

# COUPLED MODELING WATER VAPOR AND CARBON DIOXIDE FLUXES IN THE SOIL-VEGETATION-ATMOSPHERE SYSTEM

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## Summary

The chapter summarizes the different modeling approaches that have been developed for simulation of H<sub>2</sub>O and CO<sub>2</sub> exchange between soil, vegetation and the atmosphere. The main attention was paid to parameterizations for photosynthesis, respiration and transpiration of leaves, coupling of leaf photosynthesis with stomatal conductance, as well as for scaling procedure from individual leaf up to the entire plant canopy. Additionally, the modeling approaches for description of precipitation, interception and storage by a plant canopy, root water uptake, soil water exchange, and heterotrophic and autotrophic soil respiration were considered, too. Described parameterizations have a different level of complexity (e.g. model dimensionality, number of plant canopy layers), require different amount of input data and may be applied for simulation of the H<sub>2</sub>O and CO<sub>2</sub> fluxes in different temporal (from an hour to years) and spatial (from individual leaf and an ecosystem, to region and the entire globe) scales.

A coupling algorithm for H<sub>2</sub>O and CO<sub>2</sub> exchange parameterization in SVAT models considers the leaf stomatal conductance as a key parameter controlling the diffusion rate

of H<sub>2</sub>O and CO<sub>2</sub> between leaves of plants and the ambient air. It is assumed that stomatal conductance depends on biophysical and biochemical properties of the leaves and on environmental conditions (e.g. solar radiation, air temperature, water vapor deficit in the air), and it may be described by a linear function of photosynthesis rate, ambient air CO<sub>2</sub> concentration and air humidity. For description of the air humidity control in the models both air relative humidity and water vapor pressure deficit are used.

The coupled H<sub>2</sub>O and CO<sub>2</sub> exchange models may be successfully used to describe adequately the spatial and temporal patterns of H<sub>2</sub>O and CO<sub>2</sub> fluxes, to quantify the response of the water and carbon budgets for the different vegetation types to changes of environmental conditions and, especially, to CO<sub>2</sub> atmospheric enrichment and global warming.

## 1. Introduction

Photosynthesis, respiration and transpiration are most important biophysical processes determining the carbon and water budgets of land surface. During the photosynthesis the plants transform water, carbon dioxide (CO<sub>2</sub>) and minerals into oxygen (O<sub>2</sub>) and organic compounds using absorbed solar PAR. Respiration is accompanied by oxygen consumption (oxidation of sugars) in the plants and by release of CO<sub>2</sub> and water. CO<sub>2</sub> for photosynthesis reactions is obtained from the air that enters the leaves through the stomata and diffuses to the cells containing chlorophyll. The water is absorbed by the plant roots from the soil and carried to the leaves through the xylem. Some water is transpired into the atmosphere. The flow of water from soil to air via plant tissues follows a water potential gradient. Coming in leaves water provides the leaf moisture necessary for the diffusion of CO<sub>2</sub> into and oxygen out of these cells, and brings dissolved mineral elements required for biochemical reactions and plant growth.

Diffusion of CO<sub>2</sub> and H<sub>2</sub>O between leaves and ambient air is mainly controlled by leaf stomatal conductance that is strongly depended on environmental conditions (solar radiation, air temperature, water vapor deficit in the air), water status of the leaves and available in plants nutrients. Accurate parameterization of this parameter and its relationships with photosynthesis, respiration and transpiration rates should be, obviously, a key element of any mathematical model developed for description of land-atmosphere interaction and modeling of H<sub>2</sub>O and CO<sub>2</sub> between vegetation and the atmosphere. It is obvious that parameterizations of such processes in mathematical models should be based on universal coupled approaches taking into account both physical and biological mechanisms in plants influencing the leaf stomata opening and CO<sub>2</sub> and H<sub>2</sub>O exchanges.

