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**PRIMA-SECTION 2-2022**

**“Modelling and Technological Tools to Prevent Surface and Ground-Water Bodies from Agricultural Non-Point Source Pollution Under Mediterranean Conditions”**

**NPP-SOL**

**Integrated NPP-SOL MT software and related handbook**

**Deliverable number: D4.3**



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# Non-Point Pollution SOLutions (NPP-SOL)

## Deliverable 4.3: Integrated NPP-SOL MT software and related handbook

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### Deliverable D.4.3. Integrated NPP-SOL MT and related handbook

This deliverable includes the technical procedure used for coupling the agro-hydrological model, **FLAWS-HAGES** (FLows of Water and Solute Transport in Heterogeneous Agricultural and Environmental Systems) (from now on simply FLOWS) and the bio-economic model, **DAHBSIM** (Dynamic Agricultural Household Bio-economic Simulation Model). The deliverable is a product of the combined activities carried out within the **Task 1.2. Conceptualisation of an operational multidimensional and multiscale integrated Modelling Tools** and the **Task 4.1. Integrating FLOWS-HAGES and DAHBSIM for simulations at field-farm scale**.

The handbook of the two models has been provided as Deliverable D.4.1. and D.4.2.

In the following, a short of summary of the two models will be given. Then, the coupling strategy will be illustrated, along with the coupling technical procedure. The conceptual and methodological requirements of the coupled Modelling Tool (MT), to be implemented in the WP4, were identified within the activities included in the Task 1.2.

#### The FLOWS model

FLOWS (Coppola et al., 2009, 2012, 2014, 2015, 2019) is a Dynamic Physically-Based model solving the Richards equation (RE) for water flow and the Advection Dispersion equation (ADE) for solute transport, including non-linear adsorption and other non-linear processes. The model produces information on the time evolution of water and solutes balance and, specifically, of all the functional processes involved (namely, evapotranspiration, root uptake of water and solutes, irrigation volumes, groundwater recharge, drainage, runoff, and nutrient transport). As for solute transport, the model allows for **salts, pesticides, phosphorus and nitrogen transport simulations**. In the case of nitrogen transport, the model accounts for several forms (both organic and mineral) of nitrogen fertilizers: 1) Manure; 2) Cover crops; 3) Urea; 4) N-NH<sub>4</sub> and N-NO<sub>3</sub> solid and liquid fertilizers. Furthermore, the model allows nitrification, denitrification and immobilization coefficients to be given node by node in the simulation domain. The model also describes the solute flow in **the gaseous phase**, essential for **pesticide transport simulations**.

#### The DAHBSIM model

DAHBSIM (Flichman et al., 2016, Komarek et al, 2017, El Ansari et al., 2023) is a dynamic, bio-economic model of agricultural households that was designed to be applied to a rural, developing country-setting, for the purpose of addressing questions around the biophysical constraints to on-farm agricultural productivity, and the whole-farm implications of alternative strategies to sustainable agricultural intensification. DAHBSIM **maximizes household objectives** subject to constraints and resources allocation patterns by linking a number of sub-modules related to economic, production (including livestock), and consumption decisions. It is a dynamic model, where agricultural technology is explicitly represented using the engineering production coefficients generated by the DAHBSIM crop module. It allows e.g. to consider all types of crop and livestock management activities, as well as on-farm processing and marketing activities, with data collected by the farm survey. It can **assess the performances for a wide range of farm types** differing in (i) resource endowments (land, labour, equipment availability); (ii) production intensity (i.e. output per hectare); (iii) specialisation (arable, livestock, mixed); (iv) biophysical conditions (soil, weather); (v) land use (grassland, annual crops, perennial crops, agro-forestry); (vi) farm management (organic, conventional, integrated); (vii)

production orientation (market, self-consumption); (viii) socio-economic contexts (CAP reform, water policy, agri-environmental policies), and is especially suitable to describe the diversity of agricultural systems across the Mediterranean region.

### **The Models coupling strategy**

The main link between the two models was identified in the calculation of the **crop biomass growth and yield** under **water and nutrient stresses and the impact of the production process on environmental indicators such water, erosion, nitrogen, organic matter, etc.** Actually, this is the main variable calculated in DAHBSIM and used for bioeconomic analysis. In order to understand the integration strategy, it is important giving a short summary of how the two models account for the crop growth and impacts.

#### *The crop growth in the actual version of FLOWS model*

In its actual configuration, FLOWS simulates the crop in a so-called static way, so that the crop growth is not simulated dynamically by the model but the user has to specify the crop development stage by giving as input the evolution over time of the leaf area index, root depth, reference evapotranspiration, as well as the crop coefficient as a function of development stage to convert reference evapotranspiration to the potential evapotranspiration of the considered crop. With this approach, the model “sees” the crop as a root system drawing water from the soil profile according to the atmospheric water vapor demand and the soil water availability, and as a soil cover which partitions the evapotranspiration in evaporation and transpiration components, and that partly intercepts rainfall or irrigation water.

The model computes internally actual evaporation and transpiration. Transpiration is distributed in a node-by-node root uptake in the root zone according to the root distribution. Actual transpiration is calculated in FLOWS by accounting for both water and osmotic stress functions. Low water contents and/or the presence of soluble salts in the soil lower the total hydraulic head and may reduce the water fluxes to the roots, thus reducing root activity and water uptake. Reduction coefficients to decrease the maximum water uptake according to the water and osmotic stresses may be calculated independently and multiplied to calculate the actual water root uptake. Details are given in the Deliverable D.4.1. FLOWS software and related handbook). Here, only a short summary of the procedure used in FLOWS to account water stress effects on actual transpiration. No nutrient stresses are included in the actual configuration of FLOWS.

### **Predicting actual transpiration and nutrient availability in FLOWS**

Actual Transpiration: In FLOWS, the potential root water uptake flux per unit depth at a specific depth,  $S_{r,p}$  [ $T^{-1}$ ], is simulated by distributing potential transpiration,  $T_p$  [ $L T^{-1}$ ], over the root zone depth,  $D_r$  [ $L$ ], on the basis of a normalized root density distribution,  $g(z)$  [ $L^{-1}$ ], with depth  $z$ .

