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Environmental Pollution 116 (2002) S37–S44
ENVIRONMENTAL POLLUTION
www.elsevier.com/locate/envpol

# Modeling above-canopy $CO_2$ flux and evapotranspiration in wheat

Peter J. Vaughan*, Donald L. Suarez

*George E. Brown, Jr. Salinity Laboratory, 450 W. Big Springs Road, Riverside, CA 92507, USA*

**"Capsule"**: *Above-ground water vapor flux and carbon dioxide flux were measured and modeled for an Ameriflux wheat field research site.*

**Abstract**

Simulations of above-canopy water vapor and $CO_2$ fluxes were calculated by the USGF linked model of canopy gas exchange and subsurface processes for the 1996–1997 winter wheat season at the AmeriFlux Wheat Site, Oklahoma. Soil surface $CO_2$ flux plus canopy gas exchange and transpiration plus soil evaporation modeled the $CO_2$ and water vapor fluxes, respectively. Parameter values for net photosynthesis, respiration and transpiration were obtained from published sources, generated from Wheat Site data, or estimated by minimizing standard deviation between model and data. The mean measured downward flux of $CO_2$ during rapid growth and maturity of the crop was $-0.45$ mg $m^{-2}$ $s^{-1}$ compared to simulated flux of $-0.47$. Simulated downward $CO_2$ flux exceeded measured values during rapid growth of the crop but underestimated the flux during maturity. For the entire 285-day period, the mean measured upward $CO_2$ flux at night was 0.06 and simulated flux was 0.05. Published by Elsevier Science Ltd.

*Keywords:* Wheat; Evapotranspiration; NEE; Model; AmeriFlux

## 1. Introduction

The AmeriFlux program of $CO_2$ and latent heat flux measurements and the FACE (free-air $CO_2$ enrichment) experiments have provided detailed data for sites in specific ecosystems (Wofsy and Hollinger, 1997). The availability of these comprehensive data sets has provided an opportunity for development of mechanistic models that treat both subsurface and canopy processes. The *ecosys* model was applied to FACE experimental data to determine how well the model could simulate the effect of increased atmospheric $CO_2$ concentration on evapotranspiration in wheat (Grant et al., 1995). This paper reports results of a simulation of above-canopy $CO_2$ flux (net ecosystem exchange, NEE) at the AmeriFlux Wheat Site near Ponca City, OK.

Alternatives to the detailed ecosystem models are the surface-vegetation-atmosphere transfer schemes (SVATs) that are utilized in global circulation models [examples: BIOME-BGC: Hunt et al. (1996); SIB2: Sellers et al. (1996); LSM: Bonan (1995)]. These models are intended to provide spatial averaging of $CO_2$ flux and energy balance at the earth's surface. The treatment of certain processes such as water flow in the soil is simplified to provide reasonable estimates of average water flow for different soil types and topography. Furthermore, the simplification ensures rapid computation as required by the global circulation models (GCMs).

The current work discusses modeling of both evapotranspiration and above-canopy $CO_2$ flux. The model is a linkage of aboveground canopy gas exchange and subsurface water flow, $CO_2$ production and $CO_2$ transport. Our objective was the development and evaluation of a mechanistic model linking aboveground and subsurface processes for $CO_2$ and $H_2O$ flux prediction. The advantage of a mechanistic model of above-canopy CO2 flux is that model results can be compared with detailed above-canopy CO2 flux measurements. An empirical model is more suitable for estimation of, for example, yearly-averaged fluxes. The disadvantage of a mechanistic model is its specificity and its requirement that many model parameters be specified.

The USGF model for canopy gas exchange and soil processes was specifically designed to work with the types of data being recorded at AmeriFlux sites. This model links the Unsatchem model for soil water flow, $CO_2$ transport and other soil processes (Simunek et al., 1996; Suarez and Simunek, 1997) with the GAS-FLUX model for whole canopy photosynthesis (Tenhunen et al., 1994; Beyschlag and Ryel, 1999).

Eddy covariance measurements of latent heat flux, $CO_2$ flux and many other environmental variables can be recorded continuously providing extensive data sets (Verma et al., 1989). Such data sets have proved useful in model development and testing. Detailed modeling of

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* Corresponding author. Fax: +1-909-342-4962.
*E-mail address:* pvaughan@ussl.ars.usda.gov (P.J. Vaughan).