The first biophysical H<sub>2</sub>O and CO<sub>2</sub> transfer models were developed as parts of complex agricultural crop models and based on separate description of the response of photosynthesis, transpiration and stomatal conductance to environmental conditions. The new generation of biochemical H<sub>2</sub>O and CO<sub>2</sub> exchange models are focused on coupled description of H<sub>2</sub>O and CO<sub>2</sub> exchange processes, and they were developed, first of all, to describe and quantify possible effects of CO<sub>2</sub> atmospheric enrichment and global warming on biological and chemical processes in vegetation cover and on their

impact on energy and water budgets of land surface (e.g. Farquhar et al. 1980, Ball et al. 1987, Collatz et al. 1991, Leuning 1995, Sellers et al. 1997). Most attention in these models is paid to simulation of the photosynthesis, respiration and CO<sub>2</sub> fluxes between soil, vegetation and the atmosphere, and they assume a close coupling of the photosynthesis and stomatal conductance. The leaf photosynthesis in the models is usually described as a function of kinetics of the carboxylating enzyme Rubisco, electron transport, and the efficiency of the leaf light-intercepting apparatus (Farquhar et al. 1980).

A complexity of the developed coupled photosynthesis-transpiration models ranges widely and is determined by many different factors, like required prediction accuracy, spatial and temporal resolutions, properties of a vegetation cover, availability of input parameters for model calculations. In most simplified aggregated “big-leaf” models the vertical heterogeneity and structure of vegetation canopy are ignored and the aerodynamic and biological properties of the whole vegetation canopy are assumed to be equal the properties of a single leaf. These models don't need many input parameters but these parameters at the canopy level cannot be measured directly, nor defined as the arithmetic mean of leaf-level parameters because of processes nonlinearity. More sophisticated “multi-layer” SVAT models integrate the fluxes from each canopy layer to give the total flux and require obviously more input parameters with detailed information about vegetation structure and the spatial distribution of key biophysical properties of vegetation.

It is obvious, that a prediction of the total H<sub>2</sub>O and CO<sub>2</sub> fluxes in global and regional scales can be precisely enough using even simplified modeling approaches based on minimal amount of input information and on simplified parameterization of vegetation cover (e.g. one-layer “Big-leaf” models). The H<sub>2</sub>O and CO<sub>2</sub> fluxes in local (ecosystem) scale between short vegetation (e.g. grassland, some agricultural crops) with a very simplified and homogeneous structure and the atmosphere can be, in general, also very successfully simulated using similar simple models. On the other hand, modeling the energy, H<sub>2</sub>O and CO<sub>2</sub> exchanges between vertically structured vegetation cover (e.g. forest) and the atmosphere needs usually more sophisticated approaches allowing to take into account vertical heterogeneity and species composition of forest canopy, as well as to describe both the total fluxes and flux partitioning between different layers and species in a forest canopy and soil.

## **2. Modeling H<sub>2</sub>O and CO<sub>2</sub> Exchange at a Leaf Scale**

### **2.1. Leaf Photosynthesis**

Most of photosynthesis models for individual leaf are based on parameterization describing enzyme kinetics and diffusion of CO<sub>2</sub> between ambient air and leaf chloroplasts. The leaf photosynthesis rate is mainly affected by incoming and absorbed PAR, air and leaf temperatures, water vapor deficit in the air, soil moisture and available soil nutrients. Biotic factors affecting photosynthesis include growth form (e.g. herbaceous or woody, evergreen or deciduous), leaf type (e.g. leaves or needles), photosynthetic pathway (C<sub>3</sub>, C<sub>4</sub>, CAM) and longevity (annual or perennial). The supply of CO<sub>2</sub> to a leaf is determined by the concentration of CO<sub>2</sub> in the atmosphere and by diffusion through the leaf boundary layer and stomatal pores.

A photosynthesis rate in its most simple diffusion formulation can be written as

$$A_1 = \frac{(C_a - C_i)}{(r_{aCO_2} + r_{sCO_2})}$$

where  $C_a$  – ambient CO<sub>2</sub> concentration;  $C_i$  – leaf intercellular CO<sub>2</sub> concentration;  $r_{aCO_2}$  – boundary layer resistance of leaf for CO<sub>2</sub>; and  $r_{sCO_2}$  – leaf stomatal resistance for CO<sub>2</sub>.

The chemical processes of CO<sub>2</sub> fixation in the leaf may be described using the Michaelis-Menten equation:

$$A_1 = \frac{A_{1cmax}}{(1 + K/C_c)}$$

Where  $C_c$  – concentration of CO<sub>2</sub> in chloroplasts;  $A_{1cmax}$  – maximal photosynthesis rate of the leaf under saturated  $C_c$ ;  $K$  – the Michaelis-Menten constant.

