

## SUPPLEMENTARY DATA

### **Summary information for the crop model GECROS**

The crop model GECROS (for version 1.0, see Yin & van Laar 2005) predicts crop biomass and yield as affected by climatic factors (radiation, temperature, wind speed, and vapour pressure) and available amount of soil water and nitrogen. The model represents crop functions and interactive responses of contrasting processes or components to environmental variables, thereby embodying physiological mechanisms that drive crop dynamics and generate emergent feedback features. The contrasting components particularly emphasise carbon (C) vs nitrogen (N) interactions, but also include: root vs shoot, source activity vs sink capacity, and growth vs senescence relationships. Since its first release (Yin & van Laar 2005), GECROS has been updated for a couple of times. Model version 2.0, as used by Yin & Struik (2010), contains algorithms of Yin & Struik (2009) for coupled modelling of leaf photosynthesis and stomatal conductance, while accounting for mesophyll conductance (an important parameter for C<sub>3</sub> photosynthesis). Very recently, the model was further updated (version 3.0) to allow an option that stomatal and mesophyll conductance may vary in parallel in response to environmental conditions (see below). In this supplementary material, I outline model algorithms in (i) modelling carbon assimilation and growth processes, and (ii) modelling nitrogen uptake, root-shoot relation, sink demand, and senescence.

### **Modelling carbon assimilation, and growth processes**

*Stomatal conductance, leaf photosynthesis and transpiration, and their extension to canopies*

GECROS-v.1.0 calculates instantaneous leaf photosynthesis ( $A$ ) from the C<sub>3</sub>-photosynthesis model of Farquhar et al. (1980), assuming the intercellular : ambient [CO<sub>2</sub>] ratio only as a

function of leaf-to-air vapour pressure deficit. This approach was also applied to C<sub>4</sub> crops, with additional assumptions (i) to set internal [CO<sub>2</sub>] to an arbitrarily high value, and (ii) to consider the extra ATP consumption by the CO<sub>2</sub>-concentrating mechanism. In later versions, *A* was calculated from the analytical algorithms that are based on the model of Farquhar et al. (1980) for C<sub>3</sub>-photosynthesis, and its equivalent for C<sub>4</sub>-photosynthesis (von Caemmerer & Furbank 1999), coupled with a phenomenological diffusional conductance model (for overview, see Yin & Struik 2009 and references therein; Yin et al. 2009). This analytical approach was formulated according to the numerical framework of Leuning et al. (1995), with modifications to the original *g<sub>s</sub>* equation and incorporation of temperature- and leaf N-dependent mesophyll conductance *g<sub>m</sub>* (in GECROS v.2.0). The analytical cubic polynomials (see Yin & Struik 2009) simultaneously solve stomatal conductance (*g<sub>s</sub>*), internal [CO<sub>2</sub>] level, and leaf photosynthesis rate (*A*) for a given temperature. The obtained *g<sub>s</sub>* was used in the Penman-Monteith equation (Monteith 1973) for surface energy balance to model leaf transpiration and leaf temperature as affected by factors such as elevated [CO<sub>2</sub>]. Leaf temperature was then used for re-calculating leaf photosynthesis and transpiration. The effect of leaf N content on photosynthesis, *g<sub>s</sub>* and transpiration is reflected by the effect of leaf N on parameters (i.e. *V<sub>cmax</sub>*, *J<sub>max</sub>* and *TPU*; see the main text for their definition) of the photosynthesis model. This coupled approach allows the decrease of *g<sub>s</sub>* at elevated [CO<sub>2</sub>] to be well predicted, in agreement with the finding of Leakey et al. (2006) that there is no long-term acclimation of *g<sub>s</sub>* independent of photosynthetic acclimation to [CO<sub>2</sub>]. A further development of GECROS (v.3.0) was to allow an option that *g<sub>m</sub>* varies in proportion with *g<sub>s</sub>* in response to all environmental factors, given recent reports that *g<sub>m</sub>* may resemble *g<sub>s</sub>* in response to various environmental variables (e.g. Flexas et al. 2008; Yin et al. 2009).