0269-7491/01/$ - see front matter Published by Elsevier Science Ltd.
PII: S0269-7491(01)00245-7

photosynthesis, respiration, surface energy budget and soil water content is recognized as an important constituent of forcing functions for long term carbon exchange models and global circulation models [BIOME-BGC: Hunt et al. (1996); LSM-CCM2: Bonan (1995)]. Most data collection relating to these processes is done under carefully controlled conditions providing the best opportunity for extracting meaningful parameter values characterizing processes occurring at the scale of single leaves (Habash et al., 1995). At the canopy scale, experimental measurements can provide radiation capture, canopy quantum yield and carbon use efficiency for use in modeling crop productivity (Monje and Bugbee, 1998). The laboratory data, however, are not direct measurements of $CO_2$ flux from an ecosystem. Thus, the eddy covariance flux data collected by the various $CO_2$ flux measurement programs provide what may be the best opportunity for testing the models' capabilities regarding canopy-scale $CO_2$ flux prediction (Colello et al., 1998).

Accumulation of carbon in plant matter can be determined as the time integral of the $CO_2$ flux. The accumulation is divided between aboveground and subsurface plant material, a fractionation characterized by the root:shoot ratio. This ratio is likely to vary for different types of plants, different growth stages and many other factors. Calculation of carbon sequestration in soils from models of NEE, therefore, requires modeling of the root:shoot ratio. The scope of the current work is limited to modeling of NEE. In the future, as more data are gathered regarding the root:shoot ratio and soil carbon cycling, development of a soil carbon sequestration model based on NEE may be possible.

## 2. Materials and methods

The AmeriFlux Wheat site is located about 10 km northwest of Ponca City, OK. The first data set from the site was collected for the winter wheat growing season 1996–97. A hard red winter wheat (AGSECO 7853[1]) was planted 12 October 1996 and harvested 3 July 1997. Fertilizers applied in December 1996 were diammonium phosphate (type 18-46, 45 kg/ha) and anhydrous ammonia (78 kg/ha).

### 2.1. Data collection

Data discussed here were collected from 22 September 1996 through 3 July 1997 (285 days) near the center of a 64.7 ha wheat field. The eddy covariance method provided measurements of latent heat flux and $CO_2$ flux. In addition, $CO_2$ concentration, air temperature, vapor pressure, horizontal wind speed and direction, net radiation and photosynthetically active radiation (PAR) were collected at a height of 4.0–4.5 m above ground surface. Barometric pressure and precipitation were measured at a height of 2 m. Data were collected at half-hour intervals. The data were screened to remove any values that had been flagged as less than acceptable.

Gaps lasting up to several weeks occur in the data set. These are due to equipment malfunctions or removal of apparatus from the field to accommodate farm operations. Interpolation methods applied to fill gaps include curve-fitting of elementary functions to existing data to obtain interpolations of the expected value, estimation of missing data by correlation with simultaneous data take at nearby meteorological measurement sites, and linear interpolation for short gaps.

### 2.2. Model specifications

The USGF model was created through linkage of a canopy gas exchange computation (Gas-Flux: Tenhunen et al., 1994; Beyschlag and Ryel, 1999) with a model of subsurface processes (Unsatchem: Simunek et al., 1996; Suarez and Simunek, 1997). The most important feature of the Unsatchem model relating to this application is the model's inclusion of $CO_2$ production and transport enabling calculation of soil surface $CO_2$ flux. The aboveground and subsurface models are needed for calculation of NEE because the soil surface $CO_2$ flux is added to the flux due to canopy gas exchange to obtain NEE.

The two models are also linked through the soil water pressure head and the maximum stomatal conductance.

$$g_{\max} = g_l + \frac{(g_h - g_l)}{L_r}\int_0^{L_r} \alpha_s(h(z))w(z)\,dz \tag{1}$$

where $g_{\max}$ ranges between $g_l$ and $g_h$. The normalized weighting function, $w(z)$, accounts for variation in root density with depth. $L_r$ is the current rooting depth. $g_{\max}$ represents the maximum stomatal conductance for a water pressure head approaching zero throughout the root zone. The actual stomatal conductance is

$$g_s = \frac{mAh_r}{c_s} \tag{2}$$

where $m$ is the stomatal sensitivity constant, $A$ is net photosynthesis, $h_r$ is relative humidity and $c_s$ is leaf surface $CO_2$ concentration (Ball et al., 1987).