The function  $g(z)$  distributes the potential transpiration rate,  $T_p$ , through the root zone in proportion to the root distribution (Feddes *et al.*, 1978; Feddes and Raats, 2004):

$$S_{r,p}(z) = g(z)T_p \quad (1)$$

with

$$\int_0^{Dr} g(z) dz = 1 \quad (2)$$

and thus

$$T_p = \int_0^{Dr} S_{r,p}(z) dz \quad (3)$$

Several root density distributions,  $g(z)$ , may be selected in the model for simulating the sink term in equation 1, assuming root distributions to be either homogeneous (Feddes et al., 1978) or variable with depth (Raats, 1974; Prasad, 1988; Vrugt et al., 2001), the latter accounting for the fact that in a moist soil the roots can mainly extract water from the upper root zone layers.

Low water contents and/or the presence of soluble salts in the soil lower the total hydraulic head and may reduce the water fluxes to the roots, thus reducing root activity and water uptake. Reduction coefficients to decrease the maximum water uptake according to the water and osmotic stresses may be calculated independently and multiplied to calculate the actual root uptake,  $T_a$ , as:

$$S_r = \alpha_w(h)\alpha_s(h_{os})S_p = \alpha_w(h)\alpha_s(h_{os})g(z)T_p \quad (4)$$

with  $\alpha_w$  and  $\alpha_s$  being reduction factors depending on the local (at a given  $z$ ) water pressure head,  $h$  [L] and osmotic head,  $h_{os}$  [L], respectively.

Accordingly,

$$T_a = \int_0^{Dr} S_r(z) dz \quad (5)$$

and

$$\frac{T_a}{T_p} = \int_0^{Dr} g(z) \alpha_w(h)\alpha_s(h_o) dz = \beta(h, h_{os}) \quad (6)$$

with  $T_a$  being the actual transpiration rate and  $\beta$  a dimensionless water stress index integrated over the whole rooted profile (Jarvis, 1989; Shouse et al., 2011), providing a measure of total plant stress. A value of  $\beta$  equal to 1 indicates that there is no stress in the soil root zone and that the actual transpiration rate  $T_a$  is equal to the potential transpiration rate  $T_p$ .

When the soil is irrigated by keeping soil water content under optimal conditions, the eventual reduction in root uptake may only be induced by osmotic stress. Under only osmotic stresses,  $\alpha_w=1$  and root uptake parameterization is reduced to finding the factor  $\alpha_s$ , depending on the osmotic potential ( $h_{os}$ ) induced by salts in the soil water.

#### Nutrient concentrations:

FLAWS model manages the incorporation of fertilizers, including organic matter like manure and crop residue, as well as mineral fertilizers. It requires input for the depth of incorporation (referred to as "zfert")

in the FLOWS code). The model assumes that fertilizer addition is evenly distributed throughout the incorporation depth. FLOWS offers two main capabilities:

1. Simulating the decomposition of organic matter and the transport of Carbon, Nitrogen, and Phosphorus. Here, the transformations of carbon, nitrogen, and phosphorus are influenced by the dynamics of organic matter decomposition, which in turn are affected by the ratios of carbon to nitrogen (C:N) and carbon to phosphorus (C:P).
2. Simulating only the transport of Nitrogen. In this scenario, nitrogen mineralization is modelled as an empirical decay reaction, independent of organic matter decomposition dynamics, and without considering the C:N ratio in the organic matter (Stanford and Smith, 1972; Watts and Hanks, 1978; Kersebaum and Richter, 1991).

All the details on how FLOWS simulates the different transformation processes of organic carbon, nitrogen and phosphorus are explained in deliverable 4.1 (FLOWS software and related handbook). In general, FLOWS simulates the immobilization and mineralization of organic nitrogen and phosphorus based on the C:N and C:P ratios. Then, the mineralized organic N-NO<sub>3</sub>, N-NH<sub>4</sub> and P-PO<sub>4</sub> enter into the mineral fertilizers pool along with the applied mineral fertilizers. Those pools are then subjected to different transformation processes.

As for the nitrogen, ammonium can go through volatilization and urea hydrolysis. Nitrogen can undergo nitrification and denitrification. Also, N-NH<sub>4</sub> can be adsorbed to the soil solid fraction. Eventually, N-NH<sub>4</sub> and N-NO<sub>3</sub> can be subjected to root uptake and/or drawing by artificial drains.

It is worth to note that, for the nitrogen transport in FLOWS, the Advection-Dispersion Equation (ADE) is solved twice; once for N-NH<sub>4</sub> and once for N-NO<sub>3</sub>:

$$\frac{\partial \theta C_{NH}}{\partial t} + \rho_b \frac{\partial C_{a,NH}}{\partial t} = \frac{\partial q C_{NH}}{\partial z} + \frac{\left( \partial \theta D \frac{\partial C_{NH}}{\partial z} \right)}{\partial z} - S_{S_{NH}} \quad (7)$$

$$\frac{\partial \theta C_{NO}}{\partial t} + \rho_b \frac{\partial C_{a,NO}}{\partial t} = \frac{\partial q C_{NO}}{\partial z} + \frac{\left( \partial \theta D \frac{\partial C_{NO}}{\partial z} \right)}{\partial z} - S_{S_{NO}} \quad (8)$$

where the subscripts NH and NO stand for N-NH<sub>4</sub> and N-NO<sub>3</sub>, respectively. The two sink terms in the equations 7 and 8 are linked through nitrification, which transforms part of the N-NH<sub>4</sub> to N-NO<sub>3</sub>. In general, S<sub>S<sub>NH</sub></sub> is affected by mineralization, urea hydrolysis, mineral fertilizer addition, nitrification, volatilization, root uptake and artificial drainage; and S<sub>S<sub>NO</sub></sub> is affected by nitrification, mineral fertilizer addition, denitrification, root uptake and artificial drainage.

As for the phosphorus, FLOWS simulates the transformations of liquid phosphorus according to the Mansell et al. (1977a) proposed decay reaction chains. The details of phosphorus transformations are provided in deliverable 4.1 (FLOWS software and related handbook). In general, FLOWS solves the ADE for phosphorus:

$$\frac{\partial \theta C_P}{\partial t} = \frac{\partial q C_P}{\partial z} + \frac{\left( \partial \theta D \frac{\partial C_P}{\partial z} \right)}{\partial z} - S_{S_P} \quad (9)$$

The sink term S<sub>S<sub>P</sub></sub> represents phosphorus adsorption, desorption, precipitation, dissolution, root uptake, loss to artificial drainage and organic and inorganic fertilizer application.

