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Modeling water and carbon fluxes above summer maize field in North China Plain with back-propagation neural networks*

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Abstract: In this work, datasets of water and carbon fluxes measured with eddy covariance technique above a summer maize field in the North China Plain were simulated with artificial neural networks (ANNs) to explore the fluxes responses to local environmental variables. The results showed that photosynthetically active radiation (PAR), vapor pressure deficit (VPD), air temperature (T) and leaf area index (LAI) were primary factors regulating both water vapor and carbon dioxide fluxes. Three-layer back-propagation neural networks (BP) could be applied to model fluxes exchange between cropland surface and atmosphere without using detailed physiological information or specific parameters of the plant.

Key words: Carbon dioxide, Water vapor and heat fluxes, Three-layer back-propagation neural networks
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INTRODUCTION

Dynamics of carbon and water vapor fluxes exchange between the atmosphere and the ecosystem biosphere, depend on complex and non-liner interplay among physiological, ecological, biochemical and edaphic factors and meteorological conditions (Jarvis, 1995; Leuning *et al*., 1995). There are many studies quantifying the fluxes across different time and space scales as well as assessing the environment constraints on them by some kinds of biophysical or empirical models whose results were tested against measurements (Schelde *et al*., 1997; Baldocchi and Wilson, 2001; Goldstein *et al*., 2000; Pilegaard *et al*., 2001; Humphreys *et al*., 2003; Anthoni *et al*., 2002; Wilson *et al*., 2000; Hunt *et al*., 2002). Most of them were conducted in forest and grassland, and researches in cropland still remain largely undeveloped.

In the context of developmental models for surface-atmosphere fluxes exchange, this paper is aimed at conducting a robust, flexible and rapid study for modeling climatic control and environmental factors regulating water and carbon fluxes in cropland. Artificial neural networks (ANNs) are attractive and promising strategies for this work because of their capacity in prediction, control and optimization of input-output responses without a predefined mathematical model (Kosko, 1992; Demuth and Beale, 1994; Schulz and Härtling, 2003) in many research fields. A few applications of this method had been reported in modeling of ecological data since the beginning of the 90's (Thai and Shewfelt, 1991; Chao and Anderson, 1994; Murase *et al*., 1994; Cook and Wolfe, 1991; Elizondo *et al*., 1994; Batchelor *et al*., 1997; Lek *et al*., 1996; Lek and Guegan, 1999; Hecht-Nielsen, 1987; Huntingford and Cox, 1997; Francl and Panigrahi, 1997; Werner and Obach, 2001;

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Moisen and Frescino, 2002). Most of these works showed that ANNs performed better than classical modeling methods. In these researchers, studies on using ANNs in modeling carbon and water fluxes are limited except for Van Wijk and Bouten (1999)'s investigation on selecting a minimal set of input variables to model water vapor and carbon exchange of coniferous forest ecosystems with this approach. Prospects of modeling fluxes in crop field have not been examined yet.

In this work, three-layer back-propagation neural networks were developed and applied to datasets collected in a crop field in the North China Plain to explore their capability in modeling water vapor and carbon dioxide fluxes exchange between the surface of a summer maize field and atmosphere. Responses of the fluxes exchange to biotic and abiotic factors were investigated at the same time.

MATERIALS AND METHODS

Experimental site

The experiment was conducted at Yucheng Comprehensive Experiment Station (36°57′ N, 116°36′ E, 20 m a.s.l) in the North China Plain characterized by semi-humid and monsoon climate. Mean annual precipitation, temperature and global solar radiation at the station over the past 30 years are 528 mm, 13.1 °C, and 5225 MJ/m^2 respectively. Winter wheat and maize is the main crop rotation system in this region. Growing season of winter wheat is from early December to mid-June, and for maize from early-June to later September.

The measurement plot was made at the center of a 300 m×300 m field of the maize Surrounding the field was unbroken farmland of maize at similar growth stages, which extended at least 5 km in all direction (Lee *et al*., 2004).

Measurements

Continuous fluxes and meteorological measurements for this study were made in the summer maize growth period, which began from the day of sowing [day of year (DOY165)] to harvest (DOY275) in 2003.

