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DEVELOPING PLANT MODELS OF REDUCED COMPLEXITY BY CHEMICAL PROCESS ENGINEERING WAY OF THINKING

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Given the increasing complexity of agricultural systems within the broader context of the bio-based circular economy, simplified and unified plant models are needed that represent the primary biomass production by solar-driven carbon-dioxide sequestration. Utilizing experiences from process systems engineering, which was originally inspired by chemical engineering, a suitable plant model is proposed. The structure of the model is generated from the process net of the underlying state and transition elements. Two special-state elements are introduced for the short-term storage of the supplied biomass to be distributed and of the uptake of nutrient-containing water, necessary for evapotranspiration and photosynthesis. The transition-oriented description of functionalities follows the essential causalities and balances of natural self-control. Implementation of the model is illustrated by a simple example.

Keywords: plant model, reduced complexity, stoichiometric processes, process network, supply/demand logistics, natural self-control

1. Introduction

The bio-based circular economy is crucial to secure the supply of food and materials for mankind given the burden of depleting non-renewable resources and finite reservoirs. The replacement of open process systems with circular ones needs conscious engineering planning and operations while systemically overviewing the underlying processes. Multisectoral process networks require the coupling of sub-models from various disciplines on different scales. In the bio-based circular economy, the photosynthetic biosystems (plants) represent biomass production from solar energy, i.e. from the only external, unlimited energy resource for our planet. Accordingly, the model-based analysis, planning and operation of cultivated and natural plants plays an important role.

Recently, motivated also by the increasingly integrated engineering of natural and man-made systems, intensive bidirectional learning has commenced between the computational modeling of natural and man-made processes whereby:

- the principles of more sustainable and resilient natural ecosystems can be applied in the design and control of man-made systems on the one hand, while
- the experiences of industrial systems designed by engineers can be taken into account with regard to the model-based analysis, planning and operation of agricultural cultivation on the other.

Although systems of chemical process engineering played a unique role in this knowledge transfer because the underlying multidisciplinary processes were complex enough to represent various features, they were not too complex for the application of formerly applied computational tools. The lessons learnt from chemical process systems are still clearly important in terms of the rapidly developing model-supported problem-solving of complex agri-food and agro-environmental process systems. This paper shows how chemical process engineering can be used to develop plant (crop) models of limited complexity.

First, some available plant models will be overviewed in brief. Two different approaches are available, namely (i) empirical (statistical) models to calculate various specific sources of biomass production and (ii) the mechanistic (biophysical) models that describe the underlying physical, chemical and biological processes, representing causalities and balances. This overview focuses on the mechanistic crop models.

Physiological models are important to further our understanding of metabolism, growth and how plants respond to environmental conditions, e.g. climate change [1]. The detailed dynamic modeling of physiological processes is not a novel endeavor, in fact it was

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already applied at the end of the previous century [2–5]. However, because of the increasing complexity of Water-Energy-Food-Ecosystems Nexus [6–8], besides detailed biophysical models, the systemic coupling of these biophysical models from various disciplines is also necessary, which also requires flexible models to couple economic considerations [9].

Regarding the level of detail, the improved understanding of physiological characteristics and the expected response to environmental changes require mechanistic models at both the cellular and organ level [10]. However, their practical applicability, considering the available data and knowledge, also requires the development of advanced coupling models.

Various complex crop models are available. In a recent paper, eight kinds of crop models are classified and compared [11], the most important of which are as follows:

Agricultural Production Systems sIMulator (APSIM) is an actively evolving tool for the modeling and simulation of a wide range of agricultural systems, including plants, animals and soil, which also takes into consideration management actions and climatic effects [12]. The crop-related parts contain the detailed biophysical description concerning the phenology, biomass accumulation and distribution of newly synthesized biomass as well as the uptake of water and components by taking into account the related limitations and dependencies on environmental conditions.

STICS is a detailed biophysical modeling tool that considers water, carbon as well as thermal and radiation energy balances for many (ca. 20) different crops ([13, 14]). It also clearly represents the phenological stages and the most important biophysical processes, e.g. light interception, transpiration, uptake of water and nutrients, etc.

Cropping Systems Simulation Model [15] is also a frequently used simulation model that takes into consideration the soil water budget, soil-plant nitrogen budget, crop-canopy and root growth, dry matter production, yield, residue production and decomposition as well as several management options, e.g. cultivar selection, crop rotation, irrigation, fertilization, tillage operations, residue management, etc.