In case the user opts for simulating nitrogen only, FLOWS simulates nitrogen transport, primarily following the empirical approach of the RISK-N model (Gusman and Marino, 1999). It categorizes soil organic nitrogen into active and passive fractions, with the active fraction further divided into rapid and slow mineralization fractions. Rapidly mineralizing nitrogen includes recent additions like manure and crop residue, while the slow fraction comprises resident soil nitrogen still mineralizing and remaining organic nitrogen from past applications. The model handles nitrogen additions from manure, crop residue, and mineral fertilizers, assuming uniform distribution along the incorporation depth. Manure is assumed to contain 50% urea and 50% organic nitrogen, while crop residue incorporation assumes 50% rapid mineralization, 45% slow mineralization, and 5% passive fraction.

In this case, the mineralization process is assumed to follow a first-order decay which depends on the soil temperature and water content, rather than the C:N ratio. Similarly, the immobilization process does not depend on the C:N ratio, but rather on the soil temperature and the optimal temperature for immobilization, following the empirical approach proposed by Cabon et al. (1991). The other processes (i.e., urea hydrolysis, ammonium volatilization, nitrification, denitrification, root uptake and losses to artificial drainage) are simulated as previously described.

### **Predicting water and nutrient yield limitation in DAHBSIM**

In DAHBSIM, the yield may be reduced because of some water and nutrient (nitrogen) stresses. The actual yield limited by water in the summary cropping system model is calculated as follows (Doorenbos et al, 1986):

$$1 + \frac{Y_{w,act}}{Y_{w,pot}} = K_w \left( 1 - \frac{T_{act}}{T_{pot}} \right) \quad (10)$$

where  $Y_{w,act}$  is the actual yield limited by water ( $\text{kg ha}^{-1}$ ),  $Y_{w,pot}$  is the crop potential yield ( $\text{kg ha}^{-1}$ ) when no water stress exists,  $T_{act}$  is the actual transpiration ( $\text{mm day}^{-1}$ ) and  $T_{pot}$  is crop potential evapotranspiration ( $\text{mm day}^{-1}$ ) under optimal water availability.  $K_w$  is a factor accounting for the yield response to water stress and depends on cultivar properties.

There are numerous methods, but also difficulties, in modelling the uptake of nitrogen by crop, the humus and residues mineralization and the nitrogen leaching. As DAHBSIM is operating at global scale and to avoid undue complexity, DAHBSIM uses a simple module to simulate nitrogen-limited biomass by following the approach described by Stöckle et al., (1993). This approach assumes that nitrogen will act after water limiting has been accounted. In parallel, nitrogen uptake is co-regulated by both soil nitrogen availability and crop biomass accumulation (Sadras and Lemaire, 2014). For each simulation period (crop cycle period),  $NC_{crit}$  (the critical plant N concentration below which growth is reduced) and  $N_{min}$  (the minimum N plant N concentration) should be calculated as following (Stöckle et al., 1993):

$$GN = PNG \left( 1 - \frac{NC_{crit} - NC_a}{NC_{crit} - NC_{min}} \right) \quad (11)$$

where:

$GN$  = Nitrogen dependent growth ( $\text{kg ha}^{-1}$ ).

$PNG$  = Potential growth after other limiting factors have been accounted for ( $\text{kg ha}^{-1}$ ).

$NC_a$  = Crop nitrogen concentration after new growth ( $kg\ ha^{-1}$ ).

$NC_{crit}$  = Critical nitrogen concentration required by the crop to grow potential rate ( $kg\ ha^{-1}$ ).

$NC_{min}$  = Crop minimum nitrogen concentration at which growth stops ( $kg\ ha^{-1}$ ).

As the ratio between actual nitrogen absorbed ( $NC_{crit} - NC_a$ ) and nitrogen absorbed for potential growth ( $NC_{crit} - NC_{min}$ ) are correlated with the ratio actual yield to potential to potential yield, the dependent nitrogen-growth is calculated as following:

$$Y_N = Y_w \left( 1 - \frac{N_{ab}}{N_{pot}} \right) \quad (12)$$

where:

$Y_N$  = Actual yield after water stress ( $kg\ ha^{-1}$ ).

$N_{pot} = Y_{pot}/k$ , with  $N_{pot}$  the amount of N to grow at potential level ( $kg\ ha^{-1}$ ),  $Y_{pot}$  the potential yield (without N and Water stress) ( $kg\ ha^{-1}$ ),  $k$  a coefficient for N conversion.

Thus, equation 12 becomes

$$Y_N = Y_w \left( 1 - \frac{N_{ab}}{Y_{pot}/k} \right) \quad (13)$$

### Calculation of N absorbed by crop ( $N_{ab}$ )

The amount N absorbed by the crop ( $kg\ ha^{-1}$ ) will depend on N available in the soil and the N crop requirement as shown by the following two equations:

$$\begin{aligned} N_{ab} &= N_{av} & N_{av} < N_{pot} \\ N_{ab} &= N_{pot} & N_{av} \geq N_{pot} \end{aligned} \quad (14)$$

The calculation of soil available N,  $N_{av}$ , is based on a modified balance-sheet method, developed in France by Rémy and Hébert (1977), and used to calculate fertilizer N recommendation for the whole period of crop cycle. The balance-sheet method is mainly used to estimate the required N fertilizer in order to reduce at maximum the N leaching. DAHBSIM adopts the same methodology in order to calculate not the N-fertilizer application (which should be fixed by user), but the N available based on crop requirement and the changes in the soil mineral N content between the initial and the finale dates of the crop cycle as shown in the following equation 16:

$$N_{av} = N_{min} + N_o + NR + N_i + N_{comp} - N_L - N_f \quad (15)$$

In equation 15, the meaning of the different terms is as follows:

$N_{min}$  = amount of N mineralized from humus ( $kg\ ha^{-1}$ )

$N_{comp}$  = Amount of N from compost (%).