The Gas-Flux model of canopy gas exchange is a layered canopy model that calculates net photosynthesis and transpiration (Tenhunen et al., 1994; Beyschlag and Ryel, 1999). The model requires PAR as well as a variety of meteorological measurements. The incident radiation, including both direct sunlight and diffuse light from the sky, that encounters leaves within a

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[1] The use of brand names is for identification purposes only and does not constitute endorsement by the USDA.

canopy layer is determined from the PAR and various geometrical factors such as solar azimuth and inclination, leaf angles, leaf area, and vertical leaf position within the canopy (Duncan et al., 1967). Leaf temperature is calculated based on an energy balance for reflected, transmitted and absorbed infrared radiation among canopy layers (Beyschlag and Ryel, 1999). Gas exchange during the day includes gross photosynthesis, photorespiration and day respiration calculated from leaf incident radiation, leaf temperature and internal $CO_2$ concentration (Farquhar et al., 1980; Harley et al., 1992). At night, gas exchange is calculated as dark respiration. Leaf internal $CO_2$ concentration is obtained by an iterative process that balances the net rate of fixation of $CO_2$ by photosynthesis with the supply rate from the atmosphere as controlled by boundary layer and stomatal conductances. Net gas exchange for the entire canopy is a summation of gas exchange over the canopy layers.

The model employs variable time steps in the range 0.9 s to 0.5 h. Time steps are automatically shortened when water contents are highly-variable, for example, when a water front is advancing downwards within a relatively dry soil. The maximum time step is determined by the need to stop the calculation every 0.5 h to read in the next set of meteorological data.

### *2.3. Modeling approach*

Many model parameters were obtainable from existing publications. Others were determined by experimental measurements, for example, the hydraulic properties of soils at the site. Values of certain parameters were not obtainable and it was necessary to optimize parameter values based on the reported latent heat and $CO_2$ fluxes. For example, data from which average leaf angle could be calculated were not available from the site. Parameter estimation in such cases was done by calculating standard deviation ($\sigma$) for predicted vs. measured $CO_2$ flux, from calculated model results based on systematic variations of model parameter values over specified ranges. The best choice of parameter value was assumed to be that giving the lowest value of $\sigma$.

### *2.4. Photosynthesis and respiration*

The photosynthesis and leaf respiration model is a standard $C_3$ model (Farquhar et al., 1980) with certain modifications (Harley and Tenhunen, 1991). The dark respiration is given by an exponential function $[\exp(c - \Delta H/RT)]$ where $c$ is a scaling factor and $\Delta H$ is the activation energy. The scaling factor and activation energy for *Triticum aestivum* (wheat) are presumed to be similar to those of *Trisetum flavescens* (yellow oat grass) which is also in the same Pooideae subfamily. Day respiration, or the respiration that occurs during the day due to processes other than photorespiration, is set equal to one-half of the dark respiration (Niinemets and Tenhunen, 1997). For all calculations reported here $\Delta H = 39787$ J mol$^{-1}$ and $c = 16.69$ (*Trisetum flavescens*; Wohlfahrt et al., 1998).

The carboxylation rate is calculated from the maximum rate expected for a specified temperature and light intensity (Harley and Tenhunen, 1991). At low radiation levels the rate-limiting process is the regeneration of ribulose biphosphate and the maximum carboxylation rate is $P_{\mathrm{ml}}$. For PAR greater than a critical threshold, the rate-limiting process is determined by the activity of the enzyme Rubisco and the maximum carboxylation rate is $V_{\mathrm{cmax}}$.

$$[V_{\mathrm{cmax}}, P_{\mathrm{ml}}] = \frac{\exp[c - \Delta H_a/(RT)]}{1 + \exp[(\Delta S_{\mathrm{d}} T - \Delta H_{\mathrm{d}})/(RT)]} \qquad (3)$$

These two maximum rates have the form of Eq. (3) but the scaling factor c and the activation energy $\Delta H_{\mathrm{a}}$ are different for the two processes. The deactivation energy and entropy, $\Delta H_{\mathrm{d}}$ and $\Delta S_{\mathrm{d}}$, have nearly the same values for all $C_3$ species. Other parameters in the model that are constant amongst $C_3$ species including $K_{\mathrm{c}}$, $K_{\mathrm{o}}$ and $\tau$ have values identical to those utilized by Harley et al. (1992).