The dependence of leaf photosynthesis on incoming PAR as well as on some other environmental parameters may be described using an empirical equation:

$$A_1 = \frac{\alpha \cdot PAR \cdot A_{1max}}{(\alpha \cdot PAR + A_{1max})} \cdot f(T_1) \cdot f(D_a) \cdot f(\phi_1)$$

where  $A_{1max}$  - maximal photosynthesis rate at saturated PAR;  $f(T_1)$ ,  $f(D_a)$ ,  $f(\phi_1)$  – empirical functions describing dependences of photosynthesis rate on leaf temperature, water vapor pressure deficit in the air, and leaf water potential, respectively.

A biochemical model for photosynthesis of C<sub>3</sub> plants suggested by Farquhar (Farquhar et al., 1980, 2001) assumes that leaf photosynthesis ( $A$ ) is determined by the potential rate of Rubisco carboxylation ( $A_v$ ), and by the rate of CO<sub>2</sub> assimilation limited by the potential rate of ribulose-1,5 biphosphate regeneration, usually considered to be limited by the rate of electron transport ( $A_j$ ). Net CO<sub>2</sub> exchange between leaf and ambient air taking into account the mitochondrial respiration ( $R$ ) rate may be written as:

$$A = \min \{ A_v, A_j \} - R.$$

The initial slope of the relationship between  $A$  and CO<sub>2</sub> concentration in sub-stomatal air space ( $C_i$ ) can be considered as an area of  $A_v$  limitation of  $A$ .  $A_v$  can be described as:

$$A_v = V_{CM} \cdot \frac{(C_i - \Gamma^*)}{C_i + K_c \cdot (1 + O_i/K_o)} \quad , \text{ where } C_i > \Gamma^*$$

where  $V_{CM}$  is maximal carboxylation capacity of Rubisco for the leaf,  $\Gamma^*$  is compensation point,  $O_i$  is intercellular  $O_2$  concentration, and  $K_c$  and  $K_o$  are Michaelis coefficients of Rubisco for  $CO_2$  and  $O_2$ , respectively.

When the  $C_i$  is close to saturation for photosynthesis the  $A$  is limited mainly by  $A_j$  which can be written as:

$$A_j = \left( \frac{J}{4} \right) \cdot \frac{(C_i - \Gamma^*)}{(C_i + 2 \cdot \Gamma^*)}, \text{ where } C_i > \Gamma^*$$

where  $J$  is the rate of electron transport.  $J$  is related to incident photosynthetically active photon flux density ( $Q$ ) by the following equation (de Pury and Farquhar 1997, Medlin et al. 2002):

$$\Theta \cdot J^2 - (\alpha \cdot Q + J_M) \cdot J + \alpha \cdot Q \cdot J_M = 0$$

where  $J_M$  is the potential rate of electron transport,  $\Theta$  is curvature of light response curve, and  $\alpha$  is the quantum yield of electron transport.

The key parameters of the model are  $J_M$  and  $V_{CM}$  and they vary significantly among different plant species and depend strongly on atmospheric parameters (first of all, air temperature) and leaf nitrogen content.

The dependencies of  $J_M$  and  $V_{CM}$  on the temperature are usually parameterized using an equation that is based on the Arrhenius equation modified by a term that describe how conformational changes in the enzyme at higher temperatures start to negate the on-going benefits that would otherwise come from further increasing temperature (e.g. de Pury and Farquhar 1997). In general form it can be written as:

$$J_M, V_{CM} = J_{M(T=25^\circ C)}, V_{CM(T=25^\circ C)} \cdot \exp \left[ \frac{E_{a,J,V} \cdot (T - 298)}{298 \cdot R \cdot T} \right] \cdot \frac{1 + \exp \left( \frac{298 \cdot \Delta S_{J,V} - H_{d,J,V}}{298 \cdot R} \right)}{1 + \exp \left( \frac{T \cdot \Delta S_{J,V} - H_{d,J,V}}{T \cdot R} \right)}$$

where  $J_{M(T=25^\circ C)}, V_{CM(T=25^\circ C)}$  are values of  $J_M$  or  $V_{CM}$  at temperature  $25^\circ C$ ,  $\Delta S_{J,V}$  - an entropy factors for  $J_M$  or  $V_{CM}$ ,  $H_{d,J,V}$  - rates of decrease of the function above the optimum;  $E_{a,J,V}$  - activation energies for Arrhenius temperature responses for  $J_M$  or  $V_{CM}$ ,  $R$  - is the universal gas constant ( $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$ ) (Medlin et al. 2002).

