Towards universality and modularity: a generic photosynthesis and transpiration module for functional structural plant models

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Introduction

Functional Structural Plant Models (FSPMs) that combine functional and architectural submodels within the framework of an organ-based plant model are typically rather complex. To successfully overcome this problem, FSPM development requires establishing strictly modular model structures. In particular, physiological submodels should be generic and universal for different plant species, solidly tested and parameterized, provide clearly defined input-output interfaces, and facilitate the exchange between different research groups. To this end, here we present a generalized version of the nitrogen-sensitive LEAFC3-N model of the coupled CO_2, H_2O and radiation fluxes (Müller et al., 2005, 2006) that was designed to meet this requirements. The model combines and extends recent developments in ecophysiological leaf gas exchange modelling (for review, see Müller et al., 2005). It was tested and calibrated for leaves of wheat (*Triticum aestivum* L.), leaves and pods of oilseed rape (*Brassica napus* L.), and leaves and awns of barley (*Hordeum vulgare* L.). Adaptation to further plant species and organs is planned in future. The barley LEAFC3-N version was integrated into an FSPM of this crop (Wernecke et al., 2007). Here we discuss aspects of the universal formulation and parameterization of the LEAFC3-N model for different plant species and organs and its integration into FSPMs.

Model

LEAFC3-N is a nitrogen-sensitive extension of the generic steady-state flux model LEAFC3 (Nikolov et al., 1995) that couples major processes of CO_2 and H_2O gas exchange with stomatal function and the energy and mass transfer in the leaf-boundary layer. Because of the model complexity, we only outline main aspects related to the present study. A survey on combined photosynthesis-stomatal models as described in literature and further details on LEAFC3 and LEAFC3-N are given by Nikolov et al. (1995) and Müller et al. (2005).

In LEAFC3-N, biochemical processes determining net assimilation rate A_n (µmol m^{-2} s^{-1}) are modeled according to Farquhar et al. (1980). Main parameters of this submodel are: maximum carboxylation rate $V_{c,max}$ (µmol m^{-2} s^{-1}), Michaelis-Menten constants of Rubisco for carboxylation and oxygenation of RuBP, K_c and K_o (µmol mol^{-1}), CO_2 compensation concentration in the absence of mitochondrial respiration Γ^* (µmol mol^{-1}), light saturated rate of electron transport J_{max} (µmol$_{(e-)}$ m^{-2} s^{-1}), quantum yield for electron transport φ (mol$_{(e-)}$ mol$_{(quanta)}$$^{-1}$), and the rate of mitochondrial respiration in the dark R_{dark} (µmol m^{-2} s^{-1}). The parameters $V_{c,max}$, J_{max}, K_c, K_o, Γ^*, and R_{dark} are functions of temperature. Stomatal function in LEAFC3-N is modeled following Ball et al. (1987). The modified version of their model used here relates stomatal conductance g_s (mol m^{-2} s^{-1}) by a dimensionless scaling factor m to gross photosynthesis rate A_g and to the ratio of air humidity and CO_2 concentration in the leaf boundary layer. Further, a minimum value $g_{s,min}$ of g_s is considered.

Farquhar et al. (1980) gave a mechanistic explanation of the relationship between $V_{c,max}$ and nitrogen content N. A dependency of V_{cmax} and other photosynthetic or stomatal characteristics on N was incorporated into several gas exchange models (for review, see Müller et al., 2005). In developing LEAFC3-N, parameter-nitrogen relationships were subjected to special analysis and included in the model for $V_{c,max}$, J_{max}, φ, θ, R_{dark}, m, and $g_{s,min}$. For leaves, N per unit of one-sided leaf area N_a (g m^{-2}) is used. For other organs like pods of rapeseed or awns of barley ears, N must be defined in organ-specific way. Alternatively, N dependency of J_{max}, φ, and R_{dark} may be considered indirectly based on correlations between these parameters and V_{cmax}, which are stable under many conditions. Introducing N sensitivity into LEAFC3-N allows accounting for effects of organ development, mineral nutrition, and adaptation to growth conditions on gas exchange (cf. Müller et al., 2005, 2006).

Universality of parameter-nitrogen relationships

The parameter-nitrogen functions were derived from comprehensive measurements of the response of A_n and g_s to environmental factors on leaves or other organs during the course of organ and plant development. The relationships were analysed for different growth conditions and validated on the basis of field measurements of diurnal time courses of A_n and g_s. As expected, the function type of the considered parameter-nitrogen relationships differs between model parameters, but as a rule it was universal for different organs and plant species under study.

