



Coupled modeling of the hydrological and carbon cycles in the soil–vegetation–atmosphere system

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Abstract

A coupled model of the hydrological and carbon cycles in the soil–vegetation–atmosphere system is suggested. The model describes the interception and evaporation of precipitation by canopy, transpiration, vertical transfer of soil moisture, photosynthesis, the interaction between transpiration and photosynthesis, and plant and soil respiration. The validation of this model was carried out using the FIFE measurements from a grassland site in Kansas, the BOREAS measurements from a jack pine forest site in Saskatchewan, and the observations conducted within a deciduous forest in the southeastern United States. The model results show a good agreement with experimental data. The model was shown to adequately describe the influence of soil moisture and atmospheric CO₂ concentration on transpiration and net ecosystem CO₂ exchange.

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1. Introduction

Despite a large progress in understanding the role of the terrestrial biosphere in regulating energy, water, and carbon dioxide fluxes in the climate system, simulation models of these processes have not been sufficiently developed yet to yield reliable estimates of water and carbon dioxide fluxes for different types of terrestrial ecosystems. There are considerable uncertainties in calculating carbon sinks and sources in an ecosystem and variations of carbon dioxide and transpiration fluxes in space and time. At the same

time, these calculations are extremely important for determining possible changes in the climate system and the sensitivity of terrestrial ecosystems to climate change.

The complicated interactions between hydrological and biogeochemical processes and the diversity of these interactions in various vegetation ecosystems makes constructing mathematical models of water and carbon exchanges in the soil–vegetation–atmosphere system very difficult. Moisture content of the soil, vegetation, and atmosphere, as well as water evaporation and transpiration affect both directly and indirectly the photosynthesis and respiration of vegetation and microbiological processes in the soil. At the same time, vegetation controls transpiration through its internal physiology related to

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photosynthesis and respiration and through its albedo, geometric structure, and leaf area. The geometric structure of plants and the characteristics of their leaves also influence the energy and water exchange of the ecosystems. The most important interaction mechanism in the water and carbon exchange of plants is expressed in variation of the stomatal resistance to air fluxes. The stomatal openings respond very quickly to changes in the environment, and the stomatal resistance has a well-expressed diurnal cycle, as well as seasonal and inter-annual variations caused by hydrometeorological conditions or biological processes in plants.

Most studies in the investigation and simulation of the dependence of transpiration and photosynthesis on hydrometeorological variables were aimed at solving agricultural problems (first of all, irrigation and programming of harvest) (e.g. Monteith and Unsworth, 1990; Bihele et al., 1980; Hillel, 1982; Brutsaert, 1981). On the other hand, numerous studies have addressed the biophysical aspects of respiration and photosynthesis (e.g. Thornley, 1976; Farquhar, 1980; Kobak, 1988; Amthor, 1989). However, these studies did not pay proper attention to the interaction between hydrological and biogeochemical processes as parts of the climatic system. The coupling of models of the hydrological and carbon cycle provides an instrument for improving descriptions of both cycles for predicting the effects which could not be accounted for by independent hydrological or carbon models.

Large-scale international field experiments (FIFE, HAPEX-Sahel, BOREAS, NOPEX) significantly extended the possibility to integrate the descriptions of the hydrological and carbon cycles into coupled models. These experiments produced unique data collected by simultaneous short-term measurements of energy, water, and carbon dioxide fluxes in the atmosphere, vegetation, and soil for various ecosystems and created a totally new base for the development of complicated models, testing assumptions, and estimation of sensitivity of ecological systems to different environmental and human impacts. Numerous studies have been devoted to analysis of these data and their use for the development and evaluation of biophysical models of CO₂ exchange and evapotranspiration. The results of model evaluations and model comparisons for

different elaboration levels of the description of processes have been reported by Baldocchi et al. (1997); Lloyd et al. (1997); Cox et al. (1998); Baldocchi et al. (2001) and in other publications.

In this paper, we present a coupled model of heat, water, and carbon exchange in the soil–vegetation–atmosphere system, which has been constructed and evaluated on the basis of measurements carried out during FIFE and Boreas, as well as observations in a forest site, located in the southeastern United States and included in the international FLUXNET project of study of long-term carbon dioxide fluxes. The main distinction of this model from previous ones is a more detailed description of the vertical heat and water transfer in the soil–vegetation–atmosphere system. At the same time, we tried to reduce, as much as possible, the number of parameters to be calibrated.

2. Model description

It is assumed that a fraction U_k of the precipitation rate P_f is intercepted by the canopy and can be temporarily stored, evaporated, or drained to the soil surface; the remaining part $(1 - U_k)$ reaches the soil surface directly. It is supposed also that the canopy storage capacity is exponentially distributed over the canopy area with the maximum value W_{cm} and the evaporation from the wet part of canopy is equal to the water surface evaporation E_w . In this case, the precipitation rate P_s reaching the soil at the moment t can be calculated as

$$P_s = P_f(1 - U_k) + (P_f - E_w)\eta U_k, \quad (1)$$

where $\eta = 1 - \exp(-S/W_{cm})$ is the proportion of canopy area from which the stored water drains to the soil surface, $S = \int (P_f - E_w)dt$ and $W_{cm} = \mu \times LAI$, where LAI is the leaf area index and μ is an empirical coefficient (according to Dickinson (1983) μ varies from 0.05 to 0.20 mm).

Evaporation from the wet part of canopy is given by

$$E_w = \rho_a \frac{q^*(T_f) - q_a}{r_a} \eta U_k \quad (2)$$

where ρ_a is the air density, q_a is the specific air humidity, $q^*(T_f)$ is the saturated specific air humidity

at the leaf temperature T_f , r_a is the aerodynamic resistance for water vapor at the leaf surface.

Transpiration from dry leaves can be estimated as

$$E_f = \rho_a \frac{q^*(T_f) - q_a}{r_a + r_s} (1 - \eta) \text{LAI} \quad (3)$$

where LAI is the leaf area index, r_s is the stomatal resistance.

There are two main types of empirical formulas relating the stomatal resistance to the characteristics of plants and the environment. The first type is based on the assumption that the stomatal resistance depends mainly on environmental variables (the Jarvis formula (Jarvis, 1976) is a commonly used dependence of this type). The formulas of the second type are based on regarding transpiration as a physiological process and include, in addition to environmental variables, the rate of photosynthesis and the CO_2 concentration at the leaf surface. We used formulas of both types.

The first formula, which we considered as a basic one, is a modification of the Jarvis formula, and the stomatal resistance is calculated as

$$r_s = r_0 \frac{\theta_{fc} - \theta_r}{\theta - \theta_r} \left(1 + \frac{\gamma}{\text{PAR}} \right) \quad (4)$$

where r_0 is the stomatal resistance at the fully opened stomata, θ is the volumetric soil moisture content, θ_{fc} is the moisture content at the field capacity, θ_r is the residual moisture content, PAR is the photosynthetically active radiation, γ is an empirical coefficient.

The second formula, used as an auxiliary one to improve the simulations after estimating the leaf photosynthesis in a first approximation, was the relationship proposed by Ball et al. (1987)

$$r_s = \frac{C_s}{aAh_s} \quad (5)$$

where C_s is the CO_2 concentration at the leaf surface, A is the net leaf photosynthesis, a is a fitting parameter, h_s is the relative air humidity at the leaf surface.

Evaporation from bare soil E_w can be computed using

$$E_g = \rho_a \frac{rq^*(T_g) - q_a}{r_{ag}}, \quad (6)$$

where r_{ag} is the resistance of the soil to evaporation, T_g is the soil temperature, r is the relative air humidity at the soil surface. The value r is found from the assumption that

$$r = \exp \left[\frac{Mg\psi(\theta)}{R(T_g + 273)} \right], \quad (7)$$

where M is water molecular weight, R is the universal gas constant, $\Psi(\theta)$ is the soil water potential, (T_g is in $^\circ\text{C}$).

The values of aerodynamic resistance in (2) and (3) are calculated as $r_a = 1/(C_E u)$, where u is the wind speed, C_E is the foliage resistance coefficient given by

$$C_E = k^2 [\ln((z_1 - d)/z_0) \ln((z_2 - d)/z_{0v})]^{-1} \quad (8)$$

where k is the von Karman constant, z_1 and z_2 are the heights at which the wind speed and air humidity are measured, respectively, d is the displacement length, z_0 is the roughness length for momentum, z_{0v} is the roughness length for sensible heat.

The resistance in (6) is found as $r_{ag} = 1/(C_g u)$ where C_g is the soil surface resistance coefficient.

