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Modeling of CO_2 Emission from Soil in Greenhouse

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Abstract. Greenhouse industry has been growing in many countries due to both the advantage of stable year-round crop production and increased demand for fresh vegetables. In greenhouse cultivation, CO_2 concentration plays an essential role in the photosynthesis process of crops. Continuous and accurate monitoring of CO_2 level in the greenhouse would improve profitability and reduce environmental impact, through optimum control of greenhouse CO_2 enrichment and efficient crop production, as compared with the conventional management practices without monitoring and control of CO_2 level. In this study, a mathematical model was developed to estimate the CO_2 emission from soil as affected by environmental factors in greenhouses. Among various model types evaluated, a linear regression model provided the best coefficient of determination. Selected predictor variables were solar radiation and relative humidity and exponential transformation of both. As a response variable in the model, the difference between CO_2 concentrations at the soil surface and 5-cm depth showed are latively strong relationship with the predictor variables. Segmented regression analysis showed that better models were obtained when the entire daily dataset was divided into segments of shorter time ranges, and best models were obtained for segmented data where more variability in solar radiation and humidity were present (i.e., after sun-rise, before sun-set) than other segments. To consider time delay in the response of CO_2 concentration, concept of time lag was implemented in the regression analysis. As a result, there was an improvement in the performance of the models as the coefficients of determination were 0.93 and 0.87 with segmented time frames for sun-rise and sun-set periods, respectively. Validation tests of the models to predict CO_2 emission from soil showed that the developed empirical model would be applicable to real-time monitoring and diagnosis of significant factors for CO_2 enrichment in a soil-based greenhouse.

Additional key words: empirical model, real-time monitoring, regression analysis

Introduction

There has been a tremendous growth of greenhouse industry in many countries due to both an increased demand for fresh vegetables and the need for stable year-round crop production. Since CO_2 concentration plays an essential role in the photosynthesis process of crops, optimum control of CO_2 enrichment based on accurate monitoring of added CO_2 in a greenhouse is necessary to improve the efficiency and profitability of crop production and to reduce environmental impacts that may influence global warming.

The environment of a greenhouse can be modeled as a nonlinear system with multiple coupled variables. Accurate monitoring of CO_2 concentration is the key to optimal control of air fertilization by CO_2 enrichment in a greenhouse, but is complicated by a variety of factors such as temperature, humidity, and light intensity (Chen and Tang, 2010; Pohlheim and Heiβnet, 1991). Design and implementation of an effective control system for greenhouses requires continuous measurement of CO_2 concentration (Körnet et al., 2007). Although many researchers investigated CO_2 control in a greenhouse, most of them focused on long term ecological research (Caetano et al., 2008) or the mathematical model of a non-soil based agricultural facility (Körnet et al., 2007; Zhang et al., 2007). While many researchers have investigated interactive relationships between the concentration of CO_2 in the ambient air and crop growth, for example CO_2 exchange of foliage plants (Park et al., 2010) and respiration affected

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by CO_2 treatment (Jeong et al., 2006), more investigation of CO_2 interaction with soil would be useful.

In a soil-based greenhouse, there are generally three ways that CO_2 is supplied to the system. The traditional way is to supply CO_2 from the external ambient air by ventilation. The second path is to enrich CO_2 using an air fertilization device, and the third path is to supply from the soil. Presence of these different pathways creates additional difficulty in accurate monitoring of ambient CO_2 concentration. Because CO_2 concentration in the ambient air inside the greenhouse would be considerably and quickly affected by any external supplement even in a short time, our assumption was that the level or change of CO_2 concentration in soil might give us information useful for real-time monitoring.