### *2.4.1. Leaf area idex and green fraction*

The USGF model is not a plant growth model, it requires data for plant height, leaf area index (LAI) and green fraction. Total LAI was measured 11 times during the study period (Fig. 1). Because plant parameters were updated daily during a calculation, it was necessary to interpolate the measured LAI and green fraction. For

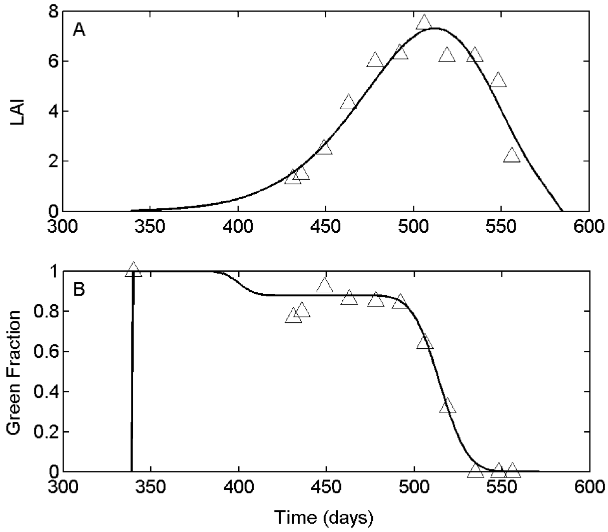

Fig. 1. Leaf area index (LAI) measured values and interpolation by a time-reversed log-normal function. Measured green fraction was fitted by the sum of two complementary error functions. Green fraction was assumed to be 1.0 at emergence.

LAI, this was accomplished by fitting a time-reversed lognormal function to the data. Green fraction was interpolated by a sum of two complementary error functions. The canopy gas exchange model is a layered model so the total LAI must be divided up among the various layers. We assumed a fixed layer height of 0.1 m and a uniform distribution of both LAI and green fraction within the canopy.

### 2.5. *Leaf angle and light absorptance*

Leaf angle was not measured at the Wheat site but our examination of plants at four locations within the site on 5 May 2000 suggested that leaf angle was quite variable within the field. Simulations were conducted for varying leaf angle in the range 55–90° with respect to horizontal. For photosynthetically active radiation (PAR, 400–700 nm) the absorptance was assumed to be 0.9, reflectance was 0.08 and transmittance was 0.02 for all layers. Leaf absorptance was consistent with measurements of 0.882 for wheat (Habash et al., 1995) and 0.85–0.95 (Monje and Bugbee, 1998).

### 2.6. *Soil hydraulic properties*

Soil characterization was obtained from unpublished data (Dept. of Plant and Soil Sciences, Oklahoma State University). Five layers of the Poncreek and Kirkland complexes (Typic & Pachic Argiustolls) were sampled in the depth range 0–1.50 m at five locations within the field. Data include soil descriptions, texture measurements with nine size classes, chemical properties, bulk density, saturated hydraulic conductivity and water retention measurements at four pressures (available for only three of five locations). The water retention data were grouped for each of the five layers generating a total of 12 data points for each layer. Each data set was fitted using the van Genuchten-Mualem water retention model (Van Genuchten et al., 1991) to obtain the water retention parameters $\theta_s$, $\theta_r$, $\alpha$, $n$ (saturated volumetric water content, residual water content and two retention curve fitting parameters). The saturated hydraulic conductivity was measured for samples taken from each layer at three sites. Measured values for the three lowest layers were believed to be artificially low because sample preparation resulted in development of a smoothed zone of artificially low permeability at the sample surface. The suspect measurements were disregarded and saturated hydraulic conductivity of the lower three layers was set to 0.1 m day$^{-1}$.

### 2.7. *Soil surface $CO_2$ flux*

$CO_2$ flux at the soil surface is controlled by production and transport of $CO_2$ in the root zone. Transport of $CO_2$ in soil occurs by advection and dispersion in the soil gas and water phases. An important simplification of the model was the assumption of equilibrium between the two phases based on Henry's Law. From this assumption a single transport equation could be written for transport in each phase (Simunek and Suarez, 1993).

Production of $CO_2$ was modeled utilizing a reduction-function approach in which soil microbial respiration and root respiration were specified as optimal $CO_2$ productions and represented as soil surface $CO_2$ fluxes. These optimal productions were multiplied by the depth integrals of products of reduction functions relating to non-optimal conditions of temperature, soil water pressure head, and $CO_2$ concentration in soil gas. For the case of root respiration an additional time-dependent function expressed the variation in root respiration due to root growth. The optimal values for soil surface $CO_2$ flux at 20C were determined from independent measurements and applied to modeling of soil surface $CO_2$ flux in wheat as $\gamma_{r0} = 0.057$ (mg m$^{-2}$ s$^{-1}$) for root respiration and $\gamma_{s0} = 0.086$ for soil microbial respiration (Buyanovsky and Wagner, 1983; Suarez and Simunek, 1993). The results of the study indicated that these optimal values of soil surface $CO_2$ flux can be successfully applied in modeling of soil $CO_2$ production in wheat (Suarez and Simunek, 1993).