To describe the vertical transfer of soil moisture, the Richards equation in the diffusion form is used

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta) \frac{\partial \theta}{\partial z} - K(\theta) \right] - S_k(\theta, z) \quad (9)$$

where $K(\theta)$ is the soil hydraulic conductivity, $D(\theta)$ is the soil diffusivity, z is the soil depth, $S_k(\theta, z)$ is the uptake of water by plant roots calculated as

$$S_k(\theta, z) = -K(\theta) [\psi_k(\theta) - \psi(\theta)] b_k \rho_k(z), \quad (10)$$

where $\psi_k(\theta)$ is the water potential of root system, $\rho_k(z)$ is the root density, b_k is an empirical coefficient related to the root structure. It is assumed that $\rho_k(z) = \rho_0 \exp(-k_1 z)$ where ρ_0 is the root density at the soil surface, k_1 is an empirical constant.

At the upper boundary of the soil, the following condition is used

$$\begin{aligned} P_s - E_g &= -D(\theta) \frac{\partial \theta}{\partial z} + K(z) \Big|_{z=0} & \text{at } P_s - E_g \leq I, \\ \theta &= \theta_s & \text{at } P_s - E_g > I, \end{aligned} \quad (11)$$

where I is the soil infiltration rate in the upper layer of soil, θ_s is the soil porosity.

The system (9)–(11) was solved numerically using an implicit finite difference scheme and the procedure described in Kuchment et al., 1989; Kuchment and Startseva (1991).

At the lower boundary of the soil layer under consideration, the water flux was assumed to be equal to the soil hydraulic conductivity at this point.

The functions $K(\theta)$, $\psi(\theta)$, and $D(\theta)$ were expressed through the soil moisture content and the soil constants (the saturated hydraulic conductivity K_s , the soil porosity θ_s , the residual soil moisture content θ_r , etc.). It was assumed that $E_f = \int_0^{z_{\max}} S_k(\theta, z)$, where z_{\max} is the depth of roots.

The soil surface temperature T_g was determined from observations. The leaf temperature T_f was calculated using the heat balance equation for canopy

$$U_k(Q_{sl} + F_a - 2F_f + F_g) = Q_{hf} + Q_{Ef} \quad (12)$$

where Q_{sl} is the short-wave radiation adsorbed by the canopy, F_a , F_f , and F_g are the long-wave radiation of the atmosphere, vegetation, and soil, respectively, Q_{hf} and Q_{Ef} are the vertical fluxes of sensible and latent heat (it was showed that the heat losses for changing the leaf temperature could be neglected).

To find the values of F_f , F_g , Q_{hf} and Q_{Ef} , the following relationships were applied

$$F_f = \varepsilon\sigma T_f^4, \quad (13)$$

$$F_g = \varepsilon\sigma T_g^4, \quad (14)$$

$$Q_{hf} = \rho_a c_p (T_f - T_{af}) / r_a, \quad (15)$$

$$Q_{Ef} = LE_f + LE_w, \quad (16)$$

where ε is the emissivity, σ is the Stefan–Boltzman constant, c_p is the specific air heat capacity, ρ_a and T_a are the air density and the air temperature, respectively.

The values of T_g , Q_{st} and F_a were taken from the observational data.

Considering the CO_2 exchange between vegetation and atmosphere as a diffusion process, we obtain the following equation for accounting for the carbon dioxide flux through the stomatal openings

(the net leaf photosynthesis):

$$A = \frac{C_a - C_i}{1.6r_s + 1.4r_a} \quad (17)$$

where C_i is the internal CO_2 concentration within the leaf; the coefficients 1.6 and 1.4 account for the different molecular diffusivities of carbon dioxide and water vapor at diffusion through the stomata and the air boundary layer.

An alternative approach to the calculation of leaf photosynthesis is based on describing the biophysical processes within leaves. We applied this approach using the model of leaf photosynthesis and carbon exchange taken from (Farquhar et al., 1980; Collatz et al., 1991; Cox et al., 1998). In this model, the gross leaf photosynthesis $P = A + R_d$ (R_d is the leaf dark respiration) is either limited by the internal CO_2 concentration C_i , or by some combination of leaf temperature and the photosynthetically active radiation.

The model can be represented by a system of two quadratics. The first equation allows us to find the largest gross leaf photosynthesis P_{\max} limited by certain combination of leaf temperature and incident photosynthetically active radiation (electron transport)

$$0.83P^2 - P_{\max}(V_T + 4.57\alpha I_p) + 4.57V_T\alpha I_p = 0 \quad (18)$$

where V_T is the carboxylation rate ($\mu\text{mol m}^{-2} \text{s}^{-1}$), α is the quantum efficiency [mol CO_2 (mol PAR photons)]. The smallest root for P_{\max} is selected as physically realistic.

The second quadratic gives the dependence of gross photosynthesis on P_{\max} and C_i

$$0.90P^2 - P(P_{\max} + K_T\nu_{\text{mol}}C_i) + P_{\max}K_T\nu_{\text{mol}}C_i = 0 \quad (19)$$

where K_T is a temperature-dependent coefficient ($\mu\text{mol m}^{-2} \text{s}^{-1}$), ν_{mol} is the molar volume ($\text{m}^3 \mu\text{mol}^{-1}$).

The dependence of the carboxylation rate on leaf temperature is given by

$$V_T = \frac{V_{\max} 2^{0.1(T_f - 25)}}{(1 + e^{0.3(13 - T_f)})(1 + e^{0.3(T_f - 36)})}, \quad (20)$$

where V_T is ($\mu\text{mol m}^{-2}\text{s}^{-1}$), V_{max} is the maximum carboxylation rate.

The leaf dark respiration and the coefficient K_T were assumed to be linearly related to V_T :

$$R_d = 0.025V_T, \quad (21)$$

$$K_T = 2 \times 10^4 V_T. \quad (22)$$

Thus the leaf photosynthesis model has two adjustable parameters: the maximum carboxylation rate, V_{max} , and the quantum efficiency, α .

To transfer from the leaf photosynthesis model to the canopy and ecosystem models, it is assumed that

$$P_c = P \times \text{LAI}, \quad (23)$$

$$R_p = R_d \times \text{LAI}_c, \quad (24)$$

where P_c is the canopy photosynthesis rate, R_p is the plant respiration, LAI_c is the plant area index which, in addition to the leaf area, also accounts for the area of canopy branches and stems. It is the simplest hypothesis without taking any explicit account of the canopy structure, which influences light extinction through the depth of the canopy. However, to account for the canopy structure, it is necessary to introduce additional a priori information, new measurements or to increase the number of calibrated parameters.

The CO_2 balance equation for the canopy can be written for a unit time as

$$N - S_t = -P_c + R_p + R_s \quad (25)$$

where N is the measured net CO_2 flux above the canopy (positive upwards), S_t is the storage of CO_2 in the canopy air layer, P_c is the gross canopy photosynthesis, R_p is the plant respiration, R_s is the soil respiration. The value $\text{NEE} = N - S_t$ is the net CO_2 exchange in the ecosystem and, at the same time, the difference between carbon gained by the ecosystem through gross canopy photosynthesis and carbon lost via respiration.

3. Model evaluation

The ability of the suggested model to reproduce evapotranspiration, soil moisture content, and the net CO_2 exchange in the ecosystem were evaluated

against experimental data for grassland and two (pine and deciduous) forest ecosystems. There are significant differences in land surface, soils, and biophysical characteristics of these ecosystems and in environmental conditions of areas where they are located. The ecosystems also considerably differ in the range of variations in the magnitudes of water and carbon fluxes, which is essential for testing the model. Besides, there is an evident difference in the quality of experimental data for the ecosystems under consideration: the data sets from FIFE and BOREAS have many long gaps, while the deciduous data sets taken from the FLUXNET observations are continuous, well-checked series.

3.1. Application to a grassland ecosystem

The data set from the FIFE experiment, carried out in a grassland area in Kansas from 28 May to 30 August 1987 (Strebel et al., 1990; Sellers et al., 1992), were used. The model has been constructed for a site of prairie with ungrazed grass species (site reference 16, 4439—ECV). The soil of the site is clay loam. Radiation components and meteorological variables were collected every 30 min at a reference height of 2.25 m. The measurements of the fluxes of sensible and latent heat as well as those of carbon dioxide were made using eddy covariance technique and averaged over half an hour interval. The soil moisture content was measured gravimetrically every week to a depth of 1.4 m by neutron probes.

Functions $\psi(\theta)$, $K(\theta)$, and $D(\theta)$ were expressed using the relationship suggested by Clapp and Hornberger (1978)

$$\psi(\theta) = \psi_s \left(\frac{\theta}{\theta_s} \right)^{-b} \quad (26)$$

$$K(\theta) = K_s \left(\frac{\theta}{\theta_s} \right)^{2b+3} \quad (27)$$

$$D(\theta) = K_s b \psi_s \theta^{b+2} \theta^{-b-3} \quad (28)$$

where ψ_s is the soil water potential at $\theta = \theta_s$, K_s is the hydraulic conductivity of saturated soil, b is an empirical constant.

