in the summer months compared with chamber-based SCE$_{ins}$ measurements. These inversely related seasonal errors in modeled SCE$_{ins}$ among our observations and those reported by Pumpanen et al. (2003) may be due to differences in soil C substrate, root and soil microbial dynamics, and plant phenology of forest vs. grassland and agroecosystems (Vargas et al., 2010). However, these differences may just as likely be due to differences in the soil depth at which SCE$_{ins}$ is best correlated to T_s (Richardson et al., 2006).

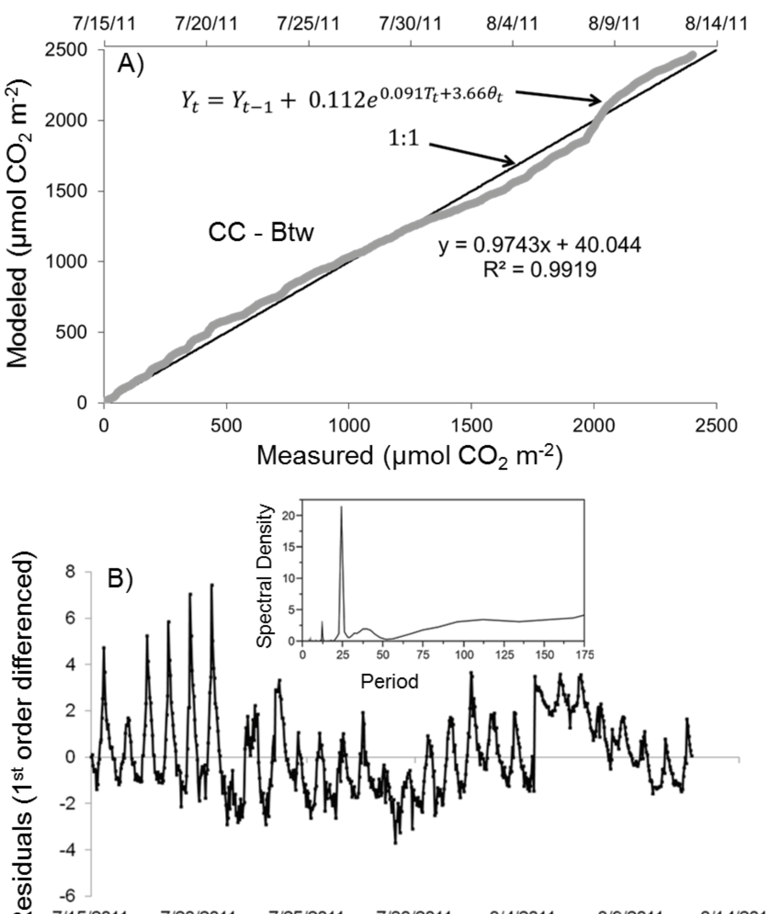

Fig. 6. Example of cumulative soil-surface CO_2 efflux (SCE$_{cum}$) across 29 d for a between-plant-row zone (Btw) in a continuous corn (CC) cropping system: (A) modeled effluxes using the second modified van't Hoff model (M2m) vs. measured cumulative effluxes, where regional errors are apparent when observing differences among the modeled data and the 1:1 line; (B) the SCE$_{cum}$–M2m residual errors transformed with a first-order differencing to enable stationary conditions for spectral analysis (upper section). The spectral analysis revealed a strong 24-h cyclic trend in the residual errors, indicating substantial temporal errors in the model at 24-h intervals that are independent of the regional (i.e., larger time scale) errors shown in (A).