Recently, the rediscovery of advantages regarding the coupling of tree and crop systems by combining their models has also come to the fore. Both APSIM and STICS follow this direction. A few validated tree models are available that are integrated in APSIM to be used in combination with plants [12]. On the other hand, a STICS crop model is embedded in the Hi-sAFe agroforestry tool [16].

2. Challenges and objective

Plant models for well-defined important crops and trees are available. These detailed, specific models require a considerable set of parameters to be identified, moreover, the increasing design space of the bio-based circular economy needs simplified, approximate, unified, flexible, extensible and connectible plant models.

The objective of this paper is to introduce the conceptual framework and experimental implementation of a unified plant model of reduced complexity. To develop the model, the following chemical process engineering-based principles were applied:

- generalized unit operations;
- specific stoichiometric composition of pseudo-components and other entities;
- stoichiometric conservation processes based on the model-specific conservation laws, e.g. conservation of atoms in chemistry; and
- demand-supply chain-like representation of material flows driven by the underlying push or pull logistics.

3. Materials and methods

3.1 *Data and calculation formulae for a typical example of a plant to be modelled*

As an illustrative example of a man-made and operational plant ecosystem, a cultivated field of maize was modeled, where 9600 individual plants were cultivated over an area of 1600 m^2. The maize-related specific data were derived from the literature [17–19].

Within the contours of the outlined system, this cultivated field was associated with the connected layers of soil and the compartment of air. The environmental conditions were taken into consideration in accordance with the data from the respective meteorological database.

The initial data of the plants refer to the stage following the sowing of the seeds when the initial biomass of the plants is contained within the seeds and sprouting has not yet occurred. The initial conditions of the seed biomass (based on estimations by experts) and its components [20, 21] are the following:

Biomass = 0.0003 kg/plant
C = 0.03747 kmol/kg
H = 0.06999 kmol/kg
O = 0.02846 kmol/kg
N = 0.00154 kmol/kg
P = 0.00011 kmol/kg
X = 0 kmol/kg
H_2O = 0.118 kmol/kg
O_2 = 0.00066 kmol/kg

Germination is an event-driven process that occurs after the time-driven sowing. Sowing, which is a management process, is modelled by putting the seeds into downflow material storage. Afterwards, in the event of the appropriate environmental (meteorological and hydrological) conditions, the seeds germinate resulting in the release of these stored materials in accordance with the following parameters (based on estimations by experts):

Seed biomass = 0.0001 kg/pc

Seed rate $= 6.579 \times 10^{-7}$ kg/h
Proportion of leaves $= 0.853$
Proportion of roots $= 0.147$
Surface area ratio of leaves $= 6.667$ m^2/kg
Surface area ratio of roots $= 3.003$ m^2/kg

In our example model, the germination period is from April 20th until May 9th.

After the leaves and roots appear, resulting from the event-driven process of germination, the life processes of plants, that is, photosynthesis, growth, respiration, evapotranspiration and uptake, start.

The rate of *photosynthesis* is calculated by the following simplified equations [19]:

$$\Delta \mathrm{BiomassDry} = \frac{\mathrm{Num\ Rad\ F_t\ E_t}}{\rho}\mathrm{DT} \qquad (1)$$

where
ΔBiomassDry = biomass produced, kg,
Num = number of plants, pc.
Rad = radiation, W/m.J^2
$\mathrm{F_t}$ = proportion of radiation absorbed by the plants
$\mathrm{E_t}$ = radiation-use efficiency,
$\mathrm{kg_{dry\ matter}/W_{absorbed\ radiation}}$
ρ = density, number of plants/m^2, where

$$\mathrm{Ft} = 1 - \mathrm{e}^{-\mathrm{k_t LAI_{act}}} \qquad (2)$$

$$\mathrm{LAI_{act}} = \frac{\mathrm{LeavesSurf\ Num}}{\mathrm{A_{act}}} \qquad (3)$$

$$\mathrm{A_{act}} = \mathrm{LAI_{ratio}\ LandSurf} \qquad (4)$$

$$\rho = \frac{\mathrm{Num}}{\mathrm{A_{act}}} \qquad (5)$$

LandSurf = surface area of land, m^2
$\mathrm{LAI_{ratio}}$ = 1 m^2 area of leaf / m^2 area of land
$\mathrm{k_t} = 0.8$ - light extinction coefficient [19]
$\mathrm{E_t} = 0.01409$ kg/MJ, radiation-use efficiency [19]