To calculate the total respiration (the respiration from leaves, roots and stems of plant plus the soil

respiration), the empirical relation received for the grassland by Norman et al. (1992) was applied in the following form

$$F_s = s_1 \left(\frac{\theta - s_2}{0.4 - s_2} \right) e^{s_3(T_a - 25)} \quad (29)$$

where the values $s_1 = 17.8 \mu\text{mol m}^{-2} \text{s}^{-1}$, $s_2 = 0.14$ and $s_3 = 0.062 \text{ }^\circ\text{C}^{-1}$ were derived from the NEE nighttime measurement data.

Most model parameters were assigned on the basis of available direct measurements; six parameters were taken from publications, and four parameters were calibrated against the field measurements of the latent heat fluxes (r_0 and C_g) and the CO_2 fluxes (α and V_{max}) for the period of the measurements from 28 May to 7 June. The values of the parameters used for model simulation are presented in Table 1.

The comparison of the measured $\text{LE} = L(E_w + E_f + E_g)$ and calculated hourly latent heat fluxes for three periods at the beginning, in the middle, and at the end of the field measurement campaign is given in Fig. 1. Fig. 2 presents the comparison of measured and simulated values of volumetric soil moisture content

at depths of 5 and 15 cm and for the 1 m upper layer. The comparison of the measured and simulated hourly values of the ecosystem CO_2 exchange for the same periods as in Fig. 1 is presented in Fig. 3. As can be seen from Figs. 1–3, the simulated variables are quite consistent with the measured ones. There are several significant discrepancies but they may be mainly explained by numerous gaps in available data or errors in measurements. It is worth emphasizing that the total period of gaps in measurements of the latent heat fluxes at the site 4439-ECV is about 70% of the entire observational period; the total period of gaps in the CO_2 measurements is about 85% of the observational period. The coefficients of determination of measured and simulated hourly values of NEE are 0.93, 0.92, and 0.92, respectively.

Fig. 4 shows the diurnal patterns of the simulated canopy photosynthesis rates, the sum of soil and plant respiration and the net ecosystem exchange averaged over the periods from May 28 to June 3, from July 1 to July 7 and August 9 to August 15, respectively. As can be seen from this figure, the simulated values are qualitatively consistent with observations and have

Table 1
Parameters used in the model (FIFE-1987, site 4439)

Parameter	Units	Values
The measured parameters		
Saturated hydraulic conductivity, K_s	m s^{-1}	0.116×10^{-7}
Soil porosity, θ_s	$\text{m}^3 \text{m}^{-3}$	0.50
Soil moisture at field capacity, θ_{fc}	$\text{m}^3 \text{m}^{-3}$	0.375
Residual soil moisture content, θ_r	$\text{m}^3 \text{m}^{-3}$	0.14
Soil water potential at saturation, ψ_s	m	-0.2
Parameter b	-	5.0
Exchange coefficient for canopy, C_E	-	0.025
The fraction of precipitation intercepted by vegetation, U_k	$\text{m}^2 \text{m}^{-2}$	0.55
Plant area index, LAI_c	$\text{m}^2 \text{m}^{-2}$	2.2
Leaf area index, LAI	$\text{m}^2 \text{m}^{-2}$	1.8
The parameters taken from publications		
Emissivity of canopy and soil, ε	-	0.98
Parameter k_1	m^{-1}	2.5
Parameter $b_k \rho_0$	m^{-2}	1000
Parameter μ	m	0.05×10^{-3}
Parameter γ	Wm^{-2}	30
The calibrated parameters		
Minimum stomatal resistance, r_0	S m^{-1}	200
Exchange coefficient for the soil, C_g	-	0.1×10^{-3}
Maximum carboxylation rate, V_{max}	$\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$	20
Quantum efficiency, α	$\text{mol CO}_2 (\text{mol PAR photons})^{-1}$	0.02

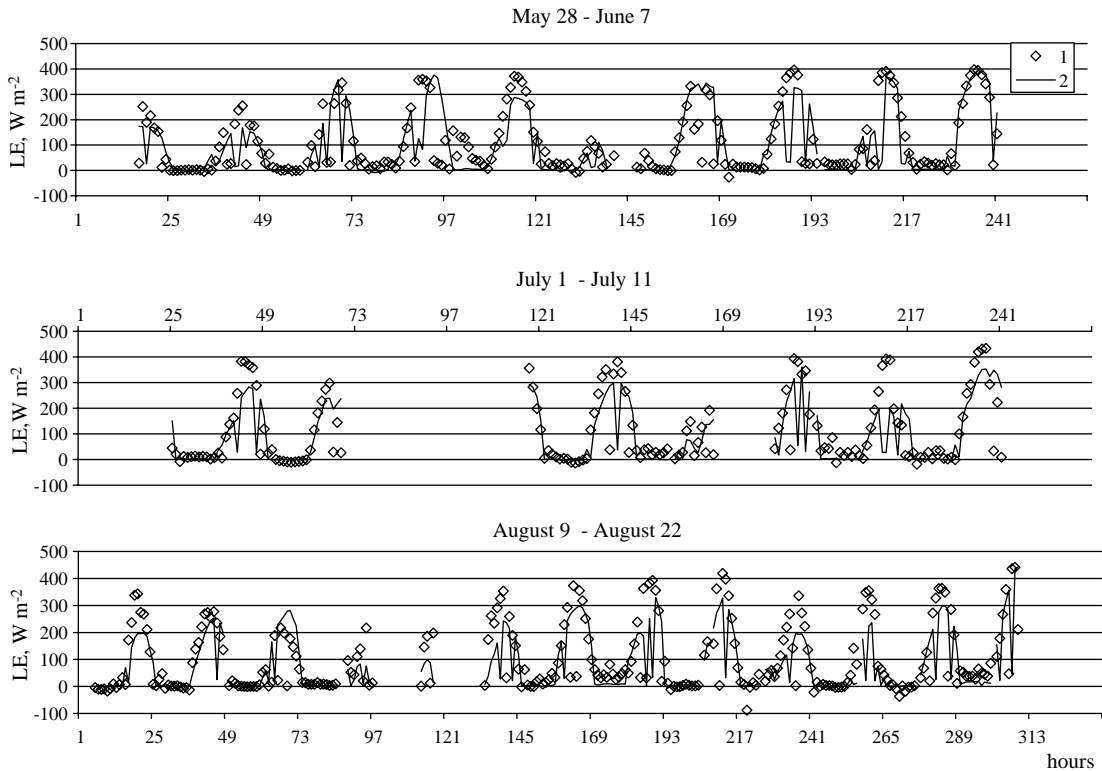


Fig. 1. Comparison of measured (1) and simulated (2) hourly latent heat fluxes (FIFE, 4439 site).

a well-expressed diurnal courses with peak rates around 13–16 h. There are also alterations of the mean diurnal courses of canopy photosynthesis rates, respiration and NEE during the growing season. The largest amplitudes of diurnal variation of all these variables have the mean diurnal courses for the period from July 1 to July 7 when the most intensive physiological processes occur.

An attempt was also made to improve the results of simulating the CO_2 exchange and the latent heat fluxes using for computing the stomatal resistance relationship (5) and the net leaf photosynthesis taken from calculation with the relationship (4) (the coefficient α in (5) was found to be equal to 7 by fitting the calculated and observed latent heat fluxes and NEE); however, this improvement appeared to be negligible.

3.2. Application to a jack pine forest

The BOREAS data for the jack pine forest near Nipawin (Saskatchewan, Canada, (SSA–OJP)),

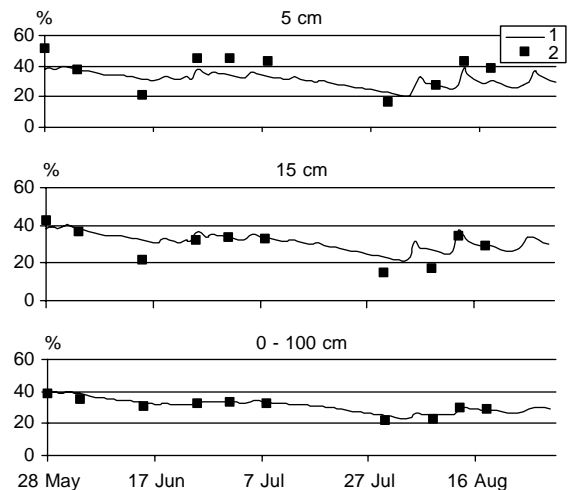


Fig. 2. Simulated (1) and measured (2) volumetric soil moisture percentage at the depths 5, 15 cm and in the 0–100 cm layer (FIFE, 4439 site).