### 2.8. *Soil surface evaporation*

An energy balance calculation was added to the model in order to determine the soil surface temperature and the latent heat flux at the soil surface (Horton and Chung, 1991). This equation was solved numerically for the soil surface temperature by a modified Newton method.

### 2.9. *Simulation specifications*

All simulations were run from 12 October 1996 to 3 July 1997 (days 266–550). In an earlier set of simulations, it was determined that the assumptions of activation energies for the maximum carboxylation rates under light-saturated and light-limited conditions ($V_{cmax}$ and $P_{ml}$, respectively) were poorly-constrained by the measured $CO_2$ flux in this data set. The values utilized in the simulations discussed here were $\Delta H_{vc} = 90$ kJ/mol and $\Delta H_{Pm} = 70$ kJ/mol. We were unable to locate values of these parameters specifically for wheat. A range of values for $\Delta H_{vc}$ for graminoids in different grassland ecosystems was 55–132 kJ/mol (Wohlfahrt et al., 1999). The selected value of $\Delta H_{vc} = 90$ kJ/mol is near the midpoint of this range. The value for $\Delta H_{Pm}$ was estimated as approximately 0.75 of the $\Delta H_{vc}$ value. The exact specification of these numbers is not particularly significant in the work reported here because there was strong correlation between the $\Delta H$

values and the scaling factors [$c$ in Eq. (3)]. If the scaling factor is estimated from fits to the data, as we have done, then the estimated value will be dependent on the choice of $\Delta H$ so as to leave the value of $V_{\mathrm{cmax}}$ approximately the same.

Sensitivity studies of the influence of leaf angle and stomatal sensitivity coefficient were conducted. Leaf angles were varied between 50 and 85° with respect to horizontal. A published range of values for the stomatal sensitivity coefficient [$m$, Eq. (2)] for six different species was 9.8–24.7 (Wohlfahrt et al., 2000). In the calculations discussed here the m was varied between 10 and 30. Dark respiration was specified by an Arrhenius expression [$R_{\mathrm{n}} = \exp(16.69 - 39787/RT)$] representing dark respiration in a closely-related species, *Trisetum flavescens* (Wohlfahrt et al., 1998). Quantum efficiencies of $\alpha = 0.046$ (Mitchell et al., 1995) and $\alpha = 0.065$ (Habash et al., 1995) were tested.

## 3. Results

### 3.1. Water flux

Water flux above the canopy was calculated from the latent heat flux reported in the data set. The measured data were compared with modeled water flux that includes soil surface evaporation and transpiration. The standard deviation of model and data was calculated for the 285-day simulation period. However, variation in the stomatal sensitivity coefficient, $m$, caused variations in the standard deviation that were only relevant during the period when the field was cropped. For this reason, the standard deviation was calculated for the period, 3 February through 13 June 1997. A value of $m = 17$ minimized the standard deviation (Fig. 2). This value of $m$, based on latent heat flux data lies within a published range of values for six other $C_3$ species (10–24.7, Wohlfahrt et al., 2000). A comparison of measured and calculated water flux for representative periods during growth of the wheat suggests that the model had reasonably good performance at times when there was no precipitation (Figs. 3 and 4). The model performance immediately after precipitation events cannot be evaluated with confidence because, for most of the larger events, resumption of data collection occurred between several hours and several days following the event.

### 3.2. $CO_2$ flux

The $CO_2$ flux data were more complete than latent heat flux. We obtained the scaling factors, $V_{\mathrm{cmax}}$ and $P_{\mathrm{ml}}$ [$c$ in Eq. (3)] by adjusting both parameters through specified ranges in order to determine a pair of scaling factors giving the minimum standard deviation for the entire 285-day period. For the activation energies $\Delta H_{\mathrm{vc}} = 90$ kJ/mol and $\Delta H_{\mathrm{Pm}} = 70$ kJ/mol the scaling factors were: $F_{\mathrm{vc}} = 41.2$, $C_{\mathrm{Pm}} = 32.2$. We found that lowering these activation energies by a factor of 2/3 did not appreciably alter the standard deviation between model and data provided that the scaling factors were changed as well. This implies that this data set was not capable of resolving the temperature-dependent and temperature-independent factors of $V_{\mathrm{cmax}}$ and $P_{\mathrm{ml}}$. Early in the period of rapid growth the model tended to over predict downward $CO_2$ flux (Fig. 3). During the stage of crop maturity, prior to senescence, the model provided reasonable predictions of downward $CO_2$ flux (Fig. 4). For the period of time when there was significant downward $CO_2$ flux due to photosynthesis (3 February through 13 June 1997), the mean of measured negative $CO_2$ flux was $-0.45$ mg m$^{-2}$ s$^{-1}$. The mean of calculated $CO_2$ flux for the same set of times as the measured data was $-0.47$ mg m$^{-2}$ s$^{-1}$. However, the