Analysis of the ratios between  $J_M$  or  $V_{CM}$  at the reference temperature  $T = 25^\circ C$  showed that the ratio for different plant species is relatively constant and according to Medlin et al. (2002) may be well approximated by 1.67.

To derive effect of leaf nitrogen content on carboxylation capacity of Rubisco the models usually used linear parameterization:

$$V_{CM} = V_{CM} \cdot f(N_1) \quad f(N_1) = \chi \cdot (N_1 - N_b)$$

Where -  $\chi$  - the ratio of measured Rubisco capacity to leaf nitrogen ( $N_1$ ) and  $N_b$  - leaf nitrogen which is not associated with photosynthesis.

Some parameterizations take into account also effect of soil moisture lack on  $J_M$  or  $V_{CM}$ :  $J_M \cdot V_{CM} = J_M \cdot V_{CM} \cdot f(\Theta_s) \quad f(\Theta_s) = 1 / (1 + \exp(0.02 \cdot (\varphi_{wilt} - \varphi_s)))$  where  $\varphi_s$  - the soil water potential,  $\varphi_{wilt}$  - the soil water potential at wilting point.

The  $CO_2$  compensation point  $\Gamma^*$  (when photosynthetic uptake is equal to the leaf respiratory losses) in equations for  $A_v$  and  $A_j$  is estimated as

$$\Gamma^* = \frac{K_c \cdot V_{OM} \cdot O_i}{(2 \cdot K_o \cdot V_{CM})}$$

where  $V_{OM}$  - oxygenation capacities of leaf Rubisco.

The  $K_c$  and  $K_o$  constants are strongly depended on the temperature and can be well derived using the Arrhenius equation (de Pury and Farquhar 1997):

$$K_{c,o} = K_{c,o(T=25^\circ C)} \cdot \exp\left[\frac{E_a \cdot (T - 298)}{298 \cdot R \cdot T}\right]$$

where  $E_a$  - activation energy for the Arrhenius temperature responses for  $K_{c,o}$ .

For simulation of the photosynthesis rate of  $C_4$  plants Collatz et al (1992) suggests to use approach based on Farquhar model (1980) for  $C_3$  plants. The approach takes into account both biophysical and biochemical processes in the leaf and describes photosynthesis as a smoothed minimum of three limiting rates: the potential rate of Rubisco carboxylation ( $A_v$ ), the amount of available light ( $A_E$ ), and the PEP-carboxylase limitation ( $A_p$ ). According to Collatz et al. (1992) the equations for  $A_v$ ,  $A_E$  and  $A_p$  for  $C_4$  plants may be written in general form as:

$$A \approx \min \begin{cases} A_v = V_{CM} \\ A_E = \alpha \cdot (1 - \omega) \cdot PAR \\ A_p = 2 \cdot 10^4 \cdot V_{CM} \cdot \frac{C_i}{P_a} \end{cases}$$

where  $V_{CM}$  – temperature and nitrogen adjusted maximal carboxylation capacity of Rubisco for the leaf,  $\alpha$  - the quantum efficiency,  $\omega$  - leaf scattering coefficient,  $P_a$  – atmospheric pressure.

Photosynthesis rate is obtained from solution of two quadratic equations:

$$\beta_1 \cdot A_p^2 - A_p \cdot (A_v + A_E) + A_v \cdot A_E = 0$$

$$\beta_2 \cdot A^2 - A \cdot (A_{VE} + A_p) + A_{VE} \cdot A_p = 0$$

where  $A_{VE}$  - the smoothed minimum of  $A_v$  and  $A_E$ ,  $\beta_1 = 0.83$  and  $\beta_2 = 0.93$  - co-limitation coefficients.