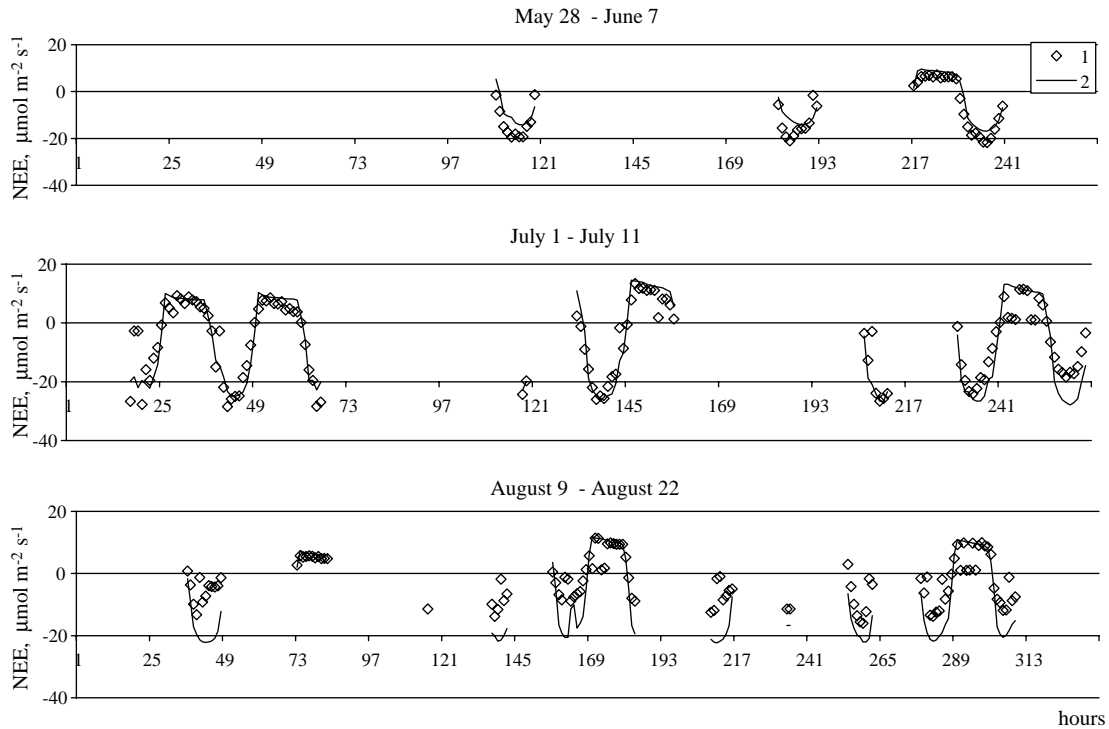


Fig. 3. Comparison of measured (1) and simulated (2) hourly values of NEE (FIFE, 4439 site).

during the period from May 24 to September 15 1994 were used. At this site, the total period of gaps in measurements of heat fluxes is about 10% of the total observational period and the corresponding period for CO₂ fluxes measurements is about 15% of the observational period.

The site is relatively flat with a mean slope of 3.5%. The mean height of the canopy is about 13.5 m. The leaf area index is estimated to vary between 1.9 and 2.2. The understory vegetation is sparse. The soil is a coarse-textured well-drained sand, containing little carbon and nitrogen.

Water vapor and sensible heat fluxes of the jack pine site were measured using two eddy flux systems. The first eddy measurement system was mounted above the forest on a three-scaffold tower. The sensors were placed on a boom 20 m above the ground. The second eddy flux system was positioned near the floor of the canopy, and the instruments were mounted 1.8 m above the ground. Soil moisture measurements were made by a neutron probe sensor. Details on the forest site measurement instrumentation and available

information are reported in Baldocchi et al. (1997); Newcomer et al. (2000).

Most model parameters were measured, some were taken from publications, parameters r_0 and r_{ag} were calibrated, the measurements of the latent heat fluxes and parameters α and V_{max} were calibrated against the measurements of CO₂ fluxes (α and V_{max}) during the period from 24 May to 20 June (Table 2). To calculate the soil respiration R_s , the empirical relationship based on the CO₂ flux and soil temperature measurements at night was fitted by the following equation: $R_s = 0.685 \exp(0.059T_g)$

To calculate the soil moisture characteristics, the relationships suggested by van Genuchten were applied

$$\psi(\theta) = \frac{1}{\lambda} \left(\left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{-1/m} - 1 \right)^{1/m}, \quad (30)$$

$$K(\theta) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{0.5} \left(1 - \left(1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{1/m} \right)^m \right)^2, \quad (31)$$

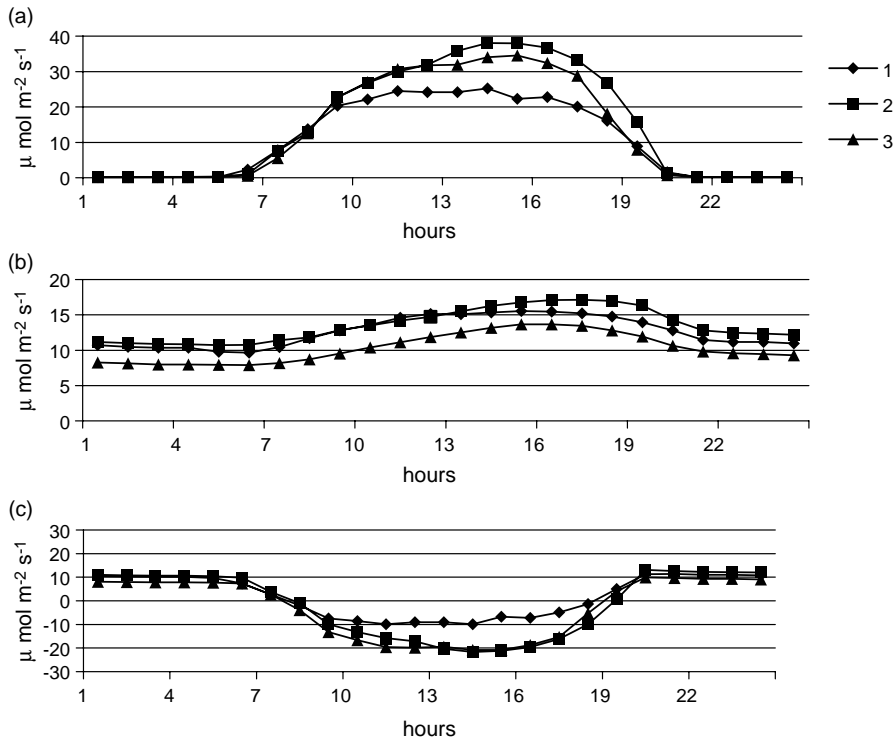


Fig. 4. Simulated mean diurnal patterns of canopy photosynthesis rates (a), soil and plant respiration rates (b) and NEE (c) for the periods: 1, May 28–June 3; 2, July 1–July 7; 3, August 9–August 15 (FIFE, 4439 site, 1987 year).

$$D(\theta) = \frac{K_s(1-m)}{\lambda m(\theta_s - \theta_r)} \left[\left(1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{(1/m)} \right)^{-m} + \left(1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{(1/m)} \right)^m - 2 \right] \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{(m-2/2m)}, \quad (32)$$

where λ is the pore distribution index, $m = 1 - 1/n$, n is a fitting constant. The stomatal resistance was calculated using relationship (4).

Fig. 5 presents the measured and calculated hourly latent heat fluxes for three 7-day periods at the beginning, in the middle, and at the end of the field observational campaign. The coefficient of determination between the measured and calculated hourly latent heat fluxes for the entire observational campaign is 0.49; for three-hourly values, this coefficient is 0.53.

The measured and calculated values of the volumetric soil moisture content for the first month of observations (before a long break in the soil moisture measurements) are shown in Fig. 6.

Fig. 7 shows the comparison of the measured and calculated hourly values of the net CO₂ exchange in the ecosystem for the same periods as in Fig. 5. The coefficient of determination between these values for entire field observational campaign is 0.41 for 1-h time interval and 0.52 for 3-h time interval.