$N_o$  = N from organic fertilization ( $kg\ ha^{-1}$ )

$N_{fert}$  = N from mineral fertilization ( $kg\ ha^{-1}$ )

NR = N from previous crop residues ( $\text{kg ha}^{-1}$ ).

NL = N leaching (fixed at 10 % of  $N_{\text{fert}}$ ) ( $\text{kg ha}^{-1}$ ).

The  $N_{\text{ab}}$  is closely correlated to the target yield, so it can be nitrogen absorbed or the potential nitrogen available to the crop. This equation assumes that deposition of N from the atmosphere (non-symbiotic fixation, wet and dry deposition) is equal to gaseous emissions (volatilization, denitrification), which explains why these two terms do not appear in the equation.

The net contributions of the various sources to mineralization (humus, crop residues, organic wastes) are evaluated separately before they are accumulated, which means that there is no interaction between the various process.

In equation 15,  $N_{\text{min}}$  is the amount of N mineralized from humus ( $\text{kg ha}^{-1}$ ) and is calculated as:

$$N_{\text{min}} = \frac{H_i \cdot K_2 \cdot da \cdot Prof \cdot 10000}{19.5} \quad (16)$$

with

$H_i$ = amount of inorganic matter (%) (specified by soil, crops techniques);

$K_2$ = mineralization rate from humus (%), which affects the total N content of the ploughed layer. It is assumed that it will depend on percentage of clay, without considering the percentage of carbonate in the soil and the mean annual temperature as suggested by Mary and Guérif (1994). Here also we assume that only the old fraction of humus can be mineralized.

$da$ = soil bulk density ( $\text{kg m}^{-3}$ )

$Prof$ = depth of the ploughed layer (m)

### Reasons for coupling DAHBSIM to FLOWS

In DAHBSIM, water and nitrogen stresses are both calculated through a simplified balance. This is mostly unable to predict in an oriented process way the effects of irrigation and nutrient management on the actual availability of water and nutrients along the root zone.

By contrast, FLOWS may provide water and nutrient (both nitrogen and phosphorus) stresses based on a physically-based approach to water and solute balance, which allows predicting the distribution evolution of water, nitrogen, phosphorus (and any other relevant nutrient) in the whole soil profile and in the root zone under different top and bottom boundary conditions and alternative irrigation and nutrient management. What's more, FLOWS also calculates osmotic stresses related to the salinity of the irrigation water, which is relevant for the objectives of the NPP-SOL project, especially when the issue of pollution prevention or reduction overlaps to that of salinity management.

In this sense, in order to make the predictions of the DAHBSIM model more physically-based, the best coupling strategy between the two models may be using FLOWS to produce water, osmotic and nutrient stresses and their effects on the crop biomass and yield under different water and nutrient managements. In sequence, the output of FLOWS in terms of yield may be passed as input to the model DAHBSIM, which in turn will provide the economics evaluation of the alternative management approaches. However, this approach required integrating a crop growth module in FLOWS.

### Integrating a crop growth module in FLOWS

Crop models estimate crop yields based on weather, soil conditions, and management practices (Hoogenboom et al., 1994). Many crop growth models have been developed over the years, such as EPIC (Williams, 1990), CROPSYST (Stockle et al., 2003), and WOFOST (van Diepen et al., 1989), which have been effectively used for simulating crop growth and yield. The DSSAT (Jones et al., 2003; Hoogenboom et al., 2015) and APSIM (Brown et al., 2014) series models are currently popular for integrating various crop models into a single platform. DSSAT is a collection of field-scale, process-based crop models capable of simulating both crop and soil processes. Additionally, in recent decades, specific models have been developed for certain crops, including SORKAM (Rosenthal et al., 1989), SorModel (Arora, 1982), SORGF (Wiegand and Richardson, 1984), and ALMANAC for sorghum management, WTGROWS (Sehgal and Sastri, 2005) for wheat, SOYGRO (Hoogenboom et al., 1990) for soybean, GOSSYM (Boone et al., 1993), and COTONS (Jallas et al., 2000).

For the integration purpose, we relied on EPIC crop growth model (Williams et al., 1989). EPIC utilises one routine to simulate all crops' growth. This facilitates the consistent calibration process development for different crops. The integration was carried out by adopting, from EPIC, the daily-scale processes of: solar radiation interception by crops and converting it to biomass; biomass partitioning into roots, above-ground biomass and economic yield; Leaf-Area Index, LAI, and root growth. Similar to EPIC model, FLOWS calculates the daily potential biomass from Photosynthetically Active Radiation, PAR, and radiation-use efficiency. The actual biomass is then calculated by reducing the potential one due to calculated daily stresses caused by either too low or high temperatures, water and nutrient limitations, and/or oxygen deficit. Eventually, the crop yield is calculated as a ratio of economic yield over the total actual above-ground biomass at maturity which is defined by harvest index.

Unlike EPIC model, the temperature, water and nutrient stresses in the crop growth module of FLOWS are computed using pressure heads and nitrate and phosphorus concentrations and temperatures simulated by FLOWS. Pressure heads are calculated by solving Richards Equation, RE, for water flow, the concentrations are obtained by solving the Advection-Dispersion Equation, ADE, for solute transport and the temperatures are simulated by van Wijk and De Vries (1963) solution for heat flow equation.

The crop's phenological development in EPIC is computed as the following equation, based on daily heat unit accumulation:

$$HU_k = \frac{(T_{mx,K} + T_{mn,K})}{2} - T_{b,j} \quad (17)$$

where  $HU_k$ ,  $T_{mx,K}$ ,  $T_{mn,K}$ , are heat units, maximum temperature and minimum temperature in °C for any day K, and  $T_{b,j}$  is the base temperature in °C (no growth occurs at or below  $T_{b,j}$ ) of crop j with no crop growth occurring at or below  $T_{b,j}$ .

Then, a Heat Unit Index, HUI, ranging between 0 and 1 for planting and crop maturity, respectively, is calculated:

$$HUI_i = \frac{\sum_{K=1}^i HU_K}{PHU_j} \quad (18)$$

where  $HUI_i$  is the heat unit index for day  $i$  and  $PHU_j$  is the potential heat units required for maturity of crop  $j$ . The value of  $PHU$  may be provided by the user or calculated by the model from normal planting and harvest dates.

