**Supplementary: Presentation of the model structure and calibration**

**Primary components of DSSAT cropping system model.** Two soil organic matter modules are provided under the Soil primary module: the CENTURY and CERES-based models (Porter et al., 2010).



**CENTURY-based soil carbon and nitrogen balance sub module** (in DSSAT V4.5, Volume 4 chapter 1. Cropping System Model Main program, Jones J.W., Hoogenboom, G. Porter C., 2010)

The CENTURY model is more appropriate for use in low input agricultural systems, for example those that use green manure where the surface layer is crucial. Gijsman et al. (2002) showed that this new component greatly improved the accuracy of simulating the long-term changes in soil carbon in the Rothamsted bare fallow experiment. The main differences between the CENTURY-based module and the CERES-based soil N module are:

(i) The CENTURY-based module divides the soil organic matter (SOM) into more fractions, each of which has variable C:N and C:P ratios and can mineralize or immobilize nutrients,

(ii) it has a residue layer on top of the soil which decomposes, and

(iii) decomposition rates are texture dependent.

The CENTURY-based module distinguishes three types of SOM: [1] easily decomposable (microbial) SOM1, [2] recalcitrant SOM2, which contains lignin and cell walls, and [3] an almost inert SOM3. At initialization of the simulation, the fractional ratio of these three pools is set, with SOM1 of only about 2% of total SOM, while SOM2 and SOM3 vary with the management history of the soil (grassland or cultivated) and the degree of depletion.

The improved SOM module also allows one to perform more realistic simulations on carbon sequestration, i.e. the accumulation or depletion of soil organic C under different management systems.

Organic phosphorus and nitrogen components are maintained in each of the SOM and fresh organic matter pools. Immobilization and mineralization of N and P are computed for each soil layer and returned to the inorganic N and P modules.

Fresh organic matter from a previous crop can be specified by the user. Both surface and soil residues are listed by dry weight of root, nodule and surface residue, all in kg ha-1. An external DSSAT data file provides additional information on lignin, nitrogen and phosphorus contents for various crop types and for surface and sub-surface crop residues. The lignin content is used to partition the crop residues into structural and metabolic components, which decompose at different rates.

**Calibration**

All simulations began two days before sowing and ended one day after harvest.

Daily temperature, solar radiation and rainfall data were recorded at the experimental site by an on-site automatic meteorological station (ENERCO 404 Series, Cimel, France).

Experiment 1 was used for calibration of the plant module, experiment 3 for the parametrization and the evaluation the soil module, experiments 2 and 3 for the evaluation of the plant module.

Input parameters for the soil were derived from measurements made on soil profiles at the site (0-20 and 20-40 cm), and for initial conditions (initial inorganic N content, initial water content) from soil measurements made in the different experiments just before sowing, to a depth of 80 cm (maximum depth of the root profile observed in experiment 2, depth 0-10, 10-20, 20-40, 40-60, 60-80 cm). The fraction of stable carbon was based on silt and clay contents (Porter et al., 2010). In order to account for subsoil retention of nitrate, the adsorption coefficient was adjusted (nitrate adsorbed/nitrate in solution; cm3 g-1, in soil setting) to 0 in the top layers, then increased to 1 cm3 g-1 in the deepest layer (Bowen et al., 1993).

Genetic coefficients were obtained by fitting the model to the observed dates of flowering and maturity, LAI at flowering, production of aboveground biomass, grain yield, and N content and uptake at maturity. The adjusted genetic coefficients mainly concerned the thermal times for the phenological stages, leaf setting and grain yield and biomass setting.