The calculated net leaf photosynthesis was also used to try to improve the accuracy of the model by using the relationship (5) instead of (4) for calculation of the stomatal resistance. This attempt largely improved the results of calculation of evapotranspiration (at $\alpha = 14$ the coefficient of determination of the hourly values increased to 0.57) and did not actually improve the results of calculation of NEE. As can be seen from Figs. 5–7, the simulated values of latent heat fluxes, soil moisture content, and net CO₂ exchange in the ecosystem are consistent with the corresponding observed data quite well; however, the coefficients of determination of simulated and measured values are relatively low. Discrepancies

Table 2
Parameters used in the model (BOREAS-1994, OJP)

Parameter	Units	Values
The measured parameters		
Saturated hydraulic conductivity, K_s	$m\ s^{-1}$	0.168×10^{-4}
Soil porosity, θ_s	$m^3\ m^{-3}$	0.40
Soil moisture at field capacity, θ_{fc}	$m^3\ m^{-3}$	0.30
Residual soil moisture content, θ_r	$m^3\ m^{-3}$	0.03
Pore size distribution index, λ (van Genuchten, 1980)	m^{-1}	7.8
Parameter n (van Genuchten, 1980)	–	1.56
Exchange coefficient for canopy, C_E	–	0.016
The fraction of precipitation intercepted by vegetation, U_k	$m^2\ m^{-2}$	0.78
Plant area index, LAI_c	$m^2\ m^{-2}$	3.0
Leaf area index, LAI	$m^2\ m^{-2}$	2.0
The parameters taken from publications		
Emissivity of canopy and soil, ε	–	0.98
Parameter k_1	m^{-1}	2.5
Parameter $b_k \rho_0$	m^{-2}	1000
Parameter μ	m	0.2×10^{-3}
Parameter γ	Wm^{-2}	30
The calibrated parameters		
Minimum stomatal resistance, r_0	$s\ m^{-1}$	400
Aerodynamic resistance of the soil to evaporation, r_{ag}	$s\ m^{-1}$	600
Maximum carboxylation rate, V_{max}	$\mu mol\ CO_2\ m^{-2}\ s^{-1}$	43
Quantum efficiency, α	$mol\ CO_2(mol\ PAR\ photons)^{-1}$	0.004

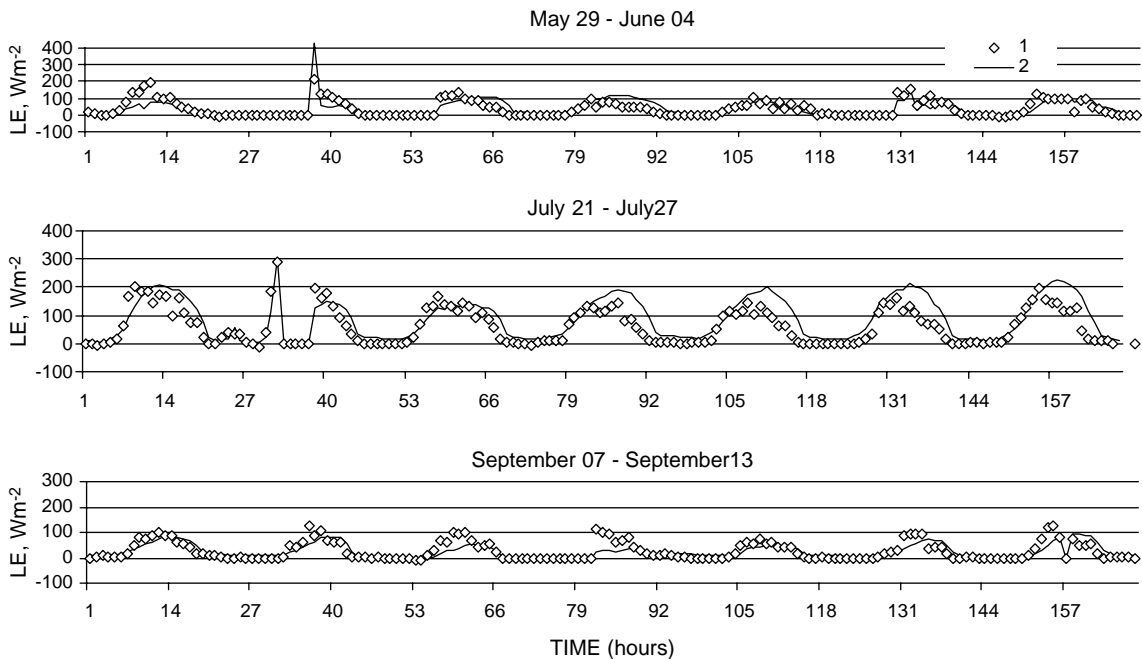


Fig. 5. Comparison of measured (1) and simulated (2) hourly latent heat fluxes (BOREAS, SSA OJP site).

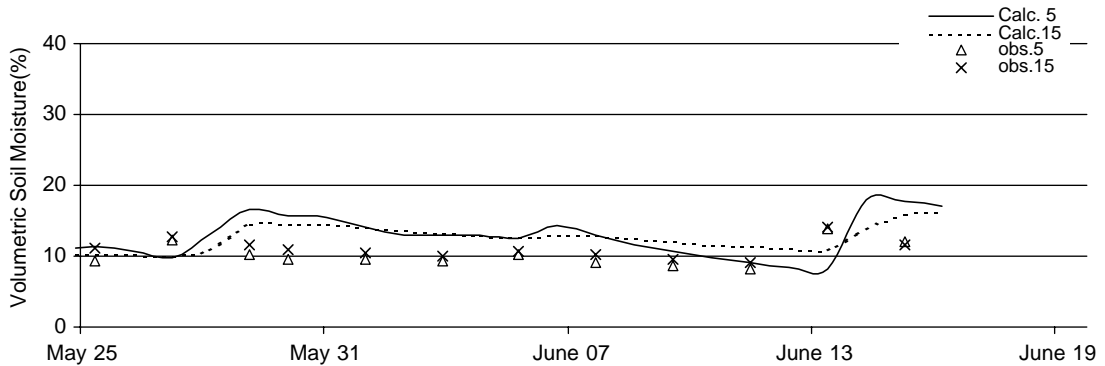


Fig. 6. Measured and simulated volumetric soil moisture percentages at the depths 5 and 15 cm (BOREAS, SSA OJP site).

between simulated and measured values can be explained by the horizontal non-homogeneity and stochastic variability of air and fluxes over the forest as well as gaps in data series and large absolute errors of eddy covariance flux measurements at small magnitudes of the measured values. To reduce the stochastic variability of eddy flux measurements in the BOREAS data, Baldocchi et al. (2001) recommended bin-averaging by hour for 2-weeks periods of eddy flux data. Applying this procedure gives the coefficient of determination between the measured

and calculated hourly latent heat fluxes of 0.78 and that between the measured and calculated hourly net ecosystem CO_2 of 0.79. In spite of significant differences in the measured and calculated values of latent heat fluxes and net CO_2 exchanges for short intervals, the differences between the sums of these values for the entire observational period are small enough (about 1% for the sum of the latent heat fluxes and about 4% for the sum of the net CO_2 exchange).

Fig. 8 shows the diurnal courses of the simulated canopy photosynthesis rates, the sum of soil and plant

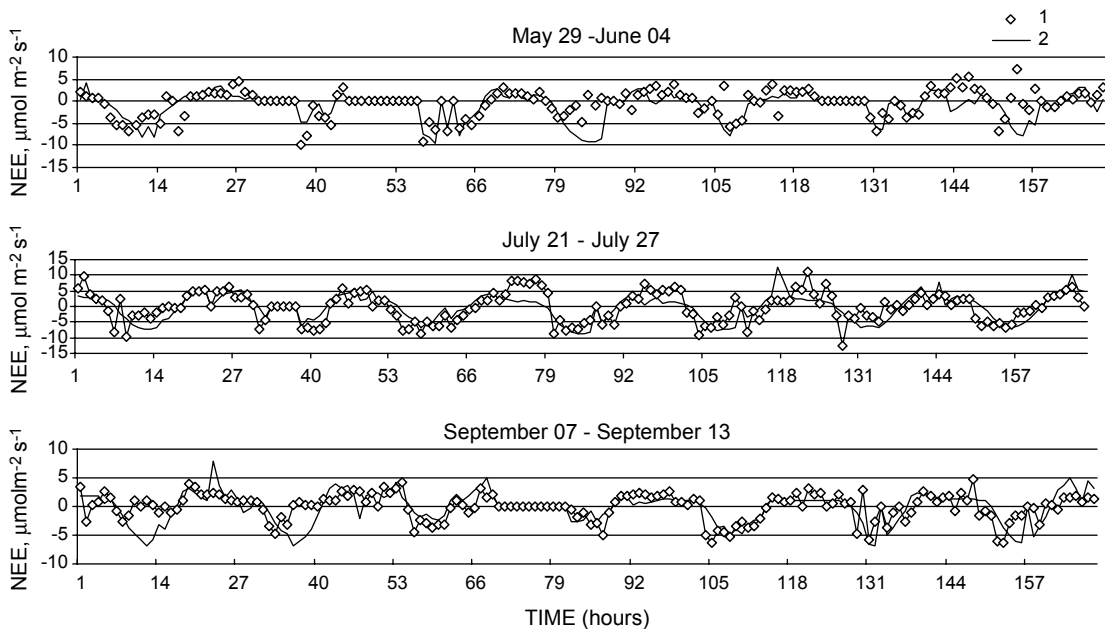


Fig. 7. Comparison between measured (1) and simulated (2) hourly values of NEE (BOREAS, SSA OJP site).

