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Towards integrating primary C-N metabolism and physiology of crop growth across different plant scales: the ProNet-CN model – a multiscale approach for functional-structural plant modeling

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Highlights: ProNet-CN is a new multiscale process network integrating biophysical, metabolic, and physiological processes of biomass formation across plant scales. It combines the LEAFC3-N model describing the exchange of CO_2, water vapor, and energy with a new model of the dynamics of mass balances of main carbon and nitrogen metabolites and its allocation between interacting compartments or organs.

Keywords: Model, multiscale, photosynthesis, carbon, nitrogen, biomass

INTRODUCTION

The understanding of biological systems may be greatly enhanced by multiscale modeling approaches that span several structural and temporal scales and enable predicting emergent properties of the system using information from – respectively models of – more basic levels (Dada and Mendes 2011; Weinan, 2011). During last years, functional structural plant models were refined by integrating classical process-based plant models (review: de Reffye et al. 2009). On the other hand, current efforts in systems biology have triggered the development of detailed kinetic models of carbon and nitrogen metabolism (e.g., Poolman et al. 2004, Foyer et al. 2006; Rasse and Tocquin 2006; Uys et al. 2007; Nägele et al. 2010). Bridging the gap between these modeling domains could facilitate integrating the knowledge on plant processes across different scales. Here we present a first version of such a multiscale modeling framework.

MODEL

ProNet-CN calculates the dynamics of mass balances of main carbon (C) and nitrogen (N) metabolites, accounting for major biochemical conversions, allocation, and biomass formation. These processes are coupled across four nested scales: (i) metabolic scale, (ii) reaction compartments, (iii) organs, and (iv) plant (Fig. 1). To keep the complexity of the model manageable and consistent with the analytical capabilities, for the present we consider plants represented by only one shoot. Photosynthetic C input and transpiration (*Tr*) are calculated by the LEAFC3-N model (Müller et al. 2005; Braune et al. 2009). The water uptake and flux through the plant is assumed equal to *Tr*. Limiting soil water availability and plant water storage are not considered. N uptake is reduced to a passive influx of nitrate with the water stream. Mass balance and rate equations are formulated in terms of moles C and N associated with the considered metabolites. Concentrations are defined per projected organ area. Both individual steps and lumped sequences of biochemical reactions or transport are modeled phenomenologically in terms of Michaelis-Menten kinetics or as driven by a concentration gradient, respectively. If appropriate, extensions were introduced to account for control by concentrations of C or N metabolites. The formation of organic N-compounds is condensed to the stoichiometry of proteins and formally included into the C and N balances of the cytosol. The calculation of respiratory C losses relies on the concept of growth and maintenance respiration (McCree 1970). Leaf area growth is assumed proportional to the rate of synthesis of cellulose and hemicelluloses in leaves.

MATERIAL AND METHODS

Data were gathered on spring barley (*Hordeum vulgare* L.) grown in partially (glasshouse, exp. 1) or fully climatized (climate chamber, exp. 2) conditions at different levels of N supply (Müller et al. 2009). In exp. 1, lateral shoots were cut immediately after emergence to get a simplified plant structure. This enables to measure twice a week the CO_2 exchange and transpiration rates on all leaves and the characteristics listed below on all 'organs' comprising visible parts of the individual leaf blades, pseudo-stem (pooled nodes, internodes, leaf sheaths, enclosed parts of leaf blades, and ear before heading), ear after heading, and roots of the entire plant. The analyses involved dry mass, leaf area, chlorophyll (leaf blades), total C, C bound to soluble carbohydrates and to fiber substances, total N, N bound to nitrate, amino acids and amids, and to proteins. In exp.