Wind velocity and virtual temperature fluctuations above the canopy were measured with a three-dimensional sonic anemometer (model CSAT3, Campbell Sci., Logan, UT). Water and CO_2 concentrations were measured at 10 Hz with an open path, infrared absorption gas analyzer (CS-7500, Campbell Scientific Inc.). Fluxes were calculated and stored using a data logger (model CR10X, Campbell Sci., Logan, UT) for 10 min periods and then averaged for 30 min periods.

Above-canopy net radiation was measured with net radiometers (model Q-7, REBS, Seattle, WA). Photosynthetically active radiation was measured with radiation sensors (LI-190SZ, LI-COR Inc., Lincoln, NE). Air temperature and relative humidity were measured with a thermistor and capacitive RH sensor probe (model HMP45C, Vaisala, Helsinki, Finland). Rainfall was measured with tipping-bucket rain gauges (model TE525MM, CSI, Logan, UT), above the canopy. Wind speed was monitored with a wind sentry set (model 03001, RM Young, Traverse City, MI). Two soil heat flux plates (model HFT-3, Seattle, WA) were positioned between-rows and between-plants at depth of 0.05 m to determine fluxes. Soil temperature was measured with copper-constantan thermocouples. Soil water content (SWC) was measured at 0.05 and 0.2 m with two soil water content sensors (model CS615, CSI, Logan, UT).

Irrigation and fertilizer were applied with the same frequency and amount as those of the local farmland. Leaf area index was measured with an electronic leaf-area meter (LAI-2000, LI-COR, Lincoln, NE) every 5 d throughout the crop growth season.

Data processing

Owing to instrument maintenance, calibration, malfunction of the sensors and supporting equipment, the missing data in the observed fluxes occupied 5.67% during the period for analysis. Unreasonable data of carbon dioxide flux (Fc), latent heat flux (LE) and sensible heat flux (Hs) rejected accounted for 0.06%, 0.48% and 0.73% respectively after all 30 min raw data were assessed for anomalous turbulent statistics and sensor malfunction (Baldocchi *et al*., 1988; Hollinger *et al*., 1995). Rejected soil heat fluxes (G) measured between-rows or between-plants comprised 3.06% and 3.41% during the growth period. Major missing fluxes data gap occurred in DOY262−267 because precipitation obscured the gas analyzer optics and sonic transducers. Measurements within 24 h after a rain event were eliminated from the dataset.

For nighttime fluxes records, a wind friction velocity (u^*) threshold (u^*>0.1 m/s) was determined (Falge *et al*., 2001; Anthoni *et al*., 2004) and fluxes measurements when u^* was smaller than the threshold were removed from the dataset to minimize problems related to insufficient turbulent mixing (Fig.1).

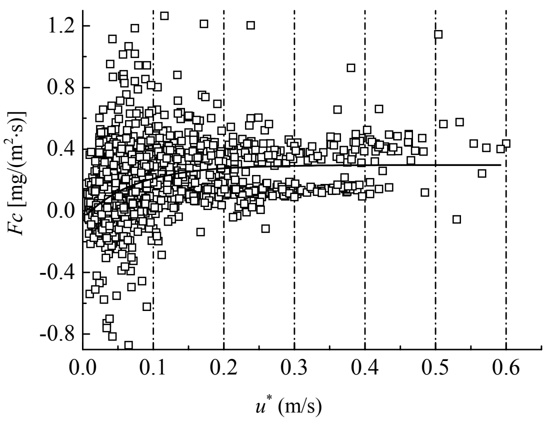

Fig.1 Measured night CO_2 flux (*Fc*) vs nighttime turbulence (u^*)

Energy closure, expressed as: $Rn-G=Hs+LE$, where Rn (W/m^2), net radiation and G (W/m^2), soil heat flux, Hs is the sensible heat flux density (W/m^2) on a 30 min basis. Liner regression indicated that agreement between the sum of the turbulent fluxes (*LE*+*Hs*) and the available energy (Ra) was generally good (Fig.2).