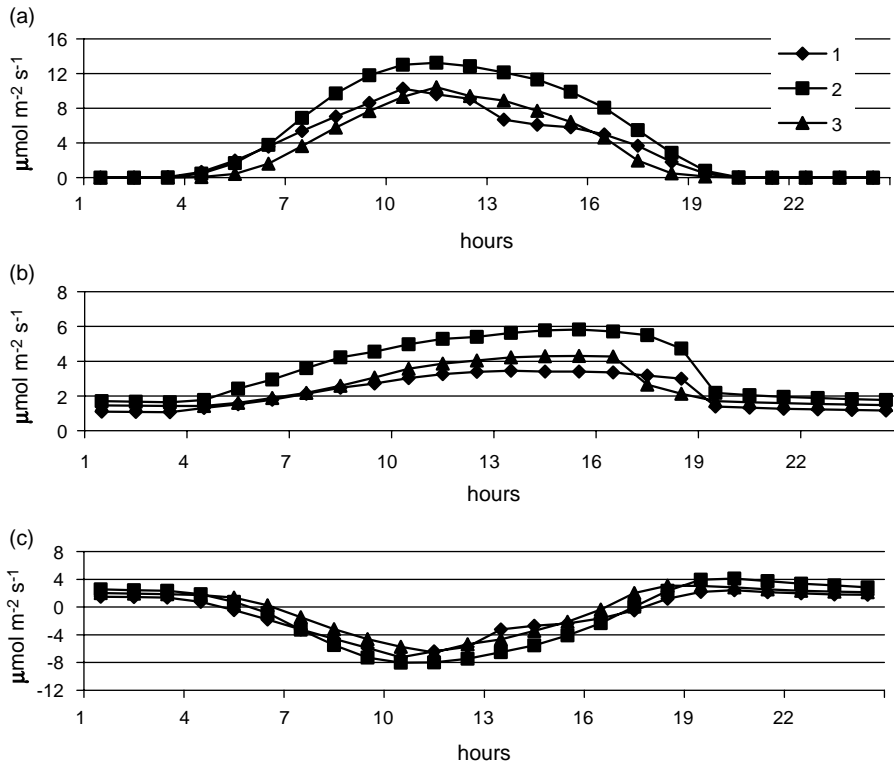


Fig. 8. Simulated mean diurnal patterns of canopy photosynthesis rates (a), soil and plant respiration rates (b) and NEE (c) for the periods: 1, May 29–June 4; 2, July 21–July 27; 3, September 7–September 13 (BOREAS, SSA OJP site, 1994 year).

respiration, and NEE averaged over the periods from May 29 to June 4, from July 21 to July 27, and from September 7 to September 13, respectively. The amplitudes of these values are not only smaller than those for the FIFE data, but diurnal courses are also well expressed.

3.3. Application to a deciduous forest site

The measurements in a mixed temperate deciduous forest in Oak Ridge, Tennessee, from 20 May to 31 August 1997 and 1998 were used. The dominant species of this forest includes oak, maple and tulip poplar. The age of the trees ranges from 60 to 120 years and the mean height is about 26 m; LAI ranges from 4 to 6. The dominant soil is silt loam.

The eddy covariance instruments for measurements of heat, moisture and CO_2 fluxes operated on a scaffold tower 36.9 m above the surface, which is on an average 10 m above the canopy. The atmospheric

CO_2 concentrations were measured at four heights (0.75, 9.1, 21.7 and 36.9 m). The soil moisture and the water potential were measured each 10–15 days at depths varying from 0 to 35 and 35 to 60 cm using gravimetric method.

As for the grassland and pine sites, most model parameters were evaluated based on measurement data and six parameters were taken from the literature. To calculate the soil characteristics, Eqs. (26)–(28) were applied.

Unfortunately, we could not find in the literature the soil moisture constants for the site under consideration, except the porosity (0.45) and the percentage of clay particles (9%). Using this constants and recommendations in (Clapp and Hornberger, 1978), we assigned the value of saturated hydraulic conductivity K_s . The parameters ψ_s and b were determined by approximating the empirical relationship between the water potential and the soil moisture content by Eq. (26). The values of constants r_0 , r_{ag} , α

Table 3
Parameters used in the model (Oak Ridge, Walker Branch)

Parameter	Units	Values
The measured parameters		
Saturated hydraulic conductivity, K_s	m s^{-1}	0.579×10^{-5}
Soil water potential at saturation, θ_s	$\text{m}^3 \text{m}^{-3}$	0.45
Soil moisture at field capacity, θ_{fc}	$\text{m}^3 \text{m}^{-3}$	0.34
Residual soil moisture content, θ_r	$\text{m}^3 \text{m}^{-3}$	0.07
Saturation suction, ψ_s	m	-0.2
Parameter b	-	5.0
Exchange coefficient for canopy, C_E	-	0.016
The fraction of precipitation intercepted by vegetation, U_k	$\text{m}^2 \text{m}^{-2}$	0.87
Plant area index, LAI_c	$\text{m}^2 \text{m}^{-2}$	5.0
Leaf area index, LAI	$\text{m}^2 \text{m}^{-2}$	4.0
The parameters taken from publications		
Emissivity of canopy and soil, ε	-	0.98
Parameter k_1	m^{-1}	2.5
Parameter $b_k \rho_0$	m^{-2}	1000
Parameter μ	m	0.20×10^{-3}
Parameter γ	Wm^{-2}	30
The calibrated parameters		
Minimum stomatal resistance, r_0	s m^{-1}	300
Aerodynamic resistance of the soil to evaporation, r_{ag}	s m^{-1}	600
Maximum carboxylation rate, V_{\max}	$\mu\text{mol CO}_2 \text{m}^{-2} \text{s}^{-1}$	40
Quantum efficiency, α	$\text{mol CO}_2(\text{mol PAR photons})^{-1}$	0.007

and V_{\max} were assigned as a result of calibration of the model against the measurements of moisture and CO_2 fluxes for the period from 20 May to 31 August 1997. The values of the parameters used in calculations are presented in Table 3.

The soil respiration was calculated using the empirical dependence received for the site under consideration in (Wilson and Baldocchi, 2001).

The comparison of the measured and simulated latent heat fluxes for three 7-day intervals characterizing the hydrometeorological and biophysical conditions at the initial period of observations (from 27 May to 2 June), the middle period (from 3 June to 9 July) and the final period (from 31 July to 6 August) is presented in Fig. 9.

The coefficient of determination between the measured and simulated latent heat fluxes is 0.72 for the period from 20 May to 31 August 1997 and 0.64 for the same period of 1998.

The comparison of the measured and simulated values of soil moisture in the soil layer from 0 to 35 cm and in the layer from 37 to 70 cm for the periods from 20 May to 31 August 1997 and 1998 is presented in Fig. 10.

Fig. 11 shows the measured and simulated net ecosystem exchanges of carbon dioxide for periods from 20 May to 31 August 1997 and 1998. The coefficients of determination between these two variables are 0.76 and 0.72 for 1997 and 1998, respectively. The integrated values of the measured and simulated latent heat fluxes and NEE are shown in Fig. 12.

The application of the relationship (5) with $a=7$ for the calculation of stomatal resistance slightly improved the results of simulations of the latent heat fluxes (the coefficient of determination increased from 0.64 to 0.71); however, the accuracy of simulations of the NEE did not change.

Most probably a better performance of the presented model for the deciduous forest than for the pine forest is explained by the better quality of measurements and the significantly larger values of the latent heat fluxes and NEE. The ecosystem of deciduous forest took up from atmosphere for the period from May to August 600 gC m^{-2} of CO_2 while the ecosystem of pine forest took up for the same period only 50 gC m^{-2} of CO_2 .