Additionally, our evaluation indicated that models with only T_s parameters had lower RMSEs than models with T_s and θ_v parameters. This contrasts with the model evaluations by Del Grosso et al. (2005) and Pumpanen et al. (2003). Pumpanen et al. (2003) reported that incorporating the same θ_v parameters as used in M1m substantially reduced the overestimation of SCE$_{ins}$. The use of θ_v parameters in the current study also reduced the tendency of SCE$_{ins}$ overestimation both early and late in the growing season but tended to induce substantial underestimation of SCE$_{ins}$ during the summer months (Fig. 5). This could be due to differences in transpiration and drainage dynamics of the field sites used by Pumpanen et al. (2003) and the current study. In their study, parameter estimations and validations were done with measured SCE$_{ins}$ from a 40-yr-old coniferous forest with glacial till soils overlain by an O horizon, with moss providing abundant ground coverage, and were naturally drained. In contrast, the current study used measurements from corn and soybean systems and mixed reconstructed prairies on mineral glacial till soils with a history of soil tillage and subsurface drainage management. Thus, the tendency of θ_v parameters was to decrease modeled SCE$_{ins}$ in both studies but at the contrasting cost of reducing overestimation vs. inducing underestimation, which may be due to differences in soil water drainage dynamics or peak photosynthesis among the ecosystems as well as to natural vs. subsurface drainage landscapes (Daigh et al., 2014b; Niinistö et al., 2011). Daigh et al. (2014a) reported that soils undergoing apparent drainage or rapid internal soil water redistribution (i.e., non-stationary conditions with time) greatly limited the effect of soil temperature on SCE$_{ins}$. These observations as well as studies of soil water potential on greenhouse gas emissions suggest that soil water potentials may be more important for predicting SCE$_{ins}$ than soil water contents or water-filled pore space (Castellano et al., 2010, 2011). Additionally, the relationship between soil water status and SCE$_{ins}$ changes seasonally with the advancement of plant growth stages, plant responses to weather, and any subsequent changes in labile C sources, thus making accurate predictions difficult for monocropped agricultural systems and for diverse, mixed perennial systems (Daigh et al., 2014a; Kirschbaum, 2013; Niinistö et al., 2011). Niinistö et al. (2011) reported that the relationship between SCE$_{ins}$ and soil water was not apparent as the annual air temperature and plant growth stage advanced. Therefore, the effects of soil moisture on SCE$_{ins}$ continue to be complex and an important challenge for improving SCE$_{ins}$ models (Howard and Howard, 1979).

To determine potential errors at finer scales, hourly measured SCE$_{ins}$ values during the summer of 2011 were compared with modeled SCE$_{ins}$ values. Similar to the residual errors of weekly modeled effluxes across a year, the residual errors of hourly modeled effluxes across a month were not stationary and displayed errors at the scale of 4 to 7 d associated with precipitation events (Fig. 6A). This is evident in the regional errors as the inflection points (where model errors change from being more positive or more negative) occur also when precipitation events occur (Fig. 6A). When these residual errors were transformed by first-order differencing, the residual errors displayed a strong spectral density signature at a 24-h frequency (Fig. 6B). Therefore, modeled SCE_{ins} from these simple models had clear residual errors at the seasonal, weekly, and daily scales (Fig. 5 and 6). Although spectral densities and wavelet analyses can sometimes aid in identifying biophysical processes, we could not attribute spectral densities in this study to any specific mechanism. However, regional variability of the residual errors at the 4- to 7-d scale was probably due to the inability of these models to adequately characterize dynamic soil water effects (e.g., soil water redistribution and changes in soil gas diffusivities) on SCE_{ins} (Daigh et al., 2014a; Vargas et al., 2010). The response of plants to changes in soil water status (e.g., plant C reallocation) may also contribute to this observed variability. During the spectral density analysis, autocorrelation functions and partial autocorrelation functions were determined for the residual errors. From this, ARIMA models were able to precisely characterize the residual errors' temporal trends and thus eliminate any significant autocorrelations and spectral-density signatures when subtracted from the modeled SCE_{ins}. In doing so, this substantially improved the modeled SCE_{ins} (Fig. 7). However, these ARIMA models are site specific and provide no information on real physical processes. If site-specific information is available, the use of ARIMA models with simple T_s– and θ_v–based SCE_{ins} models can improve estimated effluxes across time scales. However, based on these data and other evaluations in the literature, improvement of these simple T_s– and θ_v–based models is needed for accurate SCE_{ins} estimations and for downscaling SCE_{ins} estimates with time.