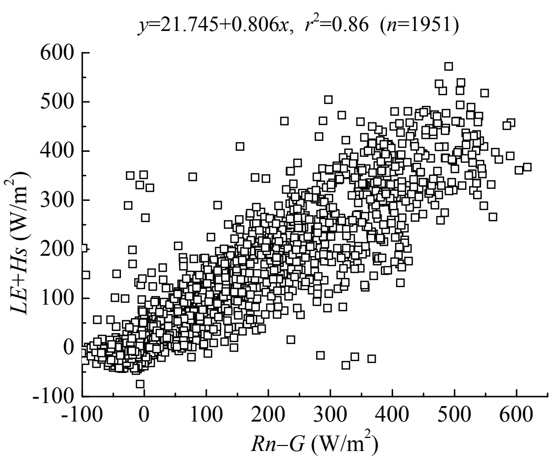

Fig.2 Half-hourly sums of *LE*+*Hs* against available energy (*Rn*−*G*) during the summer maize growth period

Model development

Back-propagation neural network (BP) is the most common multi-layer network used in 80%−90% of all ANNs applications due to its simplicity and proven learning and generalization ability (Adeli and Park, 1998; Cattan and Mohammadi, 1997; Deo and Chaudhari, 1998; Owusu-Ababia, 1998; Thirumalaiah and Deo, 1998). In this study, a feed-forward back propagation neural network with an input layer, output layer and hidden layer and output layer was employed for responses modeling. The number of input and output nodes corresponded to the number of input and output variables, while the number of the hidden nodes depended on the complexity of the relations between input and output variables.

The BP neural network was trained by repeatedly presenting a series of input-output pattern sets to the network. The network gradually "learns" the input-output relationship of interest by adjusting the weights to minimize the error between the actual and predicted output patterns of the training set. The trained network is usually examined through a separate set of data (called test set) to monitor its performance and validity (Sadeghi, 2000).

The dataset for this study was divided into three parts with the proportion of 2:1:1 for training, validation and testing respectively. To minimize the training time by eliminating the possibility of reaching the saturation regions of the sigmoid transfer function during training, both the input and output values were linearly scaled to ensure they lie within the range 0−1 using:

$$x_{\text{scaled}}=(x-x_{\min})/(x_{\max}-x_{\min})$$

$x_{\max}$ and $x_{\min}$ were equal to the maximum and minimum recorded value for each input variable.

The activation function to be used in the neural network was a sigmoidal function:

$$f(x)=\text{logsig}(x)=1/(1+e^{-x})$$

The optimization method applied in the calibration phase was the Levenberg-Marquardt method, (Marquardt, 1963; Demuth and Beale, 1994), which could minimize the total sum of squared errors (SSE) between measured and modeled values by tuning the artificial neural network parameters (e.g. scaling factors and inter-neuron connection weights). All these computations were performed in Neural Network Toolbox 2.0 in Matlab (Ver.6.5).

Input variables determination

Climate and environmental forcing variables such as photosynthetically active radiation (PAR), vapor pressure deficit (VPD) were taken as input variables. Air temperature (T), wind friction velocity (u^*), leaf area index (LAI), soil volumetric water content (W) were selected for their influences on the surface flux transfer or crop transpiration and respiration, carbon dioxide flux (Fc) and water vapor flux (LE) were outputs. All these variables have notable year round variations or different patterns in daily or seasonal periods, so two variables "Day of the year (DOY)" and "Time of the day (TOD, expressed in digital form)" should be inputted into the network to improve its results so that the best simulation model could be achieved with the driving input variables mentioned above, as Van Wijk and Bouten (1999) suggested.

Model selection

After the input layer was determined, experiments were conducted to find the combination of inputs with greatest accuracy in predicting of the validation dataset. The results of different inputs combinations were evaluated by the independent dataset. Fitness of the models were compared using the explained variance (R^2) and the root mean square error (RMSE). Main results for Fc and LE were shown in Tables 1 and 2 respectively.

In Tables 1 and 2, PAR, T and VPD contributed to the performance of the BP network significantly irrespective of the composition of the variables. For Fc, model 6 has the greatest R-square and the least RMSE. The BP network optimum topology was PAR-T-VPD-LAI-u^* in combination with TOD, only variable W was removed among the eight inputs (Table 1, Model 8). This result agreed with that obtained by Van Wijk and Bouten (1999)'s conclusion on surface CO_2 flux in forest, in which "Rg-T-VPD-LAI-TOD" was thought to be the best inputs combination except that wind speed was included in this study. Increasing the number of the hidden neurons did not improve the model performance greatly (Table 1, Models 7–8). Model 7 with 10 hidden neurons was the best-fit combination.