Spatial extension from leaf to canopy photosynthesis and transpiration was established using the sun/shade model of de Pury & Farquhar (1997). Temporal extension from

instantaneous rates to daily total was performed using the five-point Gaussian integration (Goudriaan 1986) to account for (a)symmetric diurnal course of radiation and temperature, to which photosynthesis and transpiration respond nonlinearly. These approaches for spatial and temporal extensions apply to the case in the absence of water stress.

For simplicity, diurnal course of available water is assumed to follow that of radiation. In the presence of water stress (i.e. water availability does not satisfy the requirement for potential transpiration), the available water is partitioned between sunlit and shaded leaves according to the relative share of their potential transpiration to obtain their instantaneous actual transpiration. The actual transpiration is transformed into the actual level of  $g_s$  using the Penman-Monteith equation, and the actual  $g_s$  was then used as input to the analytical quadratic model (unpublished model algorithms), to estimate the instantaneous actual photosynthesis of the sunlit and shaded leaves. The Gaussian integration is again used to obtain the daily total of the actual photosynthesis.

### *Crop respiration*

Crop respiration was modelled, based on the framework of Cannell & Thornley (2000) that recognises individual relationships between respiration and each process it supports. In this framework, component processes are differentiated: growth, symbiotic  $N_2$  fixation, root nitrogen uptake, nitrate reduction, other ion uptake, phloem loading, and residual maintenance component. Growth efficiency is obtained from the chemical composition of plant material based on carbon fraction and glucose requirement of these chemical components (Penning de Vries et al. 1989). Most of the other processes can also be well quantified and the default carbon costs used in GECROS are:  $6 \text{ g C (g N fixed)}^{-1}$ ,  $0.17 \text{ g C (g ammonium-N uptake)}^{-1}$ ,  $0.34 \text{ g C (g nitrate-N uptake)}^{-1}$ ,  $1.71 \text{ g C (g nitrate-N reduction)}^{-1}$ ,  $0.06 \text{ g C (g mineral uptake)}^{-1}$ , and  $0.06 \text{ g C (g C loaded from shoot to root)}^{-1}$ . However, the

last process maintenance respiration is less quantifiable but suggested to be related to crop N content (see the main text).

### **Modelling nitrogen uptake, root-shoot relation, sink demand, and senescence**

The following texts will mainly highlight phenomenological equations (which were largely unaltered for various versions of GECROS), further facilitating the C-N modelling.

#### *Nitrogen uptake*

In contrast to C assimilation, crop N uptake has been more empirically quantified. Usually N uptake is the minimum of crop N demand and soil N supply; the latter is presented in a soil model. Crop N demand is commonly based on the critical N concentration in above-ground biomass in the course of the growth cycle reported for various crops, in the form of either an empirical equation (Justes et al. 1994) or a tabular function. These functions were derived from experimental data, and different experiments could yield quantitatively different functions for the same crop/cultivar.

Yin et al. (2003b) used an equation to describe crop N demand ( $N_{\text{dem}}$ ):

$$N_{\text{dem}} = C_{\text{R}} \sigma_{\text{N}} = C_{\text{R}} \sigma_{\text{C}}^2 / (d\sigma_{\text{C}} / d\kappa) \quad (1)$$