Because a standard method for real-time measurement of CO_2 emission from soil is not available, many researchers have reported time-dependent mathematical models for predicting CO_2 emission from soil (Jassal et al., 2004; Kabweet al., 2002; Lou et al., 2004; Ouyang and Zheng, 2000; Smart and Josep, 2005; Takahashi et al., 2004; Zhang et al., 2007). For evaluation of their prediction models, reference values were determined using the closed chamber method (Camarda et al., 2009; DeSutter et al., 2006) or electrical sensors such as a solid fixation sensor (Tang et al., 2003) or an infrared gas sensor (Subke et al., 2003). In these studies, CO_2 emission was related to various environmental properties such as soil temperature (Fang and Moncrieff, 1999; Jassal et al., 2004), relative humidity (Granieri et al., 2003; Li et al., 2008; Ouyang and Zheng, 2000), soil water content (Jassal et al., 2004; Maestre and Cortina, 2003), solar radiation (Ouyang and Zheng, 2000), and soil physical properties (Filipovic et al., 2006; Franzlubbers et al., 1995).

Review of previous research showed that three major environmental properties; soil temperature (Jassal et al., 2004), relative humidity (Li et al., 2008) and solar radiation (Ouyang and Zheng, 2000); have been considered to have significant relationships with CO_2 movement from soil. Some researchers (Lou et al., 2004; Tang et al., 2003) tried variable transformation for predictor variables using exponential, logarithmic and inverse functions. Thus, to predict CO_2 emission from soil in a greenhouse, not only original data but also various transformed data should be considered. Additionally, the importance of investigating CO_2 concentrations at shallow soil depths (5 cm, Jassal et al., 2004; 8 cm, Tang et al., 2003) was reported.

The objective of this research was to develop empirical models for predicting CO_2 emissions from greenhouse soil, considering the effects of environmental factors such as solar radiation, temperature, and relative humidity.

Materials and Methods

Experimental Data Collection

CO_2 concentrations of ambient air and at different soil depths, and other environmental variables, including soil surface temperature, solar radiation, and relative humidity, were collected in cucumber-growing greenhouses located in Yongin-city, Korea. The greenhouses were covered with double plastic layers. Three greenhouses were selected based on different CO_2 supply practices: enrichment with ventilation only (CO_2 level: 250-360 $\mu mol \cdot mol^{-1}$), and enrichment with a commercial CO_2 fertilizer (SH-VT, Soha tech, Seoul, Korea) at 500 and 800 $\mu mol \cdot mol^{-1}$ levels. It was assumed that different enrichment practices would affect the relationships between CO_2 level and environmental factors.

Ambient temperature, solar radiation, and relative humidity were measured at the top of the cucumber tree canopy (Fig. 1A). Temperature and CO_2 concentration at the ground surface, and CO_2 levels at three soil depths of 5, 10, and 20 cm were also obtained. Data were collected at every 2 min, resulting in 720 measurements per day.

Commercial sensors were used for the data collection. An RTD (Resistance Temperature Detector) sensor (PT-100, Lake Shore Cryptronics Inc., USA) was used to measure the temperature. A pyranometer (TSL250R-LF, Taos Inc., USA) with a sensing range of 0-100 $\mu W \cdot cm^{-2}$ was used to measure solar radiation. A capacitive polymer sensor (FOST02A, BB

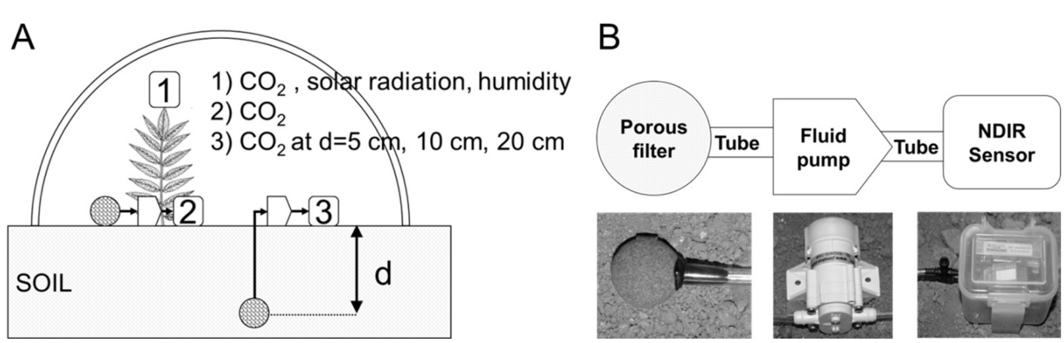

Fig. 1. Overall data collection scheme (A). Diagram explaining measurement of CO_2 concentration at different soil depths in the soil (B).