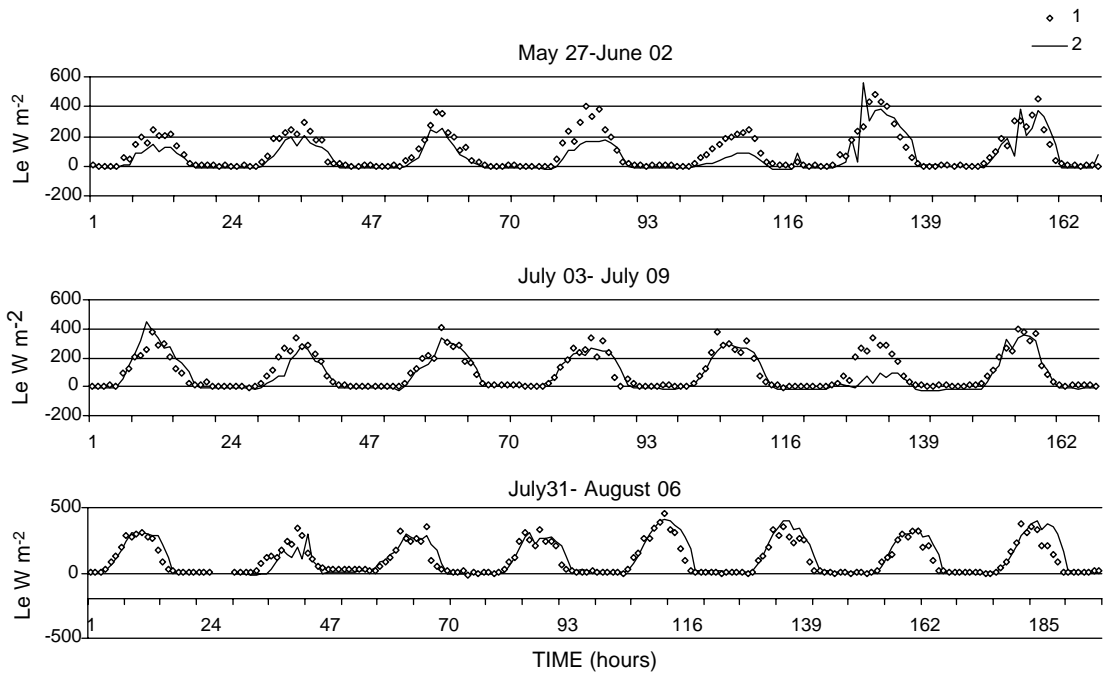


Fig. 9. Comparison of measured (1) and simulated (2) hourly latent heat fluxes (Oak Ridge, Walker Branch site).

4. Numerical experiments

To evaluate the qualitative behavior and predictive capability of the developed model, two series of numerical experiments were carried out. The first series addressed the assessment of the influence of soil

moisture on transpiration and NEE. The input hydro-meteorological data measured at the FIFE grassland from 28 May to 30 August 1987, and the BOREAS jack pine forest site from 24 May to 15 September 1994 and at the Oak Ridge deciduous forest from 20 May to 31 August 1998 were used to calculate the total

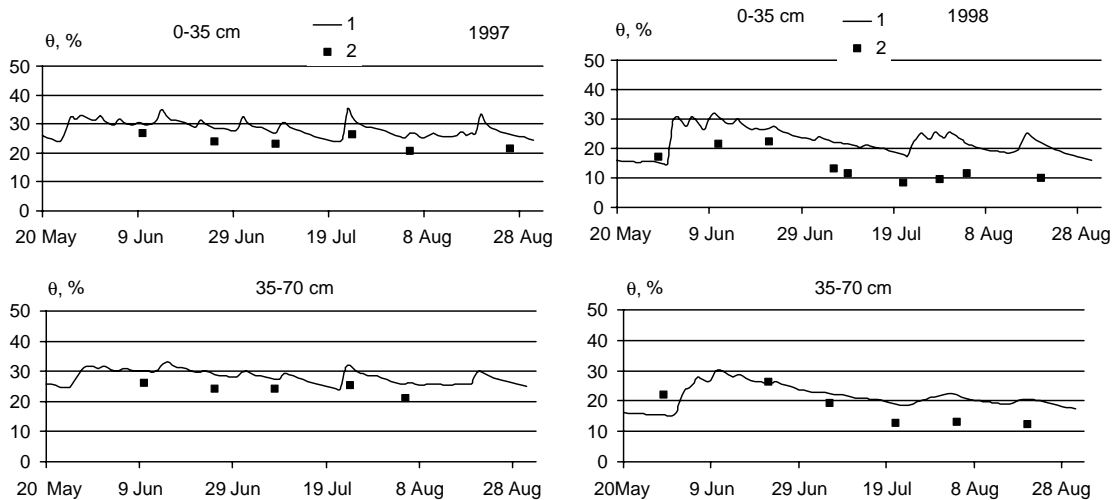


Fig. 10. Simulated (1) and measured (2) volumetric soil moisture percentages for the layers 0–35 and 35–70 cm (Oak Ridge, Walker Branch site).

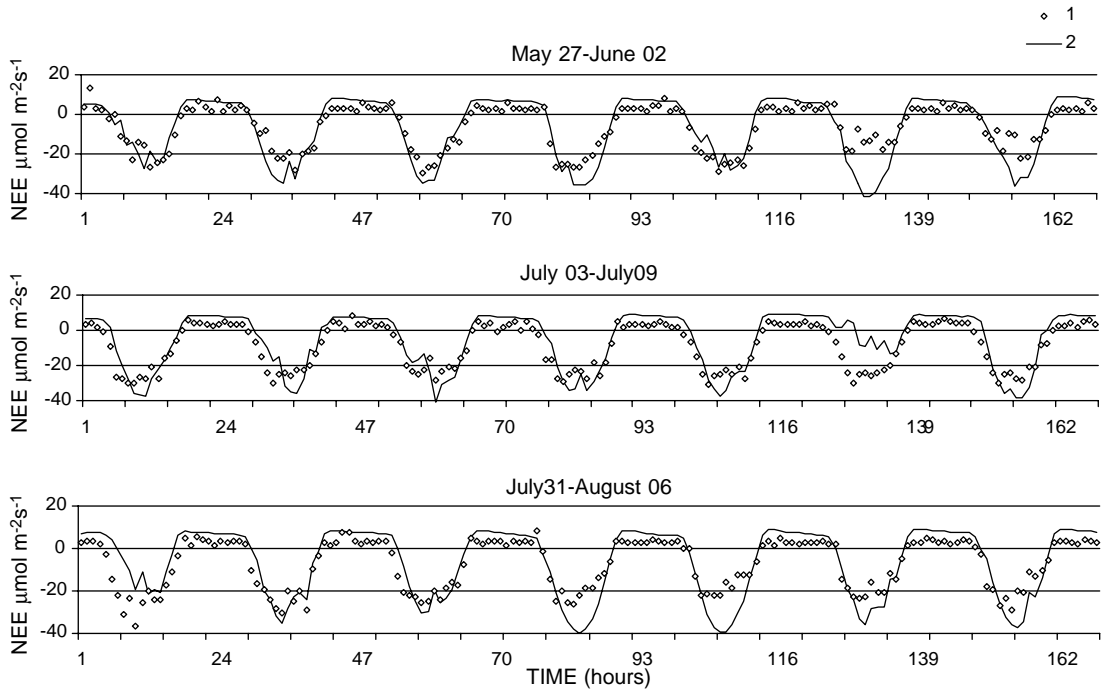


Fig. 11. Comparison of measured (1) and simulated (2) hourly values of NEE (Oak Ridge, Walker Branch site).

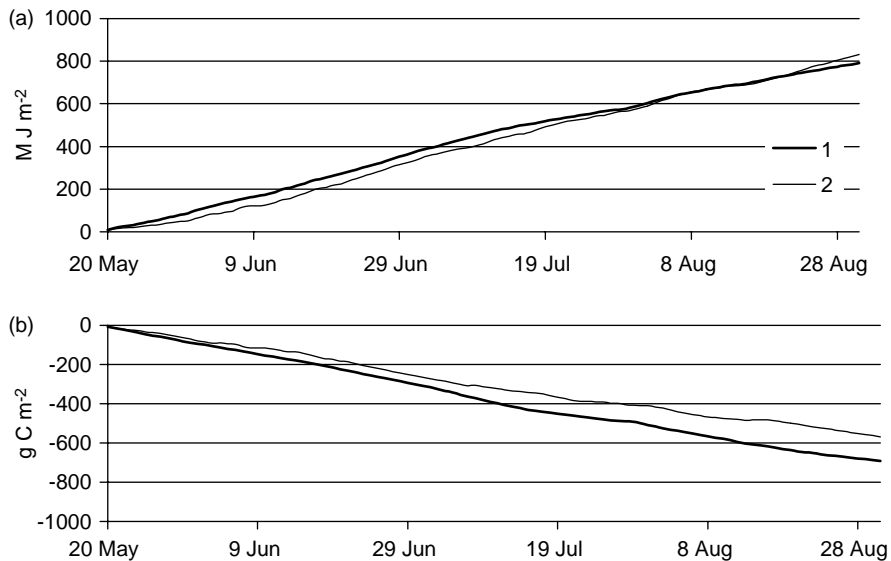


Fig. 12. Comparison of measured (1) and simulated (2) total daytime latent heat fluxes (a) and NEE (b) (Oak Ridge, Walker Branch site, 1998 year).