For LE (Table 2), Model 4 was a minimally improved after being combined with W (Model 6) while a slight decrease in model fit resulted when u^* was involved (Model 5). Model 6 could be seen as the best structure for simulation of LE. Model 7 led to little improvement in model fit of latent heat flux after DOY was inputted into Model 6. RMSE dropped and R-square increased in Model 7 when the number of hidden neurons of the network increased to 9 (Table 2, Model 8). Though this improvement was not significant, Model 8 could be chosen as the best fit.

Half-hourly modeled fluxes (Model 7 for Fc and Model 8 for LE) against measured values in summer maize field were shown respectively in Fig.3 by linear regression. The results showed that agreement between measured and BP modeled fluxes was fair to good.

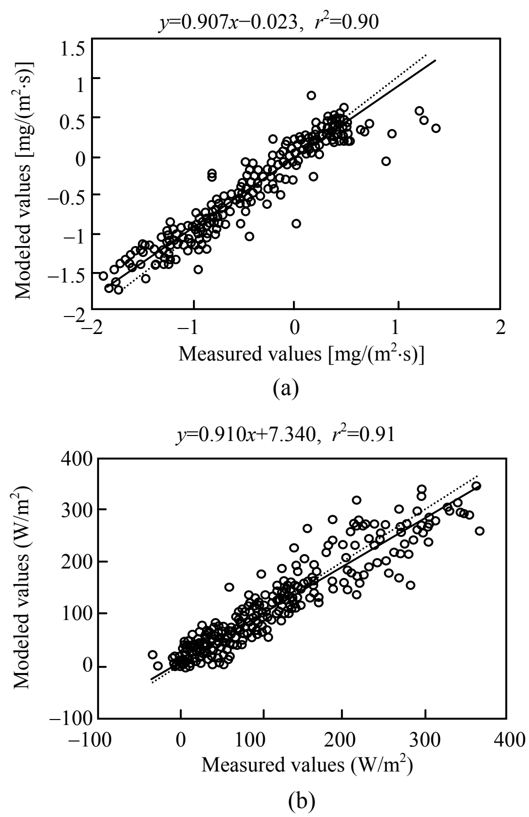

Fig.3 Simulated and measured half-hourly Fc (a), LE (b)

RESPONSES ANALYSIS

Response analysis can be used to evaluate the effects of input variables interaction (Huntingford and

Table 1 BP network topology structure and linear regression analysis for Fc

Model	Input variables combinations	Structure	Slope of the linear regression	Intercept of the linear regression	R^2	*RMSE*
1	*PAR-T-VPD*	3-5-1	0.6449	−0.0767	0.6547	0.2678
2	*PAR-T-VPD-u**	4-7-1	0.6917	−0.0547	0.6864	0.2673
3	*PAR-T-LAI*	3-5-1	0.8738	−0.0271	0.8802	0.1843
4	*PAR-T-LAI-u**	4-7-1	0.8536	−0.0322	0.8607	0.1963
5	*PAR-T-VPD-LAI*	4-7-1	0.8914	−0.0242	0.8906	0.1786
6	*PAR-T-VPD-LAI-u**	5-8-1	0.9015	−0.0189	0.9029	0.1697
7	*PAR-T-VPD-LAI-u*-TOD*	6-8-1	0.9072	−0.0218	0.9062	0.1669
8	*PAR-T-VPD-LAI-u*-TOD*	6-9-1	0.9069	−0.0231	0.9061	0.1670
9	*PAR-T-u**	4-7-1	0.7483	−0.0461	0.7508	0.2465
10	*PAR-T-VPD-W*	5-8-1	0.8820	−0.0248	0.8845	0.1822
11	*PAR-T-VPD-W-u**	6-9-1	0.9007	−0.0234	0.8940	0.1773
12	*PAR-T-W-u**	6-8-1	0.8818	−0.0268	0.8937	0.1739
13	*PAR-T-VPD-LAI-W-u**	7-15-1	0.9054	−0.0199	0.8980	0.1737