Automacao Inc., USA) was used to measure relative humidity, and a NDIR (Non Dispersive Infra Red) sensor (KCD-1, Korea Digital Inc., Korea) was used for continuous monitoring of CO_2 concentration. The NDIR sensor was a simple spectroscopic device often used to detect CO_2 molecules absorbing light at 4.26 μm. Range and resolution of the sensor were 0-2,000 $\mu mol \cdot mol^{-1}$ and 2 $\mu mol \cdot mol^{-1}$, respectively. A micro-fluid pump was positioned between the NDIR sensor and a porous filter to transfer CO_2 gas from different soil depths (Fig. 1B). Through preliminary testing in a closed chamber, flow rate of the micro-fluid pump was set to 0.9 $L \cdot min^{-1}$ to maintain sufficient gas flow from the soil. Multiple filter-pump-sensor systems were employed to measure the CO_2 concentration at the different soil depths. The benefit of this method was the ability to measure the CO_2 concentration nondestructively and continuously after the apparatus was installed at a particular soil depth.

Data were collected for 14 days for the development of empirical models estimating CO_2 levels using the environmental factors, and also for another 10 days for validation of the models. There was relatively less variance in temperature at the soil surface and CO_2 concentrations at certain soil depths (10 and 20 cm) during the calibration period (Fig. 2). CO_2 concentration was greater and the variances were lower as the measurement depth was increased. Considering the variance in CO_2 concentration, it could be recognized that there might be some relationship between the change of CO_2 in the soil and solar radiation in certain time periods (i.e., from 6:00 to 8:00 and from 16:00 to 18:00). This examination led us to conduct a closer investigation of segmentation of predictor and response variables in shorter time periods in regression analysis. Mean and standard deviation

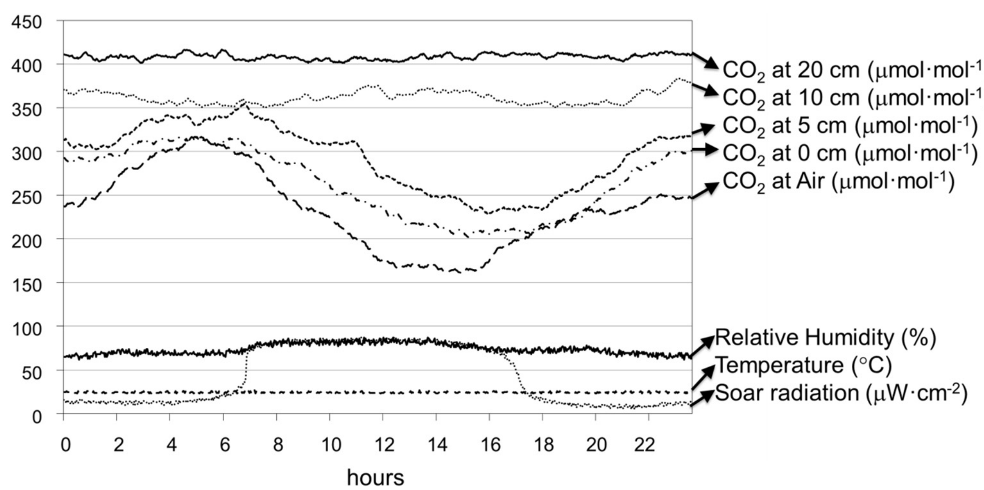

Fig. 2. Plots of averaged environmental properties obtained from the three experimental greenhouses during 14 days of calibration period.

Table 1. Descriptive statistics of measured properties for the calibration period.