$HUI$  affects the harvesting date, leaf area growth and senescence, optimum plant nutrient concentrations, and biomass partitioning among roots, shoots, and economic yield are affected by  $HUI$ .

### Potential growth

Solar radiation interception is calculated based on Beer's law (Ritchie, 1972) using an extinction factor,  $k_{ex}$ :

$$PAR_i = 0.5RA_i[1 - \exp(-k_{ext}LAI_i)] \quad (19)$$

where  $PAR$  is intercepted photosynthetic active radiation in  $MJm^{-2}$ ,  $RA$  is solar radiation in  $MJm^{-2}$  and subscript  $i$  is the day of the year. The constant, 0.5, is used to obtain the photosynthetically active radiation from solar radiation (Monteith, 1973). Experimental studies attest that foliage characteristics, sun angle, row spacing, row direction, and latitude lead to the variation of  $k_{ex}$  (Thornley, 1976). A value of 0.65 is recommended for narrowly spaced crop rows Williams (1989). Smaller  $k_{ex}$  values (0.4-0.6) are more representative of tropical areas where the sun angle is higher and the row spacing is wider.

The potential increase in biomass can be estimated as follows (Monteith, 1977):

$$\Delta B_{p,i} = 0.001 BE_j PAR_i (1 + \Delta HRLT_i)^3 \quad (20)$$

where  $\Delta B_{p,i}$  is the daily potential increase in biomass in  $t ha^{-1}$ ,  $BE$  is the crop parameter for converting energy to biomass in  $kg ha MJ^{-1} m^2$ ,  $HRLT$  is the daylength in hours and  $\Delta HRLT_i$  is the daylength's daily change in  $h d^{-1}$ .

In equation 10, the daylength increases the potential growth in the spring and reduces it in the autumn. It empirically represents the effect on plant growth by the rate of change of daylength, even if this phenomenon is poorly understood (Baker et al., 1980).

Daylength at any day  $i$ ,  $HRLT_i$ , is a function of the time of year and latitude as expressed in the equation:

$$HRLT_i = 7.64 \cos^{-1} \left[ \frac{-\sin\left(\frac{2\pi}{360}LAT\right)\sin(SD_i) - 0.44}{\cos\left(\frac{2\pi}{360}LAT\right)\cos(SD_i)} \right] \quad (21)$$

where  $LAT$  is the latitude of the simulated area in degrees and  $SD$  the sun's declination angle,  $SD_i$ , which is defined as:

$$SD_i = 0.4102 \sin \left[ \frac{2\pi}{365} (i - 80.25) \right] \quad (22)$$

For most crops, LAI value is zero or minimal at the beginning. It then increases at an exponential rate during early vegetative growth when leaf appearance, blade expansion and leaf primordia development rates are linearly proportional to the cumulative heat unit. LAI of vegetative crops, like sugarcane, reaches a plateau where the leaf area is approximately equal to leaf senescence. In other crops, LAI reaches a maximum value and then decreases, approaching zero at maturity. Also, the final LAI, leaf expansion and leaf duration are decreased by different stresses. Daily LAI is then calculated, based on heat units, crop development stages and crop stress, according to the following equations:

$$LAI_i = LAI_{i-1} + \Delta LAI \quad (23)$$

$$\Delta LAI = \Delta HUF LAI_{mx} (1 - \exp(LAI_{i-1} - LAI_{mx})) \sqrt{REG_i}$$

where HUF is the heat unit factor and REG is the value of the minimum crop stress factor, which is discussed in details later. Subscript mx is the maximum value possible for the crop and  $\Delta$  is the daily change. Equation 23 contains an exponential function that keeps LAI from exceeding  $LAI_{mx}$  when HUF is modified for certain crops vernalization. The HUF is obtained as follows:

$$HUF_i = \frac{HUI_i}{HUI_i + \exp(ah_{j,1} - ah_{j,2}HUI_i)} \quad (24)$$

For each crop j, two values for each of HUF and HUI are specified as a sigmoid relationship. Therefore, the parameters  $ah_{ji}$  and  $ah_{j2}$  can be calculated by simultaneously solving equation 14 twice using the two pairs of HUF and HUI values. Starting from leaf declining to the end of growing season, daily LAI can be estimated as:

$$LAI_i = LAI_0 \left( \frac{1 - HUI_i}{1 - HUI_0} \right)^{ad_j} \quad (25)$$

Where  $HUI_0$  is the HUI value at the beginning of leaf decline and ad is a parameter governing LAI decline rate for crop j.

Crop height is estimated as:

$$CHT_i = HMX_j \sqrt{HUF_i} \quad (26)$$

where CHT is the crop height in m and HMX is the maximum height for crop j.

According to Jones (1985), the proportion of total biomass allocated to the root system typically declines from 30-50% in seedlings to 5-20% at maturity. The model predicts that the portion of crop growth directed to the root system decreases linearly from 40% at emergence to 20% at maturity.

This method of estimating root growth yields realistic exponential decreases in root weight with depth, provided soil water and other properties do not limit growth. However, if a soil layer is dry or if root stress factors (such as strength, aluminum saturation, or aeration) restrict root function, both water uptake and root growth in that layer decrease.

Rooting depth typically increases rapidly from the seeding depth to a crop-specific maximum, which many crops reach well before physiological maturity (Borg and Grimes, 1986). Rooting depth is modeled based on heat units and the potential depth of the root zone:

$$RD_i = 2.5RDMX_jHUI_i \quad RD_i \leq RZ_j \quad (27)$$

where RD is the root depth in m, RDMX is the maximum root depth for crop j in ideal soil in m, RZ is the soil profile depth in m and the constant 2.5 allows root depth to reach its maximum when HUI reaches 0.4.

The reproductive organs represent the economic yield of most grain, pulse, and tuber crops. These crops possess various mechanisms to balance their production: it is neither too excessive to be sustained by the vegetative parts nor too minimal to ensure the species' survival. Consequently, the harvest index (economic yield divided by above-ground biomass) tends to remain relatively stable across different environmental conditions. In EPIC, crop yield is estimated using the harvest index concept:

$$YLD_j = HI_j B_{AG} \quad (28)$$

where YLD is the quantity of economic yield that could be removed from the field in  $t \text{ ha}^{-1}$ , HI is the harvest index and  $B_{AG}$  is the above-ground biomass in  $t \text{ ha}^{-1}$  for crop j.