where  $C_{\text{R}}$  is the amount of C in roots. This was based on the analysis of Hilbert (1990) for balanced growth conditions that achieving the optimum plant N:C ratio for a maximised relative C gain requires that relative root activity for N uptake ( $\sigma_{\text{N}}$ ) and relative shoot activity for C assimilation ( $\sigma_{\text{C}}$ ) be balanced as defined by eqn (1), where  $d\sigma_{\text{C}}/d\kappa$  is the first-order derivative of  $\sigma_{\text{C}}$  with respect to  $\kappa$ , the N:C ratio in the whole-plant. The value of  $\sigma_{\text{C}}$  is defined as:  $\sigma_{\text{C}} = (\Delta C / \Delta t) / C_{\text{S}}$ , where  $C_{\text{S}}$  is the amount of C in shoots;  $\Delta C / \Delta t$  is daily crop C gain (which can be calculated from the above-mentioned models for daily canopy photosynthesis and crop respiration). Because the quantity  $d\sigma_{\text{C}}/d\kappa$  in eqn (1) cannot be analytically

calculated given the sophistication of estimating  $\sigma_C$ , it can be numerically calculated by:  $d\sigma_C/d\kappa = [\sigma_{C(\kappa+\Delta\kappa)} - \sigma_{C(\kappa)}]/\Delta\kappa$ , where  $\Delta\kappa$  is a small increment of  $\kappa$ ;  $\sigma_{C(\kappa)}$  and  $\sigma_{C(\kappa+\Delta\kappa)}$  are relative shoot activities when plant N:C ratio is  $\kappa$  and  $(\kappa+\Delta\kappa)$ , respectively. This generic method is less trivial than the ‘critical N concentration’ approach, and can reflect that root N uptake may be vigorously related to crop photosynthetic activity (Triboi & Triboi-Blondel 2002). The method can produce the commonly observed sigmoid shape of cumulative N uptake over a growing season (Yin & van Laar 2005). Simulation shows that the enhancement in the N uptake predicted by eqn (1) may not keep pace with that of C gain by elevated CO<sub>2</sub>, as experimentally observed (e.g. Kim et al. 2003). As a result, N concentration of plants under elevated [CO<sub>2</sub>] may eventually be lower, which has been observed irrespective of the N availability (Wong 1990; Conroy & Hocking 1993). The ‘critical N concentration’ approach alone will yield an equal plant N concentration between ambient and elevated [CO<sub>2</sub>] if N supply is not limiting.

#### *Partitioning between root and shoot*

In some crop models, partitioning of newly formed assimilates between root and shoot is assumed simply as a fixed empirical function of development stage (e.g. Penning de Vries et al. 1989). Derivation of these partitioning functions for various crops needs substantial experimental data. More importantly, this approach does not account for the reported plasticity of root-shoot ratios in response to environmental changes (Poorter & Nagel 2000).

Yin & Schapendonk (2004) presented an equation for the partitioning of C between shoots and roots. The equation is based on the classical root-shoot functional balance theory, with an incorporation of the mechanism that plants control root-shoot partitioning in order to maximise their relative C gain. The fraction of the newly assimilated C partitioned to the shoot ( $\lambda_{C,S}$ ), calculated by:

$$\lambda_{c,s} = \frac{1}{1 + (\eta / \sigma_c) d\sigma_c / d\kappa} \quad (2)$$

where  $\eta$  is the N:C ratio in newly formed biomass,  $d\sigma_c/d\kappa$  and  $\sigma_c$  are the same as defined for eqn (1). A similar equation was derived for estimating the fraction of the newly obtained N partitioned to the shoot (Yin & Schapendonk 2004). Eqn (2) is simple and has no parameter to estimate as all the inputs can be calculated elsewhere in a crop model. The equation, strictly speaking, holds for steady-state growth conditions (Yin & Schapendonk 2004). van der Werf et al. (1993) showed an evidence that partitioning functions, if being related to plant N status, held for both steady-state and general conditions. When incorporated into a crop model, eqn (2) produces a pattern of root-shoot partitioning similar to the observed ones, yet addresses the plasticity of root:shoot ratios in response to environmental conditions (Yin & Schapendonk 2004). The simulated effects of light, nutrients and water on the partitioning agreed with the experimentally observed; the simulated effect of CO<sub>2</sub> was not consistent, which seemed to agree with the meta-result of Poorter & Nagel (2000) that a doubled [CO<sub>2</sub>] did not significantly affect the average allocation of C to roots or shoots.