## 2.2. Leaf Evaporation

Parameterization of leaf evaporation in the H<sub>2</sub>O/CO<sub>2</sub> exchange models are usually based on an integrating approach taking into account an equation of leaf energy balance

$$R_n = \lambda E + H + S$$

where  $R_n$  – net radiation of the leaf estimated as a sum of short-wave and long-wave radiation balance,  $\lambda E$ ,  $H$  – latent and sensible heat fluxes between leaf surface and the ambient air,  $S$  – storage term, and aerodynamic equations describing water vapor and sensible heat transfer between leaf and surrounding air:

$$E = \frac{1}{\lambda} \cdot \frac{\rho_a \cdot c_p \cdot (e_s^*(T_1) - e_a)}{\gamma \cdot (r_a + r_1)}; \quad H = \rho_a \cdot c_p \cdot \frac{(T_1 - T_a)}{r_a}$$

where  $\lambda$  - the latent heat of evaporation,  $\gamma$  - the psychrometric constant,  $\rho_a$  is the air density,  $c_p$  - the specific heat of the air,  $r_a$ ,  $r_1$  – aerodynamic and stomatal resistances of the leaves,  $e_a$  – air vapor pressure, and  $e_s^*(T_1)$  - vapor pressure of the air in leaf sub-stomatal cavity at saturation.

Substituting the assumption for  $e_s^*$  ( $e_s^*(T_1) \approx e_a^*(T_a) - \Delta \cdot (T_a - T_1)$ ) into equation for  $E$  and taking into account the equations of leaf energy balance and aerodynamic equation for  $H$  the final equation identifying the key abiotic and biotic factors that control leaf evaporation may be written in following form (the Penman-Monteith equation):

$$E = \frac{1}{\lambda} \cdot \frac{\Delta \cdot (R_n - S) \cdot \rho_a \cdot c_p \cdot (e_a^*(T_a) - e_a) \cdot g_a}{\Delta + \gamma \cdot (1 + g_a / g_1)}$$

where  $g_1$  – leaf stomatal conductance,  $g_a$  – leaf aerodynamic conductance,  $e_a^*(T_a)$  - vapor pressure of the air at saturation,  $\Delta$  - the slope of the saturation vapor pressure

curve evaluated at the air temperature,  $T_a$ ,  $T_l$  – air and leaf temperatures.

McNaughton and Jarvis (1983) reformulated the Penman–Monteith equation to incorporate the degree to which leaves are coupled to environmental conditions. Using a decoupling coefficient  $\Omega$ , that is the function of  $g_l$  and  $g_a$ , as well as a parameter describing the increase of latent heat content of the air per increase of sensible heat content of saturated air ( $\varepsilon = \Delta/\gamma$ )

$$\Omega = \frac{(\varepsilon + 1)}{(\varepsilon + 1) + (g_a/g_l)}$$

the Penman-Monteith equation may be rewritten then in the following form:

$$E_c = \Omega \cdot E_{eq} + (1 - \Omega) \cdot E_{st}$$

where the first term quantifies the part of evapotranspiration that depend on the available energy – equilibrium evaporation ( $E_{eq}$ ), and the second term ( $E_{st}$ ) – the part of evapotranspiration governed by stomatal control and water vapor deficit ( $D_a$ ).

An equation for equilibrium evaporation can be written as

$$E_{eq} = \frac{1}{\lambda} \cdot \frac{\Delta \cdot (R_n - S)}{\Delta + \gamma},$$

and equation for  $E_{st}$  as

$$E_{st} = \frac{1}{\lambda} \cdot \frac{\rho_a \cdot c_p \cdot D_a \cdot g_l}{\gamma}$$

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## Biographical Sketch

**Alexander Olchev** is research scientist of V.N. Sukachev' Laboratory of Biogeocenology and Historical

Ecology of A.N. Severtsov' Institute of Ecology and Evolution of the Russian Academy of Science in Moscow. He graduated from the Geographical Faculty of the Moscow State University in 1985 and got the PhD degree in Meteorology and Climatology at the end of 1998. The PhD thesis was focused on Modeling of Energy- and Mass-Exchange in Forest Ecosystems. The main scientific interests are related to modeling the land surface – atmosphere interaction in local and regional scales, measurements of H<sub>2</sub>O and CO<sub>2</sub> fluxes in forest ecosystems, and micro-meteorological measurements.

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