For conditions with no stresses, harvest index experiences nonlinear increase starting from zero at planting to HI at maturity using the equation:

$$HIA_i = HI_j \sum_{K=1}^i \Delta HUFH_K \quad (29)$$

where HIA is the harvest index on day i and HUFH is the heat unit factor that influences the harvest index, which is obtained as:

$$HUFH_i = \frac{HUI_i}{HUI_i + \exp(6.5 - 10.0 HUI_i)} \quad (30)$$

The constants in equation 30 are set to make HUFH<sub>j</sub> increase from 0.1, at HUI<sub>i</sub> = 0.5, to 0.92, at HUI<sub>i</sub> = 0.9. This is compatible with economic yield development for grain crops whose most economic yield is in the second half of the growing season.

## Nutrient uptake

### Nitrogen

Crop nitrogen, N, use is calculated based on supply and demand. The daily demand of N by crop is the difference between the crop nitrogen content and the crop ideal N content for any day i. Therefore, the demand is calculated as:

$$UND_i = c_{NB_i} B_i - \sum_{K=1}^i UN_K \quad (31)$$

where  $UND$  is the crop N demand  $\text{kg ha}^{-1}$ ,  $UN$  is the actual N uptake in  $\text{kg ha}^{-1}$ ,  $C_{NB}$  is the optimal crop N concentration of the crop in  $\text{kg t}^{-1}$  and  $B$  is the daily accumulated biomass in  $\text{t ha}^{-1}$  for day  $i$ . The optimal crop N concentration decreases with the increase in growth stage (Jones, 1983a) and is computed as a function of growth stage using the equation:

$$c_{NB_i} = b_{n1} + b_{n2} \exp(-b_{n3} HUI_i) \quad (32)$$

where  $HUI$  (heat unit index) is the fraction of the growing season and  $b_{n1}$ ,  $b_{n2}$  and  $b_{n3}$  are parameters calculated from crop-specific concentrations of N in the plant at the seedling stage, halfway through the season, and at maturity, respectively. Mineral nutrients are up taken by plant roots mainly by mass flow and diffusion.

### Growth Constraints

Potential crop growth and yield are often not fully achieved due to environmental constraints. The model estimates stresses from water, nutrients, temperature, aeration, and radiation, which range from 0.0 to 1.0 and affect plants in various ways. In EPIC, these stresses are used to estimate limitations on biomass accumulation, root growth, and yield. As for the constraint, it is determined by the lowest value among water, nutrient, temperature, and aeration stresses. As for root growth constraint, it is determined by the lowest value among soil strength, temperature, and aluminum toxicity.

As mentioned, in FLOWS, most of these limiting factors are calculated using water content, nutrient concentrations, and temperature, which are derived from solving the model's physically based equations for water flow, solute transport, and heat flow.

The following sections describe the stress factors involved in determining each constraint. For each factor, we will specify whether it is taken from EPIC or derived from FLOWS calculations.

### Biomass growth

The potential biomass in equation 10 is reduced daily if any of the five plant stress factors is less than 1.0 using the equation:

$$\Delta B = \Delta B_p \cdot REG \quad (33)$$

where  $REG$  is the crop growth regulating factor (the minimum stress factor).

**Water Stress (from FLOWS):** The water stress factor in FLOWS,  $WS$ , is calculated  $\beta(h, h_{os})$  in equation 6. It also includes the osmotic stress (due to solute concentration) and the aeration stress (oxygen deficit).

**Temperature Stress (from EPIC-FLOWS):** The plant temperature stress is estimated with the equation:

$$TS_i = \sin\left(\frac{\pi}{2} \frac{T_{gi} - T_{bj}}{T_{oj} - T_{bj}}\right) \quad 0 \leq TS_i \leq 1 \quad (34)$$

where TS is the plant temperature stress factor,  $T_g$  is the daily average temperature at soil surface in °C,  $T_{bj}$  and  $T_{oj}$  are the base and optimal temperatures for crop  $j$ , respectively. Equation 34 creates a symmetrical stress around the optimal temperature and it is driven by  $T_g$ . This approach allows for the realistic response of small plants to low soil temperatures which are found in the spring season in temperate regions. While the approach for deriving equation 34 is adopted from EPIC, the daily values of  $T_g$  is computed by FLOWS.

**Nutrient Stress (EPIC-FLOWS):** The nitrogen and phosphorus stress factors are obtained according to the ratio of simulated plant N and P contents to their optimal values. The stress factors decrease nonlinearly from 1.0, at optimal N and P concentrations, to 0.0, when N or P is half the optimal level (Jones, 1983a). In the case of N stress, the scaling equation is:

$$SN_{S,i} = 2 \left(1 - \frac{\sum_{K=1}^i UN_K}{C_{NB,i} B_i}\right) \quad (35)$$

where  $SN_s$  is a scaling factor for the N stress factor,  $C_{NB}$  is the crop's optimal N concentration on day  $i$ ,  $B$  is the accumulated biomass in  $\text{kg ha}^{-1}$  and  $UN$  is the crop N uptake on day  $i$  in  $\text{kg ha}^{-1}$ . The N stress factor is obtained as:

$$SN_i = 1 - \frac{SN_{S,i}}{SN_{S,i} + \exp(3.39 - 10.93SN_{S,i})} \quad (36)$$

where SN is the daily nitrogen stress factor. As for the P stress factor, SP, it can be obtained by rewriting equations 35 and 36 in P terms. Again, while the approach for deriving equations 35-36 is taken from EPIC, the daily value of  $UN_K$  is calculated by FLOWS. Finally, the value of REG is determined as the minimum of WS, TS, SN and SP.