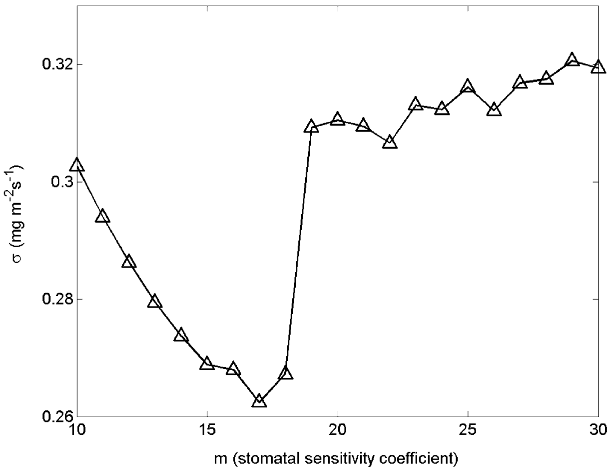

Fig. 2. Standard deviation of model result and data plotted against stomatal sensitivity coefficient.

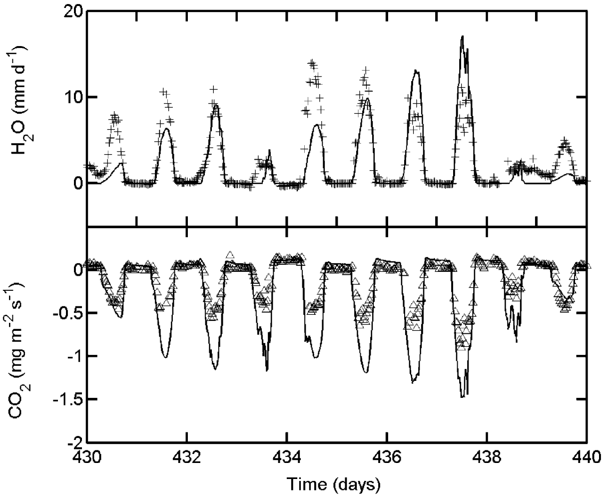

Fig. 3. Comparison of predicted and measured evapotranspiration and above-canopy $CO_2$ flux for 10 days (5–14 March 1997, tillering).

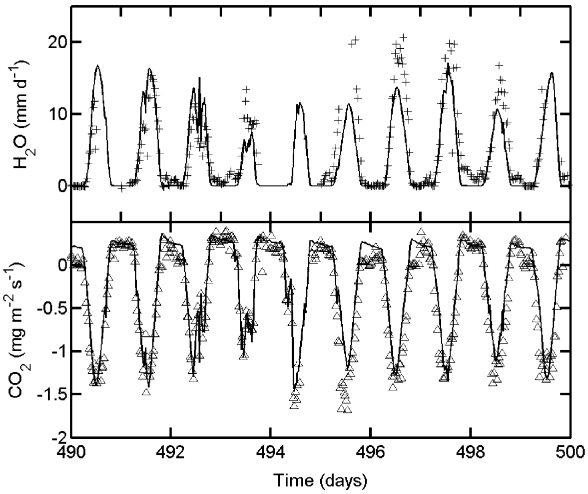

Fig. 4. Comparison of predicted and measured evapotranspiration and above-canopy $CO_2$ flux for 10 days (4–13 May 1997, heading).

standard deviation was 0.27 indicating that the model is providing a fairly good representation of $CO_2$ flux over the entire period but there are substantial compensating errors occurring at different times accounting for the large standard deviation. A gap of 30 days occurred for $CO_2$ flux data starting on 19 March and ending on 17 April 1997. The mean of calculated downward $CO_2$ flux for the 43 days prior to the gap exceeded the mean of observed downward $CO_2$ flux by 0.19 mg $m^{-2}$ $s^{-1}$. The mean difference between these fluxes for 43 days following the gap was −0.10 mg $m^{-2}$ $s^{-1}$. Standard deviations were 0.28 mg $m^{-2}$ $s^{-1}$ for the first period and 0.27 for the second. For the entire period of the simulation, a comparison of observed and predicted $CO_2$ flux resulted in $r^2 = 0.759$ as coefficient of determination.