### *Sink demand*

Assimilates distributed to the shoot need to be further modelled for partitioning among the shoot organs; and again a trivial approach is to use partitioning coefficients as a fixed empirical or tabular function of development stage (e.g. Penning de Vries et al. 1989). Alternatively, it is assumed that the strength of growing organs as sinks of available C determines the partitioning (Marcelis 1996); any surplus assimilate goes to the pool of reserves which can be remobilised later if there is assimilate deficit (Fig. 6 in the main text). To that end, the differential form of classical growth functions like the Logistic equation is often used to describe the dynamics of sink demand.

Yin et al. (2003a) developed an alternative equation for describing any asymmetric sigmoid pattern of a determinate growth. By setting the initial value of a sink organ at the start of its growth as zero, the equation uses three parameters  $w_{\max}$ ,  $\theta_e$  and  $\theta_m$  (where  $w_{\max}$  is the maximum quantity, which is reached at stage for the end of growth  $\theta_e$ ;  $\theta_m$  is the stage at which the growth rate is maximum). The differential form of the equation, when multiplied by daily development rate ( $\text{day}^{-1}$ ), can describe the daily demand of a sink (e.g. seed, or stem) for C assimilates,  $\Delta w$ , as (Yin & van Laar 2005):

$$\Delta w = \omega w_{\max} \frac{(2\theta_e - \theta_m)(\theta_e - \theta)}{\theta_e (\theta_e - \theta_m)^2} \left( \frac{\theta}{\theta_e} \right)^{\theta_m / (\theta_e - \theta_m)} \quad (3)$$

where  $\omega$  is development rate at stage  $\theta$ . The commonly used classical growth equations have an asymptotic form, meaning that an expected  $w_{\max}$  can never be achieved, even if source activity is not limiting. In contrast, eqn (3) ensures that  $w_{\max}$  is achieved exactly at  $\theta_e$ . The model uses only three parameters (i.e.  $w_{\max}$ ,  $\theta_m$  and  $\theta_e$ ) to define any asymmetric sigmoid pattern that would need at least four parameters to define with classical growth equations. Moreover,  $\theta_e$  for a given sink organ can be defined physiologically, so its timing can be predicted by the phenology part of crop model. These features allow eqn (3) to suit better than classical growth equations for being embedded in crop models to simulate sink demand.

#### *LAI and senescence*

In contrast to modelling growth, there is no well-established method for modelling senescence. A common method is to use empirical, developmental-stage dependent leaf-turnover coefficients (e.g. Penning de Vries et al. 1989; Matthews et al. 1997). These coefficients differ across crops, and across environments (e.g. N supplies), requiring specific calibration for different cases.

Yin et al. (2000) developed an equation for describing LAI ( $L$ ) in relation to the amount of canopy leaf-nitrogen ( $N$ ) as:

$$L = \frac{1}{k_n} \log_e (1 + k_n N / n_b) \quad (4)$$

where  $k_n$  is the coefficient for leaf-N extinction in the canopy, and  $n_b$  is a base N content at or below which leaf photosynthetic rate at a saturating light is nil. A broad use of eqn (4) is to describe the generic logarithmic relation between  $L$  and  $N$  for the full canopy in which the leaf N at the bottom of the canopy is as low as  $n_b$ , as confirmed by the post-panicle initiation measurements at two  $[\text{CO}_2]$  levels of an FACE experiment (see Fig. 4 in the main text). For young canopy where  $L \leq 1$ , simulation based on eqn (4) showed that the relationship between  $L$  and  $N$  is virtually linear (Yin et al. 2003b), again confirmed by the FACE data from the early-phase measurements (Fig. 4 in the main text).