### Root Growth

The root depth,  $RD_i$ , calculated by equation 27, can be limited by soil strength, temperature and/or aluminum toxicity. Thus, the root growth is constrained by the minimum of those three stress factors. Several studies showed that soil strength affects root growth. Soil strength can be determined by the soil bulk density, texture and water content (Williams, 1989). All three of these variables are considered in EPIC to estimate soil strength stress factor using the following equation:

**Soil strength stress (EPIC-FLOWS):**

$$SS_z = 0.1 + \frac{0.9BD_z}{BD_z + \exp(bt_1 - bt_2BD_z)} \quad (37)$$

where  $SS_z$  is the soil strength factor at depth  $z$ ,  $BD$  is the soil bulk density adjusted for water content in  $\text{tm}^{-3}$ , and  $bt_1$  and  $bt_2$  are parameters that depend on soil texture. The subscript  $z$  stands for the values at any depth  $z$ . The  $bt_1$  and  $bt_2$  values are calculated as:

$$bt_2 = \frac{\ln(0.112BDL) - \ln(8BDU)}{BDL - BDU} \quad (38)$$

$$bt_1 = \ln(0.112BDL) - bt_2BDL$$

where  $BDL$  and  $BDU$  are the lower and upper boundary values for bulk density for a particular sand percentage,  $SAN$  (Jones, 1983):

$$BDL = 1.15 + 0.00445 SAN \quad (39)$$

$$BDU = 1.5 + 0.05 SAN$$

The bulk density adjusted for water content, which is used in equation 27, is estimated by as (Grossman et al., 1985):

$$BD_z = BD_3 + (BDD - BD_3) \left( \frac{FC_z - WC_z}{FC_z - WP_z (4.083 - 3.33BDD^{1/3})} \right) \quad (40)$$

where  $BD$  is the daily bulk density, on day  $i$ , adjusted for water content,  $BD_3$  is the bulk density at the water content corresponding to 33 kPa of soil water pressure head,  $BDD$  is the oven-dry bulk density,  $FC$  is the field capacity,  $WP$  is the wilting point, and  $WC$  is the actual soil water content at depth  $z$  on day  $i$ . The water content,  $WC_z$ , is calculated by FLOWS.

### Special cases

**Nitrogen Fixation:** In EPIC, daily nitrogen fixation is estimated as a fraction of daily legumes N demand.

$$WFX_i = FXR_i UND_i \quad WFX_i \leq 6.0 \quad (41)$$

where  $WFX$  is the amount of N fixation in  $\text{kg ha}^{-1}$  and  $FXR$  is the fraction of uptake on day  $i$ . The fraction,  $FXR$ , is estimated as a function of soil  $\text{NO}_3$  content, water content and plant growth stage:

$$FXR = \min(1.0, FXW, FXN) \cdot FXG \quad (42)$$

where  $FXG$  is the growth stage factor,  $FXW$  is the soil water content factor, and  $FXN$  is the soil  $\text{NO}_3$  content factor. The growth stage factor prevents N fixation in: young plants before developing the functional nodules, as well as in old plants with senescent nodules (Patterson and LaRue, 1983):

$$FXG_i = 0 \quad HUI_i \leq 0.15, HUI_i \geq 0.75 \quad (43)$$

$$FXG_i = 6.67 HUI_i - 1 \quad 0.15 < HUI_i \leq 0.3$$

$$FXG_i = 1 \quad 0.3 < HUI_i \leq 0.55$$

$$FXG_i = 3.75 - 5HUI_i \quad 0.15 < HUI_i < 0.75$$

where HUI is the heat unit index for day  $i$ .

The soil water content factor reduces N fixation when the water content at the top 0.30 m of the soil is at less than 85% of field capacity (Bouniols et al., 1985) using the equation:

$$FXW_i = \frac{SW_{0.3} - WP_{0.3}}{0.85(FC_{0.3} - WP_{0.3})} \quad SW_{0.3} < 0.85(FC_{0.3} - WP_{0.3}) + WP_{0.3} \quad (44)$$

where  $SW_{0.3}$ ,  $WP_{0.3}$ , and  $FC_{0.3}$  are the water contents in the top 0.3 m of soil on day  $i$ , at wilting point, and at field capacity.

N fixation can also be affected by amount of  $NO_3$  in the root zone. Bouniols et al. (1985) determined the soil  $NO_3$  factor, FXN:

$$FXN = 0 \quad WNO3 > 300 \text{ kg ha}^{-1} \text{ m}^{-1}$$

$$FXN = 1.5 - 0.005 \left( \frac{WNO3}{RD} \right) \quad 100 < WNO3 \leq 300 \text{ kg ha}^{-1} \text{ m}^{-1} \quad (45)$$

$$FXN = 1 \quad \leq 100 \text{ kg ha}^{-1} \text{ m}^{-1}$$

where WNO3 is the weight of  $NO_3$ —N in the root zone in  $\text{kg ha}^{-1}$  and RD is the root depth in m. This approach reduces N fixation when the  $NO_3$ —N content of the root zone is greater than  $100 \text{ kg ha}^{-1}$  and prohibits N fixation at N contents greater than  $300 \text{ kg ha}^{-1}$

#### Winter dormancy:

Daylength growth constraint is applied to simulate the dormant period for crops planted in the autumn. This constraint is applied exclusively to regions with a growing season shorter than 12 months. In the model, a 12-month growing season for warm-season crops is characterized by the absence of any month with a mean minimum temperature below  $5^\circ\text{C}$ . A dormant winter period is identified as the period when the daylength is within one hour of the location's shortest daylength.

When a crop goes through a winter dormancy period, the heat unit summation is reset to zero. This facilitates the rapid new growth once temperatures rise in spring. Throughout the dormancy phase, plant growth is stopped. Additionally, the standing live biomass diminishes during this period due to frost and shorter day lengths. The reduction factor for daylength is calculated as:

$$FHR_i = 0.35 \left( 1 - \frac{HRLT_i}{HRLT_{mn} + 1} \right) \quad (46)$$

where FHR is the daylength reduction factor,  $HRLT_i$  is the daylength on day  $i$ , and  $HRLT_{mn}$  is the minimum daylength for the location. The frost reduction factor is estimated with the equation:

$$FRST_i = \frac{T_{mn,i}}{-T_{mn,i} - \exp(a_{f_{j,1}} + a_{f_{j,2}} T_{mn,i})} \quad T_{mn,i} < 1 \text{ } ^\circ\text{C} \quad (47)$$

where  $FRST$  is the frost damage factor,  $T_{mn}$  is the minimum temperature on day  $i$  in  $^\circ\text{C}$ , and  $a_{f_{j,1}}$  and  $a_{f_{j,2}}$  are parameters representing the crop's frost sensitivity.