The measured upward $CO_2$ flux at night exceeded model predictions throughout the growing season. The mean measured upward $CO_2$ flux was 0.10 mg $m^{-2}$ $s^{-1}$ and the model flux was 0.09 for the first 43-day period. For the second period the measured value was 0.17 and the model result was 0.20. For the entire period of the simulation (285 days) the mean upward $CO_2$ flux was 0.06 mg $m^{-2}$ $s^{-1}$ based on selection of positive values. The mean of calculated upward $CO_2$ flux for the same period was 0.05 mg $m^{-2}$ $s^{-1}$. Thus, the model successfully predicted upward $CO_2$ flux at night using independently-determined $CO_2$ production rates for root and microbial respiration (Suarez and Simunek, 1993).

### 3.3. Photosynthetic quantum yield

The measured true quantum yield for wheat was $\alpha = 0.065$ µmol $CO_2$ $\mu mol^{-1}$ photon flux density (Habash et al., 1995). A value of $\alpha = 0.046$ was utilized in modeling wheat growth at a $CO_2$ concentration of 350 µmol $mol^{-1}$ (Mitchell et al., 1995). Separate sets of calculations were conducted for each of these values. The fit to the data was consistently slightly better for the quantum yield of $\alpha = 0.046$. In a direct comparison of the minimum standard deviation obtained by varying $F_{vc}$ and $C$ for seven different leaf angles, $\sigma_{min}$ for $\alpha = 0.046$ was consistently 0.004 mg $m^{-2}$ $s^{-1}$ smaller than the minimum standard deviation for $\alpha = 0.065$.

### 3.4. Leaf angle

Specific measurements of leaf angle are not available so studies of sensitivity to leaf angle were performed for both values of quantum yield. Leaf angle was varied from 55–90° (Table 1). There is a trend of smaller standard deviation for larger leaf angles in the range 55–85° suggesting that values of leaf angle in the range 70–90° are preferred over those in the range 55–70°. This trend was found for both values of photosynthetic quantum yield.

## 4. Discussion

The intention of this work is modeling above-canopy $CO_2$ and $H_2O$ flux. The type of modeling discussed here involves up-scaling of photosynthesis and respiration from single leaves to canopies by means of a layered canopy gas exchange model. This model was linked to a subsurface water flow model that also calculates $CO_2$ production and transport. The combination of the two models enabled prediction of above-canopy $CO_2$ flux that included soil surface flux and canopy gas exchange. The greatest magnitude $CO_2$ fluxes that occurred during the 285-day simulation period were the downward fluxes during the middle of the day when the wheat was fully-grown. Between 14 April and 19 May 1997 the magnitude of the maximum downward $CO_2$ flux normally exceeded 1.0 mg $m^{-2}$ $s^{-1}$ as compared to a mean upwards flux of 0.06 mg $m^{-2}$ $s^{-1}$ for the entire 285 days. Clearly, modeling the downward flux as accurately as possible is an important objective.

Several parameter values were estimated from the data set. Most important of these were the scaling fac-

Table 1
Variation of minimum standard deviation of $CO_2$ flux (mg $m^{-2}$ $s^{-1}$) with leaf angle (degrees measured from horizontal); calculations for quantum yield of 0.046 mol $CO_2$ $\mu mol^{-1}$ PAR

| Leaf angle | $\sigma_{min}$ |
|---|---|
| 55 | 0.148 |
| 60 | 0.145 |
| 65 | 0.142 |
| 70 | 0.141 |
| 75 | 0.140 |
| 0 | 0.139 |
| 85 | 0.138 |
| 90 | 0.140 |

tors for $V_{cmax}$ and $P_{ml}$ [Eq. (3)]. These factors are strongly correlated with the activation energies and, because the activation energies were neither known independently nor well-constrained by the data, their assigned values can only be considered as applying to modeling of the current data set. The parameter estimation does, however, point out the importance of obtaining independent determinations of these activation energies for wheat and other crops.