The process of *evapotranspiration* is calculated from the reference evapotranspiration ($\mathrm{ET_0}$, mm/day), determined from meteorological data according to the well-known Penman-Monteith combination equation [22]. Based on this equation, the evaporation from the land and plants during a time step are calculated separately based on the following equations:

$$\mathrm{ET_{land}} = \mathrm{K_e\ ET_M\ LandSurf\ DT} \qquad (6)$$

$$\mathrm{ET_{plants}} = \mathrm{K_{cb}\ ET_M\ Surf\ Num\ DT} \qquad (7)$$

where
$\mathrm{ET_M}$ = reference evapotranspiration, recalculated from $\mathrm{ET_0}$ / kmol/h
$\mathrm{ET_{land}}$ = land-related evapotranspiration, kmol
$\mathrm{ET_{plant}}$ = plant-related evapotranspiration, kmol
LandSurf = surface area of the land, m^2
Surf = surface area of the leaves, m^2
Num = number of plants, pc
$\mathrm{K_e}$ = 1 m^{-2}, soil-related part of the dual crop coefficient [22]
$\mathrm{K_{cb}}$ = 1 m^{-2}, basal plant-related part of the dual crop coefficient [22]
DT = the time step in hours, distinguished for the changing actual daylight or night period

Growth is calculated after germination and is interpreted as the distribution of the photosynthetic biomass between the parts of the plants. Before the time- or event-driven appearance of the product, the following ratios are applied in line with estimations by experts:
Proportion of leaves = 0.853,
Proportion of roots = 0.147.
Afterwards:
Proportion of leaves = 0.637,
Proportion of products = 0.253,
Proportion of roots = 0.110.

Respiration is calculated for the individual parts of the plants. For all the parts, two kinds of respiration is simulated: one as a given proportion of the biomass synthesized and the other as a given proportion of the already existing biomass. The applied equations are the following:

$$\mathrm{R_{leaves}} = \mathrm{K\ DM_{leaves} + C\ M_{leaves}\ Num\ DT} \qquad (8)$$

$$\mathrm{R_{prod}} = \mathrm{K\ DM_{prod} + C\ M_{prod}\ Num\ DT} \qquad (9)$$

$$\mathrm{R_{root}} = \mathrm{K\ DM_{roots} + C\ M_{roots}\ Num\ DT} \qquad (10)$$

where
$\mathrm{R_{leaves}}$ = respired biomass of leaves, kg
$\mathrm{R_{prod}}$ = respired biomass of product, kg
$\mathrm{R_{root}}$ = respired biomass of roots, kg
$\mathrm{DM_{leaves}}$ = synthesized biomass of leaves, kg
$\mathrm{DM_{prod}}$ = synthesized biomass of product, kg
$\mathrm{DM_{roots}}$ = synthesized biomass of roots, kg
$\mathrm{M_{leaves}}$ = existing biomass of leaves, kg
$\mathrm{M_{prod}}$ = existing biomass of product, kg
$\mathrm{M_{roots}}$ = existing biomass of roots, kg
K = the constant of 0.1 h^{-1} [22]
C = the constant of 0.0001 h^{-1} [22]
Num = number of plants, pc.
DT = the time step in hours, distinguished for the changing actual daylight or night period

The *uptake* of water, nitrogen and phosphorus (or of other optional elements) is calculated as the minimum amount:

- required for evapotranspiration and photosynthesis together and
- available in the soil.

3.2 Non-conventional methodology of Programmable Process Structures

Programmable Process Structures (PPS, [23–26]) have developed from its antecedent, that is, Direct Computer Mapping [27]. PPS offers automatic generation of easily extensible, connectible and combined dynamic balance- and rule-based models for the analysis, planning and operation of complex process systems, even beyond industries that apply CIM (Chemical Integrated Manufacturing). These models consist of unified state and transition elements, transition-oriented representations of structures as well as locally programmable functional prototypes.

The main sources of inspiration behind PPS are: 1) the general functional definition of process systems in Kalman's State Space Model [28]; 2) the structural representation of General Net Theory [29]; 3) the concept of communicating autonomous programs in terms of Agent-Based Modeling [30].

Accordingly, PPS models are derived from two general (state and transition) "meta-agents," namely the structure of the generated state and transition elements form a net structure, moreover, the locally programmed state and transition prototypes represent the distributed functionalities in terms of Kalman's model. In addition, PPS can consciously make a distinction between model-specific conservation laws based on additive measures and signals.

In fact, PPS models can be generated from two general meta-prototypes and from the corresponding description of the process net. The local program containing prototype elements (that are responsible for the case-specific calculations), are also derived from the same meta-prototypes. The simulation can be executed according to the connections between the actual state and transition elements, accompanied by the data transfer between the actual elements and their calculated prototypes. This architecture and its AI programming language-based (SWI-Prolog to be exact) implementation strongly support the integration of various field- and task-specific models.