The standing live biomass reduction is estimated with the equation:

$$\Delta B_{AG,i} = 0.5 B_{AG,i} (1 - HUI_i) \cdot \max(FHR_i, FRST_i) \quad (48)$$

where  $\Delta B_{AG,i}$  is the reduction in above ground biomass in  $\text{t ha}^{-1}$  on day  $i$ ,  $HUI$  is the heat unit index, and  $B_{AG,i}$  is the above ground biomass in  $\text{t ha}^{-1}$  on day  $i$ . The frost damage is greater when plants are small, i.e., when  $HUI_i \approx 0$ , and approaches zero near maturity.

### **The FLOWS-DAHBSIM coupling procedure**

For the coupling with DAHBSIM, we opted for a “sequential approach”. First, we simulate water flow, nutrient transport and crop growth using FLOWS. Within FLOWS, the pressure head and nutrient concentrations in the root zone, as well as the temperature distribution, are used to calculate the stress factors, to be used to reduce the potential biomass and yield. The actual biomass and yields are thus used as input in the DAHBSIM model for bioeconomic simulations. **This procedure mostly makes the hydrological component of the model more physically based.**

The figure 1 provides a schematic view of the FLOWS – DAHBSIM model coupling approach. The coupling is obtained by firstly integrating an EPIC-based crop growth model in FLOWS. EPIC uses some vegetation input related to the crop type and, in turn, produces other vegetation output to be used by FLOWS. In order to emphasize this circular feedback, in the figure the vegetation data window is partially represented outside the FLOWS input data block. FLOWS, in turn, produces distributions of soil water, temperature and nutrient (nitrogen, phosphorus, etc.) concentrations along the soil profile, which are input for the growth model. Finally, the latter gives the time evolution of the above ground biomass and yield, to be used as input for the bioeconomic analysis in DAHBSIM. FLOWS and the growth model are fully integrated, using the same simulation  $\Delta t$ . By contrast, FLOWS and DAHBSIM are used in sequence, with DAHBSIM using as input the time evolution of biomass and yield provided by FLOWS.

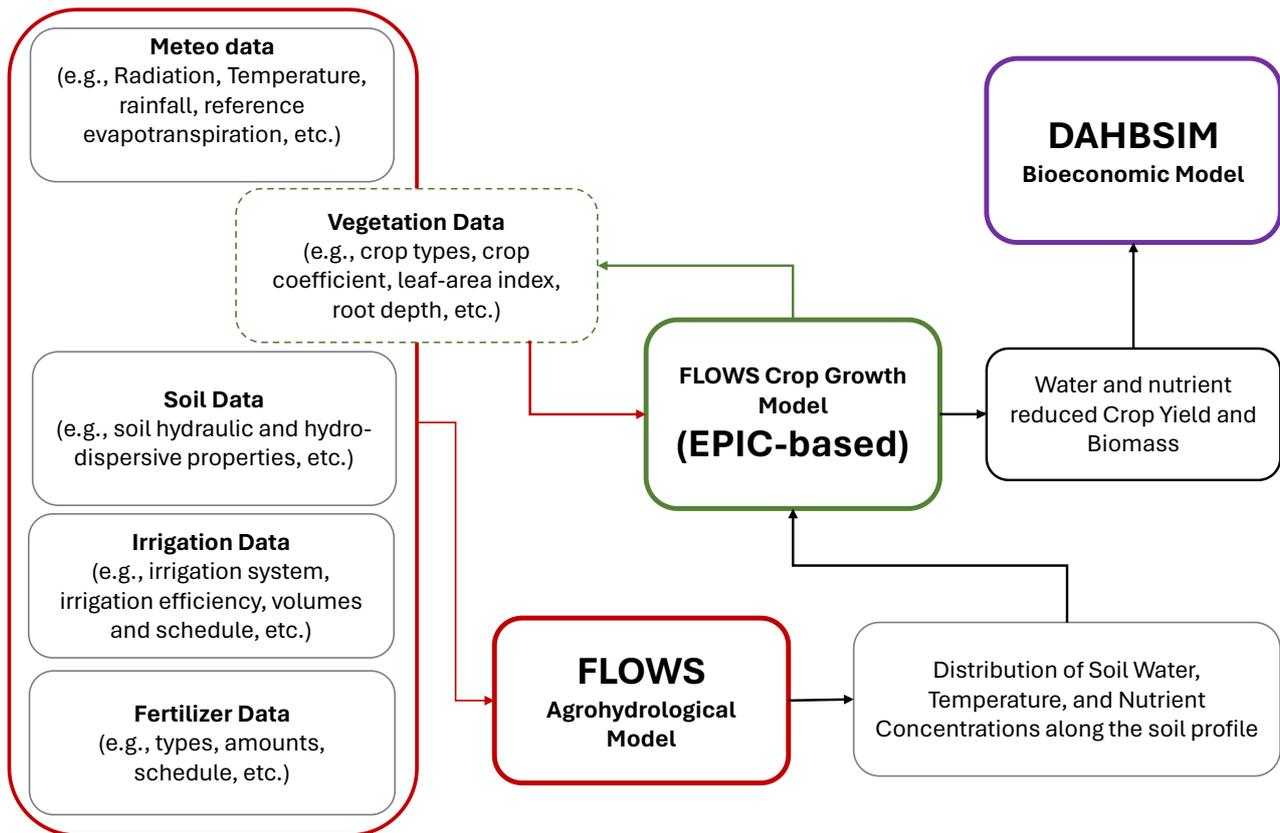


Figure 1. Schematic view of the FLOWS – DAHBSIM model coupling approach. The coupling is obtained by firstly integrating an EPIC-based crop growth model in FLOWS. The latter uses some vegetation input related to the crop type and, in turn, produces other vegetation output to be used by FLOWS. This is the reason why the vegetation data window is partially represented outside the FLOWS input data block. FLOWS, in turn, produces distributions of soil water, temperature and nutrient (nitrogen, phosphorus, etc.) concentrations along the soil profile, which are input for the growth model. Finally, the latter gives the time evolution of the above ground biomass and yield, to be used as input for the bioeconomic analysis in DAHBSIM. FLOWS and the growth model are fully integrated, using the same simulation  $\Delta t$ . By contrast, FLOWS and DAHBSIM are used in sequence, with DAHBSIM using as input the time evolution of biomass and yield provided by FLOWS.



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