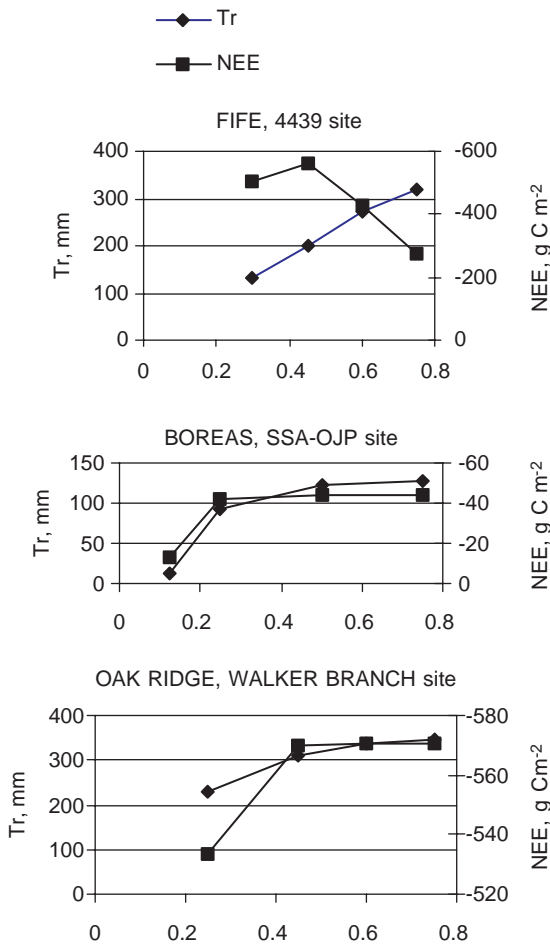


Fig. 13. Effects of the initial soil moisture content (θ/θ_{max}) on the total transpiration and the total NEE.

transpiration and the total NEE for these periods at different initial soil moisture contents. The total transpiration of grass vegetation almost linearly grows with increasing initial soil moisture content (Fig. 13).

Table 4

Direct impact of possible change of atmospheric CO₂ content and increasing air temperature on transpiration and NEE

N exp	FIFE, 4439 site		BOREAS, SSA OJP site		Oak Ridge, Walker Branch site	
	Tr, mm	NEE, $g\ C\ m^{-2}$	Tr, mm	NEE, $g\ C\ m^{-2}$	Tr, mm	NEE, $g\ C\ m^{-2}$
1	329	-286	105	-44	286	-569
2	171	-309	53	-45	148	-572
3	196	-342	57	-11	162	-522

Calculated transpiration and NEE for the chosen periods: (1) at the measured hydrometeorological values; (2) at the measured hydrometeorological values and a twofold of the atmospheric CO₂ concentration; (3) at a twofold of the CO₂ concentration and a 2 °C increase of air temperature.

However, the NEE slightly increases from $\theta/\theta_{max} = 0.3-0.4$ and after that an increase in soil moisture leads to a decrease in NEE. The main cause of this decrease is the growth of soil respiration. For the pine and deciduous forests, a considerable growth in transpiration and NEE caused by increasing soil moisture is observed only at small values of soil moisture content.

In the second series of numerical experiments, the sensitivity of transpiration and NEE to possible increases in atmospheric CO₂ concentration and air temperature variations were estimated. The total measured values of transpiration and NEE for the same periods, as in the first series of numerical experiments, were compared with the corresponding calculated values of transpiration and NEE, assuming a two-fold increase in the atmospheric CO₂ concentration separately or simultaneously with a 2 °C growth of air temperature (the most probable scenario of climate change to the end of this century). The results of these numerical experiments are presented in Table 4. As can be seen from this table, a two-fold increase in CO₂ concentration leads to an almost two-fold decrease in transpiration for all three ecosystems. However, a simultaneous two-fold increase in CO₂ concentration and a 2 °C growth in air temperature can give a decrease in transpiration of about 30% (these results are close to calculations carried out in Kuchment and Startseva, 1991). The change in the total NEE at a two-fold increase in atmospheric CO₂ concentration is insignificant. In the case of a simultaneous two-fold increase in CO₂ concentration and 2 °C growth of air temperature, the assimilation of CO₂ increases in the grass ecosystem and decreases in the forest ecosystems. It can be caused by different sensitivity of soil respiration to air temperature.

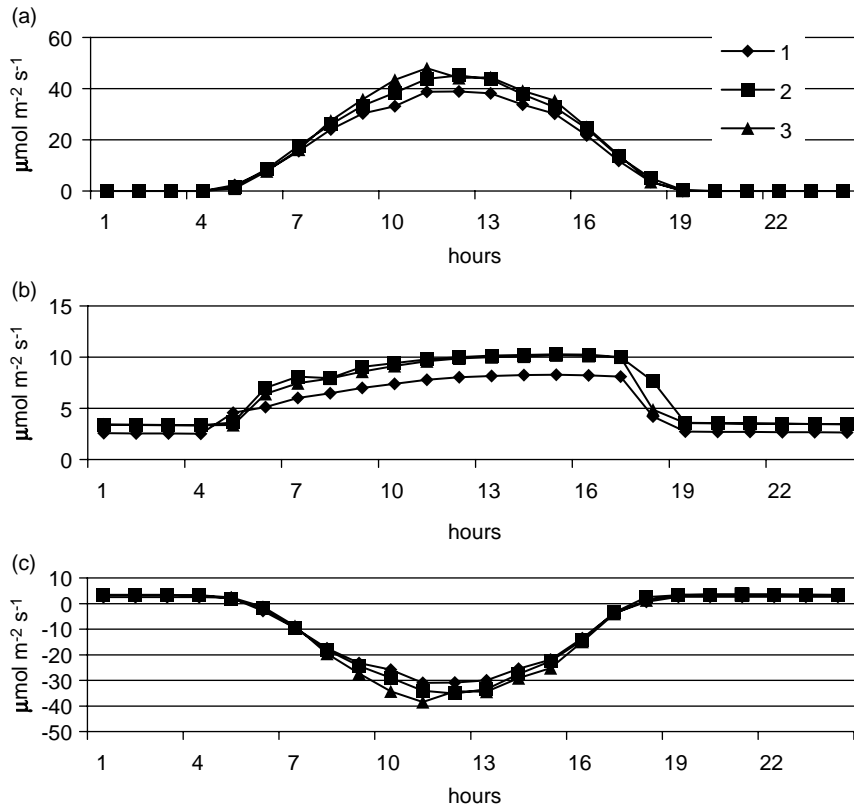


Fig. 14. Simulated mean diurnal patterns of canopy photosynthesis rates (a), soil and plant respiration rates (b) and NEE (c) for the periods: 1, May 27–June 2; 2, July 3–July 9; 3, July 31–August 6 (Oak Ridge, Walker Branch site, 1998 year).

5. Discussion

According to Lloyd et al. (1997), the error of eddy covariance flux measurements for homogeneous steppe areas is about 20%. For the forest area with pronounced horizontal non-homogeneity, the errors of these measurements may reach 30%. As can be seen from comparisons of the measured and simulated values of soil moisture content, latent heat fluxes, and net CO_2 exchanges, presented in Figs. 1–12 and 14, the developed model gives in general, the accuracy of the same order as the accuracy of eddy covariance flux measurements and provides reasonably realistic simulation of the variables under consideration. The best results were obtained in the simulation of the broadleaved deciduous forest ecosystem with an intensive CO_2 exchange, where continuous long series measurements were available. The model also gives

qualitatively reasonable mean diurnal patterns of net photosynthesis, and respiration rates and NEE.

6. Conclusion

The presented model describes the interaction between heat, water, and carbon exchanges in the soil–vegetation–atmosphere system taking into account the dependence of the stomatal resistance on atmospheric, soil moisture and physiological factors, photosynthesis and plant and soil respiration. The model includes only four parameters to be calibrated. The test of the model against experimental data has shown in general a good agreement between measured and simulated water and carbon fluxes. The numerical experiments carried out using the presented model have shown

that the model can be applied for predicting ecosystem responses to changes in atmospheric CO₂ content and soil moisture. There are several simplifications of the modeled processes, which can be easily refined if the observational data series are available for calibration of additional parameters. The improvements of the model seem necessary, first of all, for a more detailed description of the transfer from the leaf photosynthesis and leaf respiration model to the canopy carbon dioxide cycle model, subdivision accounting for change of radiation balance inside the canopy, as well as application of a perceptual model of soil respiration instead of empirical relationships.

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