Table 2 BP network topology structure and linear regression analysis for LE

Model	Input variables combinations	Structure	Slope of the linear regression	Intercept of the linear regression	R^2	*RMSE*
1	*PAR-T-VPD*	3-5-1	0.7681	21.1550	0.7746	38.8409
2	*PAR-T-VPD-u**	4-7-1	0.8035	18.0332	0.7867	39.2250
3	*PAR-T-LAI*	3-5-1	0.9000	9.2300	0.9052	27.2992
4	*PAR-T-VPD-LAI*	4-7-1	0.9178	7.5646	0.9143	26.3406
5	*PAR-T-VPD-LAI-u**	5-8-1	0.9039	7.7923	0.9101	26.5981
6	*PAR-T-VPD-LAI-W*	5-8-1	0.9131	7.4051	0.9153	26.0346
7	*PAR-T-VPD-LAI-W-DOY*	6-8-1	0.9164	7.3359	0.9225	24.9054
8	*PAR-T-VPD-LAI-W-DOY*	6-9-1	0.9273	6.0639	0.9264	24.5040
9	*PAR-T-VPD-W-u**	6-8-1	0.9145	7.3373	0.9144	26.2316
10	*PAR-T-VPD-W*	5-8-1	0.8505	12.8883	0.8588	32.3297
11	*PAR-T-VPD-LAI-W-u**	5-8-1	0.9171	10.0673	0.9101	27.0157

Cox, 1997). In this study, this evaluation was made with figures interpretation in which two variables were varied together while the others were set to their mean values (Figs.4, 5).

Fig.4a showed CO_2 fluxes response to T and LAI at certain vapor pressure deficit and wind speed condition (or soil water volumetric content) during nighttime. With the maize at its jointing stage (1.2<*LAI*<3.5) and T greater than 20 °C, measured upward flux indicate that CO_2 efflux is mostly due to respiration of the soil microbes and the roots. The value of flux increased thereafter (*LAI*>3.5) during the courses when crop respiration and soil CO_2 efflux increased.

At an early stage with an incomplete canopy (*LAI*<4.0) or leaf senescence, limited canopy cover led to low Fc. Meanwhile, more solar radiation went to soil heat flux than to canopy transpiration caused partially high VPD, dry soil surface, so LE was relatively small (Fig.5a). When the canopy was fully established with a larger LAI, both Fc and LE became higher, LE increased with T if soil water content was adequate.

LAI had direct effect on soil surface cover, canopy area for transpiration and the canopy ventilation condition. Evaporation is under a low LAI and sufficient soil water content, decreases as the soil surface becomes dry. Canopy transpiration of the summer maize comprises the major part of evapotranspiration, and gradually increases to a stable value under the condition that the there is no soil water deficiency (Fig.5a).

In Fig.4c, at a fixed PAR, surface-atmosphere carbon flux exchange intensifies with increasing LAI,