2, main shoots were analyzed in similar way, whereas lateral shoots were pooled and analyzed for overall dry mass, total C, and total N. For parameterizing the LEAFC3-N photosynthesis model, light and CO_2 response curves of net photosynthesis rate were recorded in exp. 1 on all leaves and in exp. 2 on leaves of rank 4 and the leaf below the flag leaf (Braune et al. 2009; Müller et al. 2009). As additional information, data were available on the content of glucose, fructose, sucrose, starch, fructans (M.-R. Hajirezaei, IPK Gatersleben, Germany), and cell wall compounds (B. Usadel, MPI Potsdam-Golm, Germany) in barley leaves, as well as on the diurnal dynamics of main carbon metabolites in grasses grown under different N supply and CO_2 concentration (Isopp et al. 2000). Matlab-Simulink (The Mathworks®) was used as simulation environment. Simulation studies covered the development of barley plants from leaf emergence until ripeness. The environmental data recorded at plant height in exp. 1 were used in the simulation studies (time step 5 min).

RESULTS AND DISCUSSION

Generally, the simulated dynamics of the conversion and transport rates of the considered metabolites and of the related mass balances were in good agreement with both the expected response and the experimental data. As an example of the simulations, the net rate of the interconversion of two central metabolites of the carbon metabolism, namely of cytosolic hexose (Hex) and sucrose (Suc) for leaves 1 to 10 during plant ontogenesis are shown in Fig. 2 (in terms of mol C). This simulation output reflects that leaves 2 to 10 during their early phase of development are sinks for C (import of Suc and thus Suc → Hex dominates) and thereafter act as a source of C (export of Suc and thus Hex → Suc dominates). This is mirrored by similar patterns of the net transport rate of Suc into/out of the phloem (simulation not shown). Skipping a large number of analogous simulation results for other C and N metabolites, the growth patterns are shown in Fig. 3. Again, the simulation results were generally in good agreement with the data. A more detailed comparison with data is planned after further refinement of the model and improved calibration. Simulink was proved to represent a powerful tool for developing a multiscale dynamic systems model that integrates C and N metabolism, organ based C and N mass balances, and process up-scaling to biomass formation.

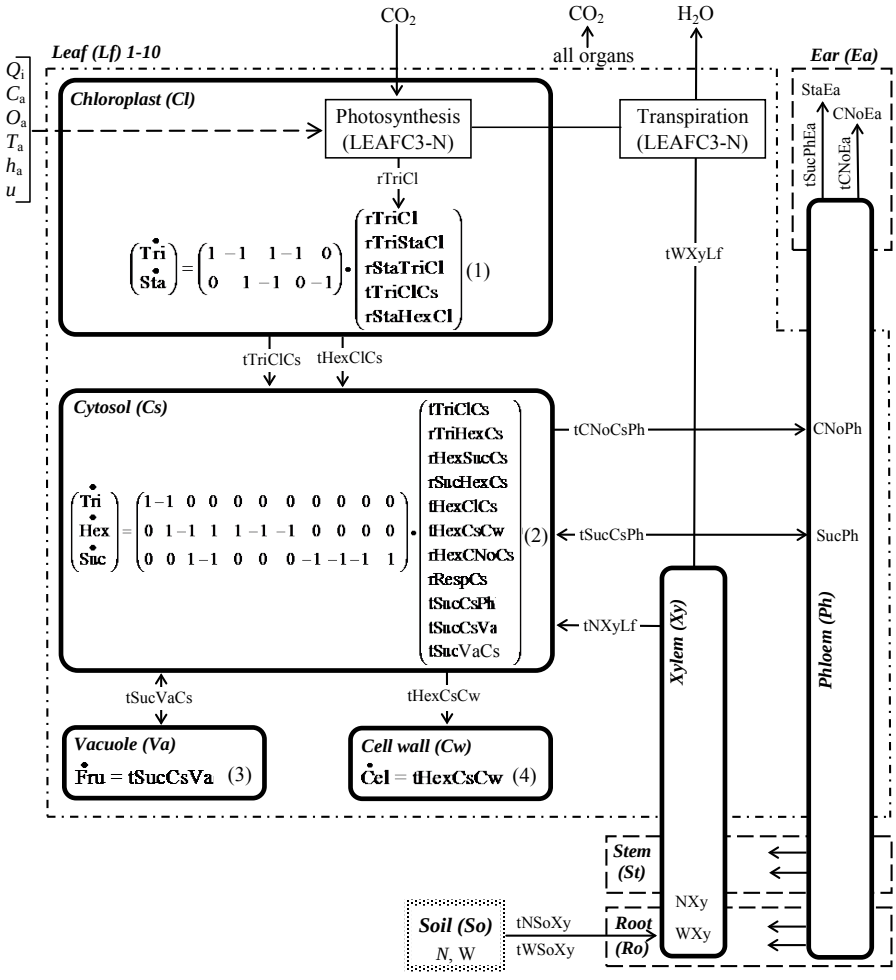

Fig. 1. Model scheme.