Properties	Sensor location	Greenhouse 1 (CO_2: 250-360 $mol \cdot mol^{-1}$)		Greenhouse 2 (CO_2: 500 $mol \cdot mol^{-1}$)		Greenhouse 3 (CO_2: 800 $mol \cdot mol^{-1}$)		Mean of all data	
		Mean	SD[z]	Mean	SD	Mean	SD	Mean	SD
Ambient temperature (°C)	1[y]	23.61	0.59	23.63	0.61	0.62	0.64	23.62	0.61
Soil surface temperature (°C)	2	20.11	0.62	19.11	0.63	18.61	0.67	19.23	0.63
Solar radiation ($\mu W \cdot cm^{-2}$)	1	39.32	31.75	35.85	31.75	35.82	31.76	35.75	30.99
Relative humidity (%)	1	71.41	6.05	68.90	6.04	68.91	6.04	68.04	5.89
$CO_{2(air)}$ ($mol \cdot mol^{-1}$)	1	207.09	45.10	231.85	45.17	241.98	45.68	222.02	44.19
$CO_{2(surface)}$ ($mol \cdot mol^{-1}$)	2	237.16	38.98	262.44	39.83	272.48	39.83	251.66	38.32
$CO_{2(5cm)}$ ($mol \cdot mol^{-1}$)	3 (d = 5)	267.22	25.12	264.72	25.12	264.73	25.13	259.2	24.52
$CO_{2(10cm)}$ ($mol \cdot mol^{-1}$)	3 (d = 10)	334.25	6.37	331.76	6.38	337.74	6.39	324.63	6.23
$CO_{2(20cm)}$ ($mol \cdot mol^{-1}$)	3 (d = 15)	339.24	2.44	336.74	2.42	336.75	2.45	329.50	2.28

[z]SD: Standard deviation (n = 720).
[y]Index of sensor location in Fig. 1.

of the measured environmental properties for each experimental greenhouse was shown in Table 1.

Analytical Procedures

To determine the relationships between CO_2 concentration vs. environmental properties, various regression models were tried: linear regression (LR), robust linear regression (RR), second order (quadratic) polynomial regression (P2), third order (cubic) polynomial regression (P3), and a generalized linear model using the inverse of the normal cumulative distribution function as the link function (GN). Preliminary analysis (Lee et al., 2011) showed that no significant regression models were found between the CO_2 concentration and environmental variables such as soil temperature, solar radiation, and relative humidity. When using the difference between CO_2 concentrations at different soil depths as a response variable, however, relatively strong and significant relationships were obtained with solar radiation and relative humidity as predictor variables in some cases. Based on the preliminary analysis, a line arregression model as in equation 1 was introduced and multiple linear regression analysis was performed to determine the regression coefficients. Models were evaluated with original and transformed forms of solar radiation (W) and relative humidity (H) data (Table 2).

$$C_{surface} - C_{5\ \mathrm{cm}} = \beta_0 + \beta_1 W + \beta_2 H + e \qquad (1)$$

Table 2. Models, variables, and variable transformations used in the regression analysis.

Type	Model function	Predictorvariable (x)		Response variable (y)
LR	$y = \beta^z x + \varepsilon^y$	Environmental variables	Transformation	CO_2 concentration at
RR	$y = \beta x + \varepsilon$		x	Ambient air,
P2	$y = \beta_1 x + \beta_2 x^2 + \varepsilon$	Soil temperature	$\frac{1}{x}$	Surface of soil 5 cm depth of soil
P3	$y = \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \varepsilon$	Solar radiation Relative humidity	$\log(x)$	10 cm depth of soil 20 cm depth of soil
GN	$y = \beta(x)^x + \varepsilon$		$e^{\frac{x}{100}}$	And their difference

[z]Coefficient.
[y]Error term.
[x]Inverse of the normal cumulative distribution function.