**Genetic coefficients for the DSSAT CERES-Wheat model.**

File CULTIVARS WHCER046

Name Value Coefficient definition

P1V 0 Days optimum vernalizing temperature required for vernalization

P1D 0 Photoperiod response (% reduction in rate/10 h drop in pp)

P5 400 Grain filling (excluding lag) phase duration (oC.d)

G1 25 Kernel number per unit canopy weight at anthesis (#/g)

G2 30 Standard kernel size under optimum conditions (mg)

G3 3.2 Standard non-stressed mature tiller wt (incl grain) (g dwt)

PHINT 83 Interval between successive leaf tip appearances (oC.d)

File ECOTYPES WHCER046

 PHENOLOGY (PHASE\_DURATIONS) P.MOD MAX\_RUE

Name P1 P2FR1 P2 P3 P4FR1 P4FR2 P4 VEFF PARUE PARU2

Unit oC.d fr oC.d oC.d fr fr oC.d fr g/MJ g/MJ

Value 1150 .25 750 300 .25 .10 200 0.0 2.7 2.7

LEAF PRODN LEAF\_SIZES LEAF\_SENESC TILLER\_PRODUCTION TILLER\_DEATH

PHL2 PHF3 LA1S LAFV LAFR SLAS LSPHS LSPHE TIL#S TIPHE TIFAC TDPHS TDPHE TDFAC

Lf# Fac cm2 fr/lf fr/lf cm2/g GrStg GrStg Lf# GrStg Fac GrStg GrStg. Fac

13 1.0 1.5 0.05 0.20 400 5.7 6.3 4.5 2.0 0.5 2.2 6.0 20.0

ROOTS CANOPY COMPOSITION KILL

RDGS HTSTD AWNS KCAN RS%S GN%S GN%MN TKFH

cm/d cm Score Exp % % % oC

3.0 100 0.0 .85 60 2.0 1.2 -1

Coefficient definition

! AWNS Awn score (0-10; 10=very long)

! ECO# Code for the ecotype (code)

! GN%MN Minimum grain N (%)

! GN%S Standard grain N (%)

! HTSTD Standard canopy height (cm)

! KCAN PAR extinction coefficient (#)

! LA1S Area of standard first leaf (cm2)

! LAFR Increase in potential area of leaves reproductive phase (fr/leaf)

! LAFV Increase in potential area of leaves vegetative phase (fr/leaf)

! LARS Area of standard reproductive phase leaf (cm2)

! LAVS Area of standard vegetative phase leaf (cm2)

! LLIFE Life of leaves during vegetative phase (phyllochrons)

! LSPHE Final leaf senescence ends (GrowhStage)

! LSPHS Final leaf senescence starts (GrowhStage)

! P1 Duration of phase end juvenile to terminal spikelet (PVTU)

! P2 Duration of phase terminal spikelet to end leaf growth (TU)

! P2FR1 Duration of phase terminal spikelet to jointing (fr P2)

! P3 Duration of phase end leaf growth to end spike growth (TU)

! P4 Duration of phase end spike growth to end grain fill lag (TU)

! P4FR1 Duration of phase end spike growth to anthesis (fr P4)

! P4FR2 Duration of phase anthesis start to anthesis end (fr P4)

! PARU2 PAR conversion to dm ratio after last leaf (g/MJ) (If -99, set to PARUE)

! PARUE PAR conversion to dm ratio before last leaf stage (g/MJ)

! PHFn Factor by which PHINTS is multiplied -> PHINT for phase (#)

! PHLn Leaf # produced during phyllochron phase (#)

! PPFPE Daylength factor,pre emergence (#,0-1)

! RDGS Root depth growth rate,early phase (cm/standard d)

! RS%S Reserves part of assimilates going to stem (%)

! SLAS Specific leaf area standard first leaf (cm2/g)

! TDFAC Tiller death factor (%/st.day when tiller wt 2xstandard wt)

! TDPHE Tiller death ending stage (Growth Stage)

! TDPHS Tiller death start stage (Growth Stage)

! TIFAC Tiller initiation (rate) factor (fr of phyllochron based) (#)

! TIL#S Tiller production starts (leaf #)

! TIPHE Tillering phase end stage (Growth Stage)

! TKFH Temperature at which killed when fully hardened (oC)

! VEFF Vernalization effect (Rate reduction when unvernalized (fr)

! WFGU Water stress factor growth upper (fr)

! WFPU Water stress factor photosynthesis upper (fr)

**References**

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