Model inputs: C_a – ambient CO_2 concentration, h_a – air humidity, N – nitrogen bound to nitrate in soil water, O_a – ambient oxygen concentration, T_a – air temperature, Q_i – incident irradiance, u – wind speed, W – water.

Carbon entities: Cel – C in cellulose and hemicelluloses, CNo – C in organic N compounds (mol), Fru – C in fructans (mol), Hex – C in hexoses (mol), Sta – C in starch (mol), Suc – C in sucrose (mol), Tri – C in trioses (mol).

Organs and compartments: see figure.

Composite symbols as in the following examples: HexCs – C in hexoses in the cytosol (mol), rTriHexCs – rate of C flux from triose phosphate to hexoses due to transformation of triose phosphate to hexoses in the cytosol (mol s^{-1}), tTriClCs – rate of C flux due to transport of trioses from chloroplast into the cytosol (mol s^{-1}).

Other symbols: rRespCs: rate of release of C from the sucrose pool in leaf cytosol due to growth and maintenance respiration.

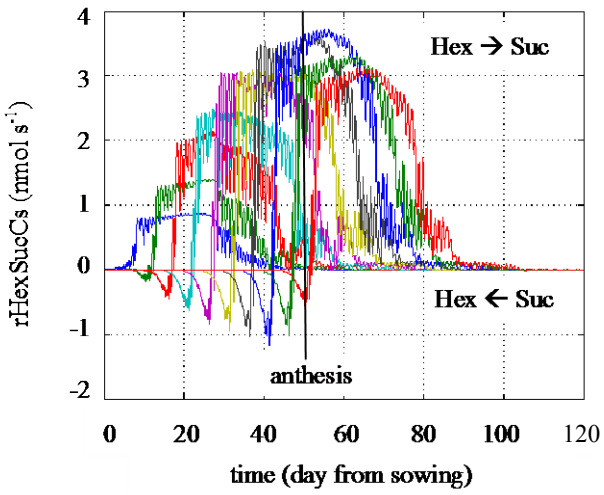

Fig. 2. Simulated ontogenetic courses of the rate of conversion hexose ↔ sucrose (rHexSucCs) in the cytosol of leaves of rank 1 to 10 (in terms of mol C s^{-1}). The fluctuations represent the diurnal cycles.

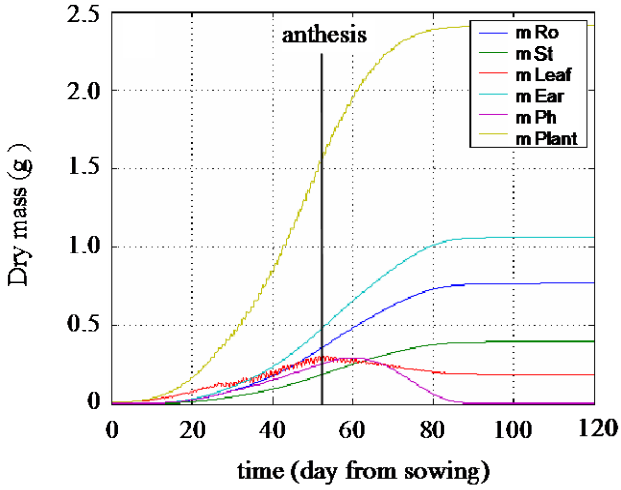

Fig. 3. Ontogenetic courses of dry mass of the whole plant (m Plant) and plant organs (Ro: root, St: fiber substances of the stem, m Ph: substances transported via phloem).

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