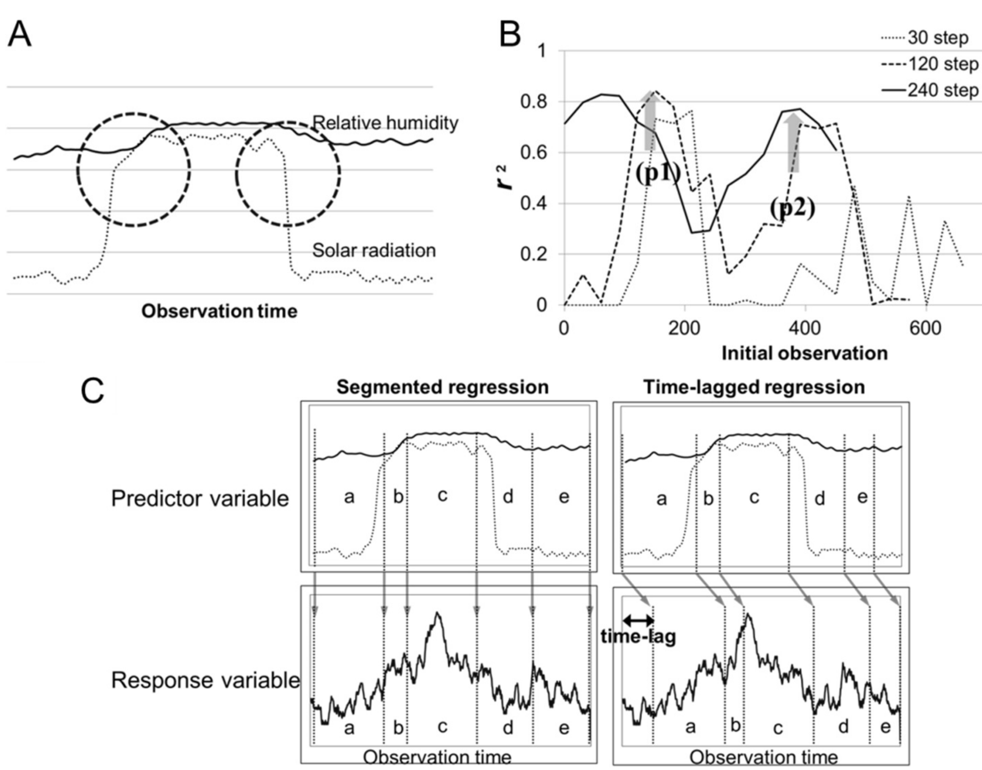

Fig. 3. Considerable variability found within the region of dotted circle in plots of solar radiation and relative humidity (A). Plots of coefficient of determination from regression analysis as a function of observation width and initial observation (B). An illustration of the time-lag between predictor and response variables in time-lagged regression (C).

where,

Csurface	: CO_2 concentration at soil surface,
C_{5cm}	: CO_2 concentration at a 5-cm soil depth,
W	: original or transformed solar radiation,
H	: original or transformed relative humidity,
β_0, β_1, β_2	: constant and regression coefficients, and
e	: error term.

During multiple linear regression analysis, calibration of the model was carried out in several ways. Through observation of the data (Fig. 3A), regression was applied for segmented sub-data sets of short time periods to obtain different regression coefficients for different portions of the whole data. Segmented regression (Berman et al., 1996; Cox, 1996; Shuai et al., 2003) is useful when the relationship between dependent and independent variables is different in these segments. The boundaries between the segments are called 'breakpoints'. To determine the breakpoints, regression analysis was performed iteratively by varying the initial observation and observation width (Fig. 3B). By taking the maximum coefficient of determination indicated by p1 (Fig. 3B), the first segmented partition (from initial observation point to initial point plus observation width) was determined. For the second segmented partition, the next representative peak value (p2 in Fig. 3B) was selected. Another iterative time-lagged regression analysis (Körnet et al., 2007) was also used to develop a more practical model considering the time dependent nature of change in CO_2 emission from the soil affected by solar radiation and relative humidity. With this method, each observation in the response variable (CO_2) is shifted by a time-lag per iteration step, after the determination of breakpoints (Fig. 3C).

Results and Discussion

First, the type of regression model and optimum transformation of the independent (predictor) variables were determined. Different regression methods and transformations as listed in Table 2 were applied to the calibration dataset. Comparison of the results showed that the best coefficients of determination were obtained with linear regressions using original and exponential forms of predictor variables, as shown in bold in Table 3. Based on these results, linear regression was used for the remainder of the analysis.