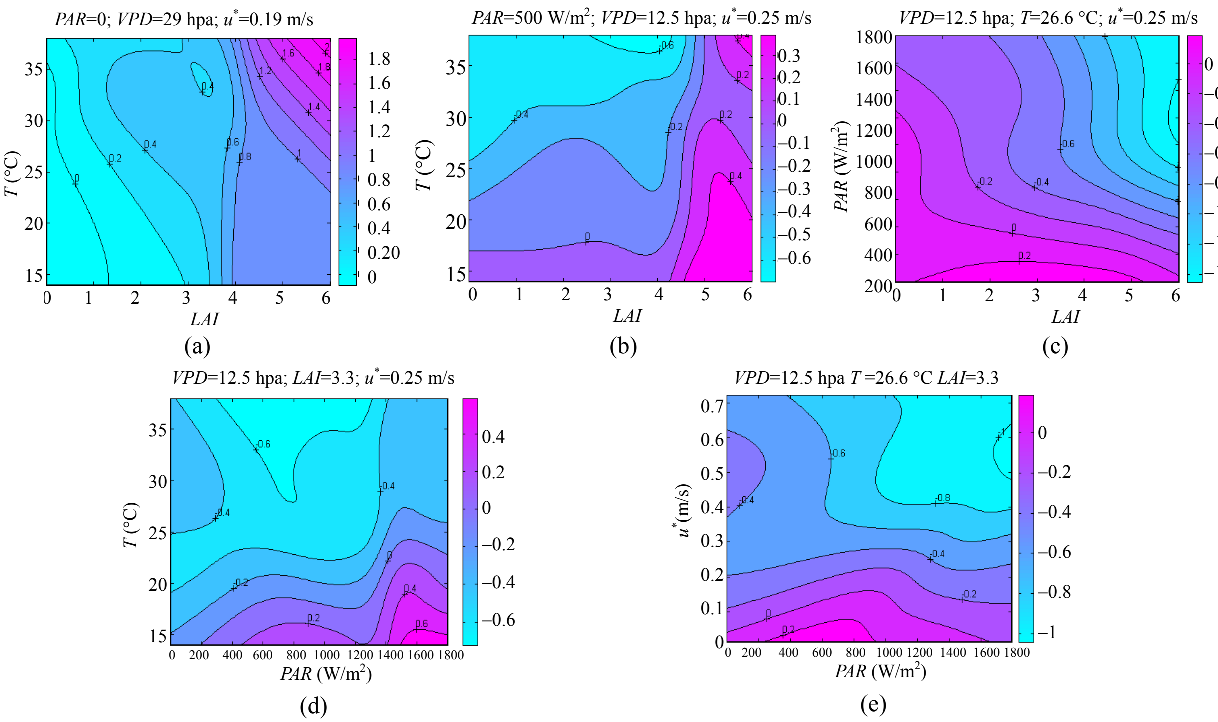

Fig.4 Responses analysis of carbon dioxide flux (Fc)

(a) Nighttime Fc when PAR, VPD and u^* fixed; (b) Daytime Fc when PAR, VPD and u^* fixed; (c) Daytime Fc when T, VPD and u^* fixed; (d) Daytime Fc when LAI, VPD and u^* fixed; (e) Daytime Fc when T, VPD and LAI fixed