A more important use of eqn (4) is to engender a simple robust method to predict the onset and quantity of leaf senescence. The LAI calculated by eqn (4) can be designated as the N limited LAI ( $L_N$ ). Conventionally, LAI has been calculated from C partitioned to or biomass accumulated in leaves (e.g. Matthews et al. 1997), denoted here as  $L_C$ . The rate of the LAI decrease due to senescence can be formulated as  $[L_C - \min(L_C, L_N)] / t_c$ , where  $t_c$  is the time constant, which can be equal to or more than the time step for simulation (Yin et al. 2000). This approach is generic and avoids the use of time-dependent, crop-specific, empirical leaf-turnover coefficients. The input parameter  $n_b$  is required anyway in a crop model for simulating leaf photosynthesis, and the other parameter  $k_n$  may be calculated theoretically from light extinction coefficient (Yin et al. 2003b). The approach agrees with a coherent biological picture of leaf senescence in relation to the decreasing amount of N in the bottom canopy, especially during seed growth (Sinclair & de Wit 1975). A similar approach was used in GECROS for describing root senescence, based on root N content. The approach can



also predict, to a large extent, high temperature-induced senescence as high temperature accelerates seed filling that requires a fast remobilisation of leaf and root N, thereby causing fast senescence. However, any direct impact of extreme high temperature on senescence needs further modelling studies.

## References

- Cannell, M.G.R. and Thornley, J.H.M., 2000. Modelling the components of plant respiration: Some guiding principles. *Annals of Botany* 85: 45-54.
- Conroy, J. and Hocking, P., 1993. Nitrogen nutrition of C<sub>3</sub> plants at elevated atmospheric CO<sub>2</sub> concentrations. *Physiologia Plantarum* 89: 570-576.
- de Pury, D.G.G. and Farquhar, G.D., 1997. Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models. *Plant, Cell and Environment* 20: 537-557.
- Farquhar, G.D., von Caemmerer, S. and Berry, J.A., 1980. A biochemical model of photosynthetic CO<sub>2</sub> assimilation in leaves of C<sub>3</sub> species. *Planta* 149: 78-90.
- Flexas, J., Ribas-Carbó, M., Diaz-Espejo, A., Galmes, J., and Medrano, H., 2008. Mesophyll conductance to CO<sub>2</sub>: current knowledge and future prospects. *Plant, Cell and Environment* 31: 602-621.
- Goudriaan, J., 1986. A simple and fast numerical method for the computation of daily totals of crop photosynthesis. *Agricultural and Forest Meteorology* 38: 249-254.
- Hilbert, D.W., 1990. Optimization of plant root:shoot ratios and internal nitrogen concentration. *Annals of Botany* 66: 91-99.
- Justes, E., Mary, B., Meynard, J.-M., Machet, J.-M. and Thelier-Huche, L., 1994. Determination of a critical nitrogen dilution curve for winter wheat crops. *Annals of Botany* 74: 397-407.
- Kim, H.Y., Lieffering, M., Kobayashi, K., Okada, M. and Miura, S., 2003. Seasonal changes in the effects of elevated CO<sub>2</sub> on rice at three levels of nitrogen supply: a free air CO<sub>2</sub> enrichment (FACE) experiment. *Global Change Biology* 9: 826-837.
- Leakey, A.D.B., Bernacchi, C.J., Ort, D.R. and Long, S.P., 2006. Long-term growth of soybean at elevated [CO<sub>2</sub>] does not cause acclimation of stomatal conductance under fully open-air conditions. *Plant, Cell and Environment* 29: 1794-1800.
- Leuning, R., Kelliher, F.M., De Pury, D.G.G. and Schulze, E.-D., 1995. Leaf nitrogen, photosynthesis, conductance and transpiration: scaling from leaves to canopies. *Plant, Cell and Environment* 18: 1183-1200.
- Marcelis, L., 1996. Sink strength as a determinant of dry matter partitioning in the whole plant. *Journal of Experimental Botany* 47: 1281-1291.
- Matthews, R.B., Kropff, M.J., Horie, T. and Bachelet, D., 1997. Simulating the impact of climate change on rice production in Asia and evaluating options for adaptation. *Agricultural Systems* 54: 399-425.
- Monteith, J.L. 1973. *Principles of environmental physics*. Edward Arnold, London, 241pp.
- Penning de Vries, F.W.T., Jansen, D.M., ten Berge, H.F.M. and Bakema, A., 1989. Simulation of ecophysiological processes of growth in several annual crops. IRRI, Los Banos and Pudoc, Wageningen.
- Poorter, H. and Nagel, O., 2000. The role of biomass allocation in the growth response of plants to different levels of light, CO<sub>2</sub>, nutrients and water: a quantitative review. *Australian Journal of Plant Physiology* 27: 595-607.
- Sinclair, T.R. and de Wit, C.T., 1975. Photosynthate and nitrogen requirements for seed production by various crops. *Science* 189: 565-567.
- Triboi, E. and Triboi-Blondel, A.-M., 2002. Productivity and grain or seed composition: a new approach to an old problem. *European Journal of Agronomy* 16: 163-186.