4. Results and discussion

4.1 Chemical process engineering-inspired principles and hypotheses of plant models

Natural and cultivated plants, including crops, vegetables, herbs, grasses and bushes, trees, etc. in a broader context, cover a wide variety of biological species embedded in a naturally occurring and partly human-controlled process system. Since many different species exist, at first glance this resembles the early stages of chemical engineering when individual technologies were interpreted as a system of various case-specific reactors, separators, etc. The essential invariant elements were later generalized according to the concept of unit operations. Similarly, the unified, essential features of agricultural models can be formulated as "biological engineering unit operations" within the complex system of the connected agrotechnological, ecological and environmental systems.

Considering the need for unified and simplified biological, ecological and environmental engineering process units, these systems must be represented by the necessary and sufficient types as well as numbers of state and transition elements calculated by a limited set of generally usable program prototypes.

The coherent and connectible set of the underlying 'first principles'-based mechanistic (physical, chemical and biological) models must be based on causally correct, model-specific conservation laws-based material and energy balances. Considering the numerous biochemical compounds and biological objects, that is, organs, etc., synthesized from these compounds, the various typical biological units can be characterized by their specific stoichiometric composition that facilitates the representation of balances in accordance with the conservation of atoms and in line with chemical principles.

Besides the conservation-based balances, the causally determined (driving force-based) transformations and transportations are the second pillar of process engineering models. In this regard, plant-like biological process units represent a special case because the major driving force is solar radiation originating from beyond the contours of the system. This feature determines the unique position of plants in the bio-based circular carbon economy.

In fact, solar radiation-driven photosynthesis produces a stoichiometric composition of biomass that supplies biomass in the various state elements of plants through downflow transporting short-term storage. Moreover, the forces of solar radiation-driven evapotranspiration result in the uptake of water and dissolved nutrients through upflow transporting short-term storage that supplies the additional resources required for photosynthesis as well as removes the by-products of the energy-producing respiration.

Accordingly, the essential self-control of plant life is organized by the solar radiation-driven push logistics of downflow as well as by the solar radiation-driven pull logistics of upflow. The daily and seasonal changes in plant behavior are determined by the temporally changing environmental functionalities, while human intervention can be taken into consideration by the respective managerial events.

The hypotheses for the simplified and unified plant model can be summarized as follows:

- The state elements are described by the specific biomass (or mass); the stoichiometric amounts of C, H, O, N, P and optional X atoms; as well as those originating from H_2O, O_2 and CO_2.
- The transition elements, e.g. photosynthesis, growth, respiration, evapotranspiration, uptake, etc., determine the functionalities resulting in stoichiometric changes in the aforementioned sources

of biomass, mass, atoms and components in the respective state elements.

- The life processes of plants as self-controlled living systems can be characterized by (i) the supply logistics of the photosynthesis-driven utilization of CO_2 from air and H_2O, N, P, etc. (from top soil) to produce O_2 which is emitted into the atmosphere in addition to stoichiometric pools of C, H, O, N and P that is incorporated into downflow material storage, as well as by (ii) the demand logistics of the solar energy-driven evapotranspiration-controlled uptake of H_2O, N and P from the soil and the emission of CO_2 and H_2O into the air.

4.2 Structure of the investigated process system

The process net structure of the simplified plant model, embedded in its natural environment and extended with human managerial interventions, is illustrated in Fig. 1. In the net model, the dots and bars represent the state and transition elements, respectively. The state and transition elements of the simplified plant model are the following:

Plant-related model elements:

- State elements:
  - roots (responsible for the water uptake, transportation of dissolved nutrients and long-term biomass storage that is also capable of generating useful products);
  - leaves (including stems which are responsible for solar radiation-driven photosynthesis and evapotranspiration);
  - products (which facilitate the storage of biomass for reproduction that also generates useful products);
  - downflow of material (short-term storage of photosynthesized biomass to be distributed amongst the roots, leaves and products);
  - upflow of material (short-term storage of uptaken water and nutrients as well as of respired components to be distributed between evapotranspiration and photosynthesis).
- Transition elements:
  - photosynthesis: utilizes solar radiation to synthesize biomass from atmospheric carbon dioxide, uptaken water and dissolved components, e.g. nitrogen, phosphorus, etc.;
  - growth: distributes the photosynthesized biomass between the parts of the plant according to the phenological phase-specific stoichiometry;
  - respiration: creates energy to synthesize tissues from already synthesized biomass and in part maintain existing plant biomass;
  - evapotranspiration: which is determined by the atmospheric conditions, i.e. level of solar energy, generates the driving force for the uptake of water and dissolved nutrients from the soil as well as releases the CO_2 and H_2O produced by respiration;
  - uptake: supplies the necessary water and dissolved nutrients from the soil.