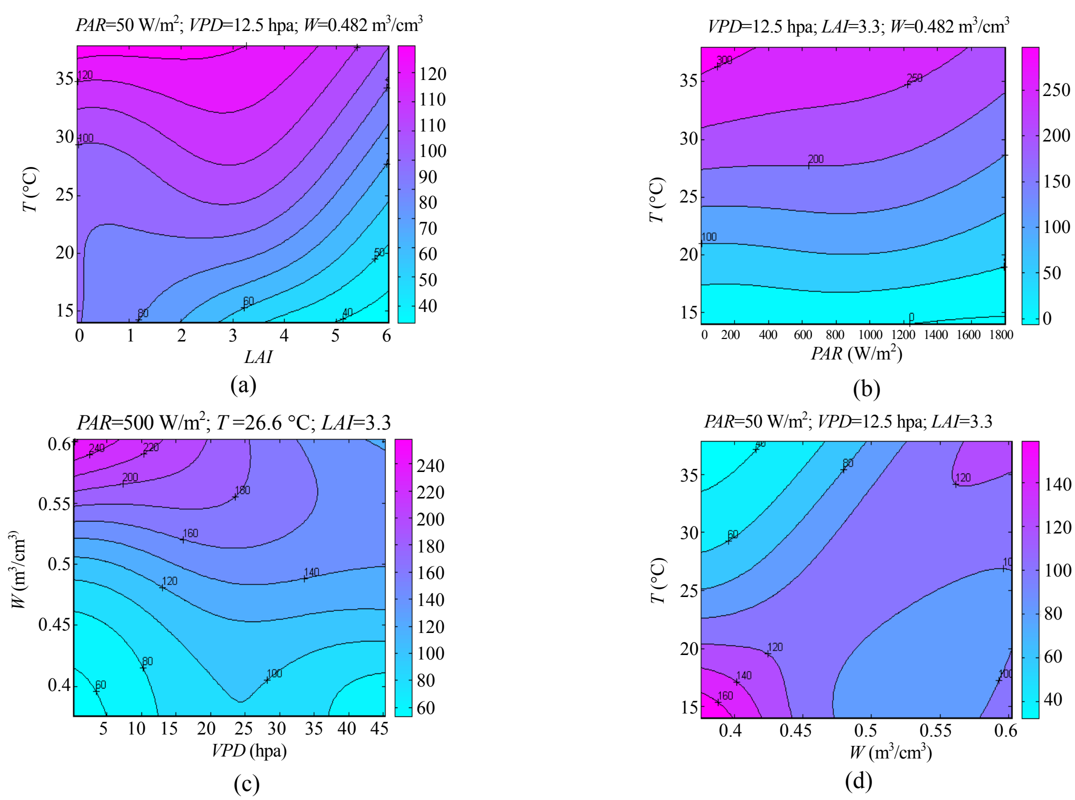

Fig.5 Responses analysis of water vapor flux (LE)

(a) LE when PAR, VPD and W fixed; (b) LE when LAI, VPD and W fixed; (c) LE when PAR, T and LAI fixed; (d) LE when PAR, VPD and LAI fixed similar trends can be seen when LAI is fixed. Greater LAI, lack of significant soil moisture limitation on carbon assimilation results in much higher rates of carbon uptake.

Wind speed greatly influences air turbulence and carbon dioxide transfer. For calm conditions (u^*<0.1 m/s) in our experiment site, respiration in the crop field was very likely under-estimated. This underestimation of respired CO_2 at low u^* was commonly observed at other research sites (Goulden *et al*., 1996; Massman and Lee, 2002). Wind friction velocity of 0.15 to 0.4 m/s represents the most of the actual wind conditions, especially for the midday and afternoon period (Fig.4e).

It must be noted the existence of interactions among the variables. For instance, air temperature is usually 20–35 °C during jointing-milking filling stage when LAI is around 3.2; temperature beyond this variance requires extrapolation of the neural network response.

UNCERTAINTIES

It has been reported that stomatal response is the main mechanism through which a crop can influence carbon and water exchange with the ambient atmosphere (Katerji and Perrier, 1983; Jarvis, 1976; Stewart, 1988; Bosveld and Bouten, 1992). However, it is inconvenient to measure the magnitude of stomatal conductance directly, the most applicable way for a wide knowledge of surface fluxes exchange is to examine the relationship between the fluxes and the environmental variables associated with the variation of stomatal conductance.

Artificial Neural networks enable a mapping between a set of inputs and corresponding outputs (Adeli and Hung, 1995), especially when the apparent relationship between them exists, but they ignored the existence of the Penman-Monteith equation of surface energy partitioning; this can be an advantage or a disadvantage. In this sense, neural networks can only be used in the absence of enough weather, soil, and crop physiological information or process-based knowledge despite their completely unconstrained optimization capability without a predefined mathematical model.

It is important to be careful when introducing additional variables for optimization of neural network. Sometimes increase of the ability to fit just because there is simply more degrees of freedom, but not necessarily mean that the new parameter indicates a strong physical dependence. For instance, in Table 1 Model 6 yields R^2=0.9029 (with PAR, T, VPD, LAI, u^* dependence) while R^2=0.9062 (with the addition of TOD) in Model 7, performance of the Model 6 was improved. However, this slight improvement may not suggest that interface carbon dioxide flux exchange depends on TOD. Inter-relationship between the input variables might lead to unintended side effects in the responses that the network finds. In addition, the dependence of BP model performance on locations with other crop species and meteorological conditions was not evaluated in this study. A thorough study on ANN model performance in different kinds of cropland without detailed physiological or site-specific information will be carried out in future.

CONCLUSION

Three-layer back propagation trained with Levenberg-Marquardt algorithm was developed and tested for simulation of instantaneous surface water and carbon fluxes responses to local environmental variables in a summer maize field. PAR, VPD, T and LAI were primary factors regulating both water vapor and carbon dioxide fluxes. These four input variables together with u^* and TOD led to a little accuracy in estimating carbon dioxide flux, while the model involving PAR, VPD, T, LAI as well as W and DOY could improve the model performance in estimating water vapor flux. BP neural networks provided an interesting and viable alternative method for modeling surface-biosphere fluxes exchange when compared with existing methods for doing the same task.

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