- van der Werf, A., Enserink, T., Smit, B. and Booij, R., 1993. Allocation of carbon and nitrogen as a function of the internal nitrogen status of a plant: Modelling allocation under non-steady-state situations. *Plant and Soil* 155/156: 183-186.
- von Caemmerer, S. and Furbank, R.T., 1999. Modeling C<sub>4</sub> photosynthesis. *In* Sage R.F. and Monson R.K. (eds) C<sub>4</sub> Plant Biology. Academic Press, Toronto, pp. 173-211.
- Wong, S.-C., 1990. Elevated atmospheric partial pressure of CO<sub>2</sub> and plant growth. II Non-structural carbohydrate content in cotton plants and its effect on growth parameters. *Photosynthesis Research* 23: 171-180.
- Yin, X. and Schapendonk, A.H.C.M., 2004. Simulating the partitioning of biomass and nitrogen between root and shoot in crop and grass plants. *NJAS-Wageningen Journal of Life Sciences* 51: 407-426.
- Yin, X. and Struik, P.C., 2009. C<sub>3</sub> and C<sub>4</sub> photosynthesis models: An overview from the perspective of crop modelling. *NJAS-Wageningen Journal of Life Sciences* 57: 27-38.
- Yin, X. and Struik, P.C., 2010. Modelling the crop: from system dynamics to systems biology. *Journal of Experimental Botany* 61: 2171-2183.
- Yin, X. and van Laar, H.H., 2005. *Crop Systems Dynamics: An Ecophysiological Simulation Model for Genotype-by-Environment Interactions*. Wageningen Academic Publishers, Wageningen, The Netherlands, 155pp.
- Yin, X., Goudriaan, J., Lantinga, E.A., Vos, J. and Spiertz, J.H.J., 2003a. A flexible sigmoid function of determinate growth. *Annals of Botany* 91: 361-371 (erratum in 91: 753, 2003).
- Yin, X., Lantinga, E.A., Schapendonk, A.H.C.M. and Zhong, X., 2003b. Some quantitative relationships between leaf area index and canopy nitrogen content and distribution. *Annals of Botany* 91: 893-903.
- Yin, X., Schapendonk, A.H.C.M., Kropff, M.J., van Oijen, M. and Bindraban, P.S., 2000. A generic equation for nitrogen-limited leaf area index and its application in crop growth models for predicting leaf senescence. *Annals of Botany* 85:579-585.
- Yin, X., Struik, P.C., Romero, P., Harbinson, J., Evers, J.B., van der Putten, P.E.L. and Vos, J., 2009. Using combined measurements of gas exchange and chlorophyll fluorescence to estimate parameters of a biochemical C<sub>3</sub> photosynthesis model: a critical appraisal and a new integrated approach applied to leaves in a wheat (*Triticum aestivum*) canopy. *Plant, Cell and Environment* 32: 448-464.