The next step was to optimize the exponential transformation of the input predictors. Initial screening used a transformation of the form exp (x/100), but for final model development the optimum value of the constant was determined. Multiple linear regression (MLR) analysis runs were completed iteratively varying the constant, k, in exp (x/k) from 1 to 100. Examination of the coefficient of determination across the range of k in the exponential formula for solar radiation showed that the transformation exp (x/12) was the best. Thus, the transformation exp (x/12) was used for solar radiation for the remainder of the analysis. Two candidate multiple linear regression models developed were summarized in Table 4.

Through iterative regression analysis, optimum segmented partitions of the measurements were determined for each greenhouse (Table 5). The whole data were partitioned into five segments, and the breakpoints determined were different for the different greenhouses. The two most important partitions were segments b and d, sub-data sets for after sun-rise and before sun-set, since these two breakpoint ranges gave the best coefficients of determination. For the calibration of the candidate models 1 and 2 using data from all of the greenhouses, the breakpoints for the mean data from all greenhouses were selected.

The two candidate models were evaluated by the segmented and time-lagged regression analyses. While r^2 values were relatively low when MLR analysis was applied to the other segments, good fits were obtained for segments b and d. Model 1 gave the best coefficient of determination for the

Table 3. Coefficient of determination (r^2) obtained with different transformations of predictor variables for the calibration dataset. Predictor variable x_1 is solar radiation, predictor variable x_2 is relative humidity, and response variable y is $CO_{2(surface\text{-}5\ cm)}$.

Transformation of thepredictors					
x_1, x_2	$\frac{1}{x_1}, \frac{1}{x_2}$	log (x_1), log (x_2)	$e^{\frac{x_1}{100}}$, x_2	x_1, $e^{\frac{x_2}{100}}$	$e^{\frac{x_1}{100}}, e^{\frac{x_2}{100}}$
0.7963	0.7378	0.7693	0.8031	0.7981	0.8044

Table 4. Results of multiple linear regression using optimized regression type and variable transformation for the calibration dataset.

Model ID	Predictor variable x_1 = solar radiation Predictor variable x_2 = relative humidity	Response variable y = $CO_{2(surface\text{-}5\ cm)}$				
		r^2	RMSEC	β_1	β_2	β_0
1	x_1, x_2	0.7963	5.08	0.1749	0.7410	-31.233
2	$e^{\frac{x_1}{12}}$, x_2	0.8293	4.65	0.0217	0.3369	-2.0473

Table 5. Breakpoints from the segmented regression for datasets from each greenhouse and mean values of all greenhouses.

Segment ID	Greenhouse 1 (CO_2: 250-360 mol·mol^{-1})		Greenhouse 2 (CO_2: 500 mol·mol^{-1})		Greenhouse 3 (CO_2: 800 mol·mol^{-1})		Mean of all data	
	Initial	Width	Initial	Width	Initial	Width	Initial	Width
a	1^z	169	1	169	1	139	1	180
b	170	35	150	50	140	60	181	24
c	206	173	201	149	201	149	205	163
d	380	130	380	190	350	150	368	199
e	511	209	511	179	501	219	567	153

^{z}1 unit = 2 min.

Table 6. Results of validation of each candidate regression model on the three experimental greenhouses.

Greenhouse ID		Greenhouse 1 (CO_2: 250-360 mol·mol^{-1})		Greenhouse 2 (CO_2: 500 mol·mol^{-1})		Greenhouse 3 (CO_2: 800 mol·mol^{-1})	
Candidate model	Regression method (segment id)	r^2	RMSEV^z	r^2	RMSEV	r^2	RMSEV
Model 1b	Segmented (b)	0.88	2.34	0.84	8.82	0.61	5.86
	Segmented and time-lag (b)	0.84	4.46	0.84	6.41	0.70	7.73
Model 2d	Segmented (d)	0.79	4.18	0.72	4.60	0.64	8.38
	Segmented and time-lag (d)	0.85	4.64	0.74	4.80	0.75	9.04

^{z}RMSEV: Root mean square error of validation.

b segment, measurements from 6:02 to 6:50 AM (from 181 to 181 + 24 in Table 5), model 2 performed well in the d segments, measurements of 12:16 to 6:54 PM (from 368 to 368 + 199 in Table 5). Model 1 with the b segment (indicated by Model 1b) and the d segment (indicated by Model 1d) gave coefficient of determination of r^2 = 0.93 and r^2 = 0.85, respectively. Model 2 with the b segment (indicated by Model 2b) and the d segment (indicated by Model 2d) both gave coefficients of determination of r^2 = 0.87. The two models showed the same optimum time lag (8 min or 4 measurements) in the b segment but different lags in the d segment (0 and 10 min). These results suggested that the model could estimate the response values better with the determined time-lag.