CONCLUSIONS

Although model selection has been shown to significantly affect modeled SCE_{ins} across a range of cropping systems and land management practices, both SCE_{ins}–Km and SCE_{ins}–VHm have similar RMSEs and tended to produce lower RMSEs than those for SCE_{ins}–M2m and SCE_{ins}–M1m by 0.17 and 0.62 μmol CO_2 m^{-2} s^{-1}, respectively. Regardless of the model, similar temporal errors were observed at monthly, weekly, and daily time scales. Monthly errors were attributed to changes in the sensitivity of soil CO_2 production to T_s across a crop growing season (Yu et al., 2011). Weekly errors were at least attributed to the lack of incorporating parameters to account for the periodic effects of soil water redistribution on SCE_{ins} (Daigh et al., 2014a). In general, our results substantiate the poor performance of these simple models as reported by Richardson et al. (2006) and Tuomi et al. (2008), and these simple models have limited versatility when modeling SCE_{ins} across time scales during the growing season. However, time series analysis, such as ARIMA models, in conjunction with simple soil temperature and soil water content based SCE_{ins} models can substantially reduce residual errors. The ARIMA models may be useful in this context but are site specific, require detailed information with regard to temporal autocorrelations, and provide no insight into real physical processes. To accurately model SCE_{ins} and to scale it with time, improvements of these simple T_s– and θ_v–based SCE_{ins} models are needed if accurate and precise closure of C balances for managed and natural ecosystems are to be obtained.

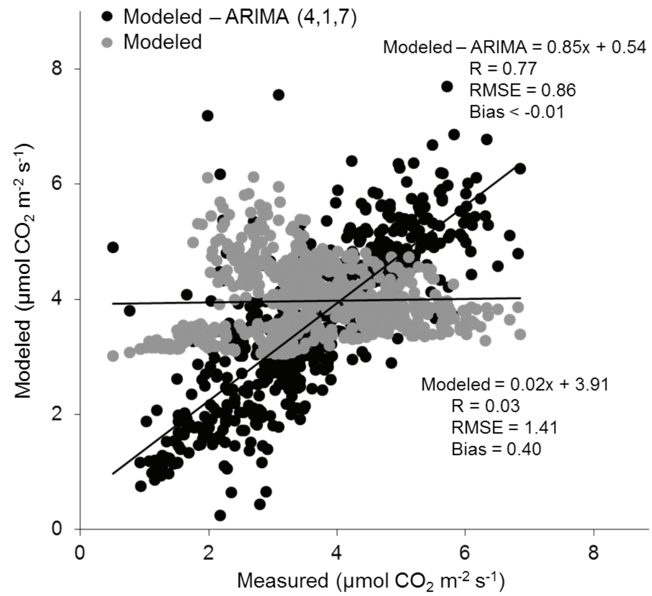

Fig. 7. Example of soil-surface CO_2 effluxes modeled using the second modified van't Hoff model (SCE_{cum}–M2m) and modeled using an autoregressive, differenced, moving average (ARIMA)-(4,1,7) vs. measured values for a between-plant-row zone (Btw) in a continuous corn cropping system (CC).

Abbreviations and Variables Used in This Study

ACF	autocorrelation function
AIC	Akaike information criterion
ARIMA	autoregressive, differenced, moving average model
Btw	interrow without sidedress N injection or tire traffic
CC	continuous corn with stover harvest without winter rye cover crop
CCW	continuous corn with stover harvest and winter rye cover crop
C-s	corn phase of the corn–soybean rotation
c-S	soybean phase of the corn–soybean rotation
Fert	interrow with sidedress N injected
PACF	partial autocorrelation function
Pr	reconstructed mixed prairie without N fertilization
PrF	reconstructed mixed prairie with N fertilization
RMSE	root mean squared error
Row	plant row
RSS_{avg}	average residual sum of squares
SCE_{ins}	instantaneous soil-surface CO_2 efflux
SCE_{ins}–Km	Kirschbaum model for instantaneous soil-surface CO_2 efflux
SCE_{ins}–M1m	van't Hoff first modified model for instantaneous soil-surface CO_2 efflux
SCE_{ins}–M2m	van't Hoff second modified model for instantaneous soil-surface CO_2 efflux
SCE_{ins}–VHm	van't Hoff model for instantaneous soil-surface CO_2 efflux
SCE_{cum}	growing-season cumulative soil-surface CO_2 efflux
SCE_{cum}–Km	Kirschbaum equation with values integrated across the growing season

SCE_{cum}–M1m	van't Hoff first modified equation integrated across the growing season
SCE_{cum}–M2m	van't Hoff second modified equation integrated across the growing season
SCE_{cum}–NI	numerical integration
SCE_{cum}–VHm	van't Hoff equation with values integrated across the growing season
Traf	interrow with tractor tire traffic
T_s	soil temperature
θ_v	volumetric water content

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