Basic parameter-nitrogen relationships mainly determining the response of the model to the effects listed above are those for V_{cmax}, J_{max}, φ, and m. Typically, the relationships between $V_{c,max}$ or J_{max} and N_a may be expressed by the linear function:

$$p_{max} = \begin{array}{ll} s_{Na}\left(N_a - N_{a,min}\right), & \text{if } N_a > N_{a,min} \\ 0, & \text{if } N_a \le N_{a,min}\ , \end{array} \tag{1}$$

where p_{max} stands for $V_{c,max}$ or J_{max}, s_{Na} (µmol g^{-1} s^{-1}) is the slope of the relationship, and $N_{a,min}$ is a minimum value of N_a at which p_{max} approaches zero. Alternatively, the nitrogen dependency of J_{max} may be accounted for indirectly using a correlation between J_{max} and $V_{c,max}$ (Leuning et al., 1997). The relationship between φ and N_a typically shows a saturation pattern as described by:

$$\varphi = \gamma_{Na1}\left(1-\exp\left(-\gamma_{Na2}\ N_a\right)\right), \tag{2}$$

where γ_{Na1} (mol mol^{-1}) is the value of φ at high N_a, and γ_{Na2} (m^2 g^{-1}) defines the saturation pattern. Alternatively, nitrogen dependency of φ was accounted for indirectly based on the correlation between φ and $V_{c,max}$, where the same type of function applies. To compare φ for different organs and species, the characteristic φ_{ref} calculated for a reference concentration $N_{a,ref}$ (e.g, 3.5 g m^{-2}) may be derived from eq. (2).

The parameter m typically drops with increasing N_a according to the relationship:

$$m = \delta_1\, N_a^{-\delta_2}\ , \tag{3}$$

where δ_1 (m^2 g^{-1}) and δ_2 (dimensionless) are empirical coefficients. However, in rapeseed leaves the m-N_a dependency tended to a linear one, whereas none dependency was found for pods. Again, most appropriate for comparisons is the characteristic m_{ref} calculated for $N_{a,ref}$.

For different plant species and organs, the values of key characteristics of the parameter-N_a relationships except of m_{ref} for awns and pods generally are in close range (Table 1). The values of s_{Na} for $V_{c,max}$ and J_{max} as well as those for φ_{ref} correspond well to those theoretically expected. The range of values given for several parameters of wheat and rapeseed is related to the method of its determination (for further detail, see the literature cited in Table 1). The upper values of these ranges were derived from parameter optimization based on adapting the complete model to data from diurnal time courses of gas exchange rates measured in the field. Therefore, these parameter values may be recommended for applying the model under comparable conditions. Nevertheless, it should be pointed out that further information is needed on the effects of growth conditions and genetic factors on the stability of parameter values.

Table 1. Characteristics of parameter-N_a relationships.

Object		**$V_{c,max}$ vs. N_a**		**J_{max} vs. N_a or $V_{c,max}$**			**φ vs. N_a**	**m vs. N_a**
Species	**Organ**	s_{Na}	$N_{a,min}$	s_{Na}	$N_{a,min}$	$J_{max}/V_{c,max}$	φ_{ref}	m_{ref}
Wheat	leaves	58-76[a]	0.1-0.3[a]	116-152[ac]	0.1-0.3[ac]	2[c]	0.43[a]	6.2[a]
Barley	leaves	63	0.2	151	0.2	2.2	0.44	7.4
	awns	52	0	108	0.1	1.9	0.41	2.6
Rapeseed	leaves	54-67[b]	0.3-0.4[b]	108-134[bc]	0.3-0.4[bc]	2[c]	0.32[b]	6.0-8.7[b]
	pods	49[b]	0.1[b]	98[bc]	0.1[bc]	2[c]	0.25[b]	11[b]

[a] from Müller et al., 2005; [b] from Müller et al., 2006; [c] value re-calculated or adopted based on Leuning, 1997.

Universality of temperature dependencies

The applicability of the parameter values of temperature dependencies of photosynthetic characteristics given for C_3-plants in literature was confirmed for the wheat, barley and rapeseed model versions by analysis of diurnal time courses of A_n and for the barley model version additionally by measurements of temperature response curves of temperature-sensitive parameters.

Model application

LEAFC3-N can be integrated into plant models via an interface providing local environmental characteristics and organ-based state variables (*N*, chlorophyll content, characteristic dimension of area elements, specific area). It was tested successfully with an FSPM for barley (cf. Müller et al., 2007, Wernecke et al., 2007) and with 1D multi-layer models for rapeseed (Müller et al., 2005) and wheat (Müller, unpublished). In principle, the LEAFC3-N model can be used with FSPMs of different level of discretization of the 3D structure, depending on the discretization of absorbed radiation provided by the light model used as well as on the discretization of organ-based state variables provided by the FSPM. However, in simulation studies covering the entire growth period, assembling individual polygons according to a 1D multi-layer scheme may be useful to reduce computational time. Concerning the choice of the time step for using LEAFC3-N as submodel of an FSPM, it must be noted that model calibration was derived from steady-state response curves of gas exchange rates and validated against diurnal time course data given with a measuring time interval of 10 s for the barley data and a time interval resulting from averaging of the measurement data in order of 2 or 6 minutes for the rapeseed and wheat data, respectively. Thus, by using LEAFC3-N with other time steps, the resulting biases must be analyzed and, if required, corrected.

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