The model was capable of generating reasonable fits to the data by adjusting various parameter values such as the scaling constants for photosynthesis under RuBP-limited and RuBP-saturated conditions, $C$ and $F_{vc}$, respectively. A crude optimization was performed to determine what adjustments to these parameter values might be necessary to best fit the above-canopy $CO_2$ flux data. The study of leaf angle effect indicated the importance of leaf angle as a factor determining above-canopy $CO_2$ flux. In future field experiments of the type discussed here, we recommend measurement of leaf angle at least at several locations in the vicinity of the eddy covariance flux towers. Also, the stomatal conductance should be measured to permit an independent determination of the stomatal sensitivity coefficient.

Some important simplifications were made in this study. We assumed that leaf angle had a constant value for all layers in the canopy. There was no separation of leaf and stem photosynthesis, rather, the entire leaf area index was presumed to be leaves. We have assumed that the concentration of $CO_2$ external to the leaf is equal to the measured $CO_2$ concentration above the canopy. There was adequate fertilization of the field with respect to phosphate so the assumption of no limitation of the regeneration of RuBP due to lack of inorganic phosphate appears reasonable. Measurements of leaf nitrogen content were not available but the two types of nitrogen fertilizers were applied in December, 1996 so an adequate nitrogen supply was available. There is no mechanism in the current model to account for aging of leaves with associated buildup of starches, loss of chlorophyll content, or anatomical changes (Harley et al., 1992). However, the model over predicted downward $CO_2$ flux during the rapid growth stage and under predicted downward flux when the crop was mature. A model that reduced photosynthesis with age would not address this discrepancy.

The measured above-canopy $CO_2$ flux at night was determined by both the dark respiration in the canopy and the soil surface $CO_2$ flux. The dark respiration parameters, activation energy and scaling factor, were presumed to have values identical to those of Trisetum flavescens (yellow oat grass). Modeling $CO_2$ production in the subsurface utilized a reduction-function approach with optimal values for surface $CO_2$ flux in wheat (Suarez and Simunek, 1993). We assumed that the optimal soil $CO_2$ production values and other parameter values, determined in this earlier work, are applicable at the Wheat Site. These assumptions appear supported by the successful predictions of upward $CO_2$ flux for all times during the simulation period. Soil surface $CO_2$ flux measurements would be useful in evaluating, more precisely, the contributions of dark respiration and soil surface $CO_2$ flux to the above-canopy $CO_2$ flux.

Several reasons can be given to account for the overestimate of downward $CO_2$ flux during rapid growth of the wheat. The LAI may be overestimated relative to its estimated value later in the season or the assumption of a uniform distribution of LAI within the canopy may be incorrect. The assumption of uniform distribution of LAI within the canopy might be invalid during the rapid growth stage but valid when the crop was mature. There could be seasonal changes in parameter values, for example, leaves growing during the late spring might be better adapted to higher temperature than those that had grown earlier. This could be reflected in parameters used to calculate $V_{cmax}$ and $P_{ml}$.

## 5. Conclusions

The above-canopy water vapor flux and $CO_2$ flux were measured at the AmeriFlux Wheat site by researchers at the University of Nebraska, Lincoln. Using the USGF linked model of canopy gas exchange and subsurface processes we have computed above-canopy water vapor flux and $CO_2$ flux for the 1996–1997 winter wheat season. Many of the model parameter values could be obtained from published work or by analysis of data gathered at the Wheat Site. Certain critical parameters for $CO_2$ flux such as the scaling factors for $P_{ml}$ and $V_{cmax}$ were not obtainable from published work and these were estimated by adjusting them to minimize the standard deviation between the model and the data. Model results overestimated maximum downward $CO_2$ flux during the rapid growth of the crop and underestimated downward flux when the crop was mature. Upward $CO_2$ flux at night was successfully predicted by the model. Modeling of above-canopy water vapor flux was more problematic than $CO_2$ flux. Water flux has the inherent problem that meaningful eddy covariance measurements can only be made when there is no precipitation. Only 59% of the measurements during the 285-day period were considered valid. The model made reasonably good predictions of water vapor flux at these measurement times.

## Acknowledgements

This study was supported by the National Institute for Global Environmental Change (NIGEC) under grant 92-0294 NEBR. Prof. Shashi Verma, Director of the Great Plains Regional Center of NIGEC, consulted with us and provided essential data that his group collected at the Wheat Site. Dr. Ronald Ryel assisted us in linking the canopy gas exchange model with the Unsatchem model and provided valuable advice regarding operation of the model. This paper was presented at the USDA Forest Service Southern Global Change Program sponsored Advances in Terrestrial Ecosystem: Carbon Inventory, Measurements, and Monitoring Conference held 3–5 October 2000 in Raleigh, NC.

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