The four models were evaluated with the validation datasets from three experimental greenhouses with using the defined segments and time-lags. Two models showed relatively high coefficients of determination throughout all greenhouses (Table 6). Model 1b gave greater coefficients of determination in the b segment (Table 5) of all the greenhouses, while model 2d gave greater coefficients of determination in the d segment (Table 5) of all the greenhouses. The models showed relatively high correlation in the different segments regardless of the type of CO_2 enrichment, the correlation between the concentration of $CO_{2(surface\text{-}5cm)}$ and the solar radiation, but greenhouses with greaterCO_2 enrichment setting resulted in a greater root mean square error of validation (RMSEV) for most of the models.

Based on these results, we suggested two empirical models to estimate the difference of CO_2 concentrations at different depths. Equation 2 is one part of the suggested empirical model to estimate the concentration of $CO_{2(surface\text{-}5cm)}$ between observations 182 and 205 (between 6:02 and 6:50 AM) with an 8-min time-lag Equation 3 represents the other partition between observations 368 and 567 (between the time range of 12:16 and 6:54 PM) with a 10-minute time-lag.

$$(C_{surface} - C_{5\ cm})_{(t+8)} = 0.9618W_t + 0.4502H_t - 28.464 \quad (2)$$

$$(C_{surface} - C_{5\ cm})_{(t+10)} = 0.0217e^{\frac{W_t}{12}} - 0.1238H_t + 30.373 \quad (3)$$

where,

C : CO_2 concentration at a soil depth,
t : observation time in minutes,
W_t : solar radiation at time t,
H_t : relative humidity at time t.

Using the validation dataset, the concentration of $CO_{2(surface\text{-}5cm)}$ was predicted by the empirical models as described by Equation

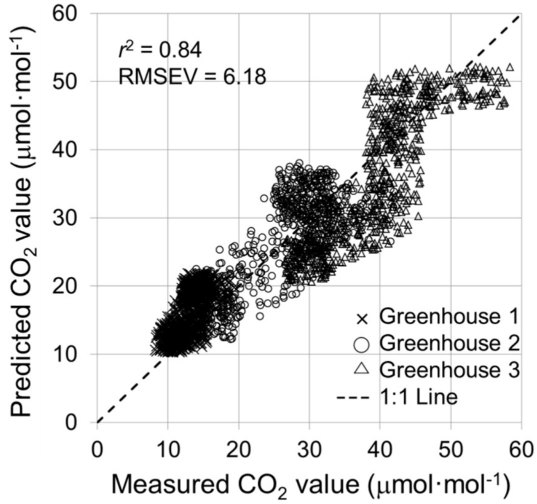

Fig. 4. Scatter plot of measured and predicted $CO_{2(surface-5cm)}$ values for the validation dataset.

2 and 3. The coefficients of determination for each greenhouse were not strongly high, but the empirical model was somewhat more robust against the different CO_2 enrichment methods considering the overall coefficient of determination was 0.84 (Fig. 4).

In this study, a mathematical model was developed to relate key environmental factors to CO_2 concentrations measured at different depths. Predictor variables selected were original and exponential transformation of solar radiation and relative humidity. The difference of CO_2 concentrations between the surface and 5-cm soil depth was chosen as the response variable. The models were applied to segmented sub-datasets of shorter time periods, and better models were obtained for measurements at "after sun-rise" and "before sun-set" periods when there was more variability in solar radiation and relative humidity than in other time frames. To consider time delay in the response of CO_2 concentration, time-lagged regression analysis was used. As a result, there was an improvement in coefficients of determination (0.93 and 0.87) with the segmented time frames. The developed model resulted in an overall coefficient of determination of 0.84 forthe 10-day validation dataset.

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