Soil-related model elements:

- State elements:
  - residue (only in the topsoil): contains organic residues, e.g. from leaf littering or the ploughing of roots;
  - humus (only in the topsoil): transformed organic biomass in the soil;
  - solution containing water and dissolved components;
  - inorganic solid phase.
- Transition elements:
  - transform (only in the topsoil): describes the production of humus and dissolved nutrients from the residues;
  - air_land (only in the topsoil): calculates the levels of precipitation and nitrogen fixation from the atmosphere into the soil as well as those of evaporation and CO_2 emission from the soil into the atmosphere;
  - miner_deminer: determines the degrees of mineralization and demineralization of dissolved components in the soil;
  - seepage: calculates the vertical downflow of water and dissolved components between the layers of soil.

Human interventions in terms of cultivation:

- Typical state elements: manure, seeds, harvested products, etc.
- Typical time- and/or event-driven transition elements: manuring, sowing, harvesting, ploughing, etc.

Other environmental state elements: the atmosphere (air), solar radiation-related meteorology, ground layer below the soil that absorbs water and nutrients.

4.3 Solar radiation-driven “natural supply logistics” of plant biomass generation

The essential functionalities of the investigated process system can be represented as solar energy-driven as well as predominantly self-regulated, natural supply-and-demand logistics. Moreover, the respective supply-and-demand processes are causally connected that establish a natural (basically cooperative) feedback between each other.

Solar radiation facilitates the synthesis of biomass, the latter is calculated according to Eqs. 1-5. The related subprocesses of the plant model are denoted in green lines in Fig. 1.

The synthesis of biomass is driven by solar radiation but limited by the available amounts of water, nitrogen and phosphorus with regard to the upflow material to be

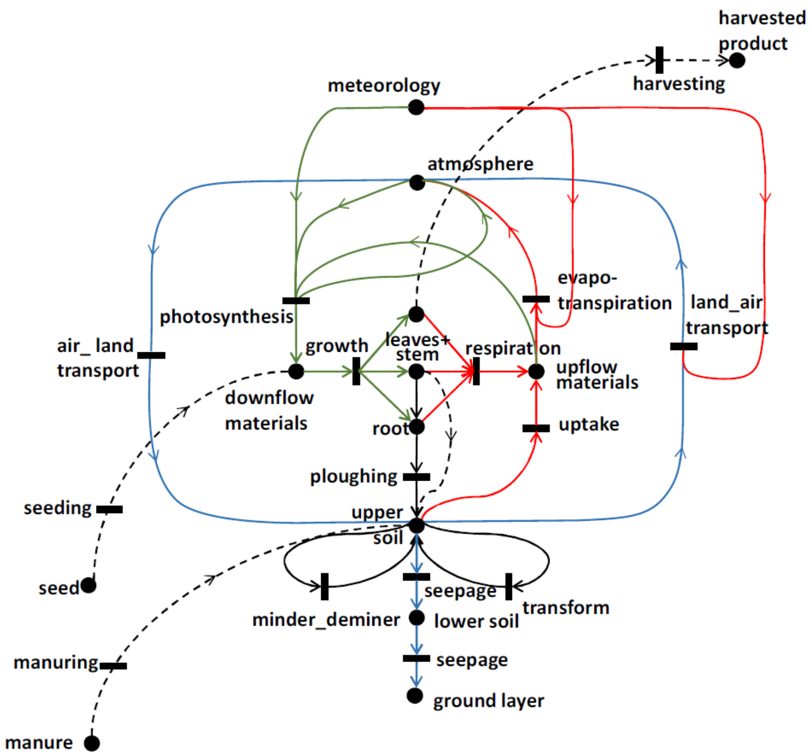

Figure 1: Process network of the simplified plant model

stored. The rate of photosynthesis also depends on the surface area of the leaves and stem. Controlled by these conditions and limitations, the synthesis sequestrates the calculated amount of the practically unlimited supply of atmospheric CO_2 in the biomass. Simultaneously, photosynthesis emits O_2 into the atmosphere as a result of the oxidation of uptaken water, while the associated hydrogen is incorporated into the synthesized biomass. The photosynthesized biomass supplies the downflow of material to be stored according to the plant-specific atomic stoichiometry. In the case of the studied maize, the stoichiometry of the synthesized dry matter was as follows [20, 21]:

[C, H, O, N, P, X] = [0.037, 0.062, 0.029, 0.00087, 4.8×10^{-5}, 0]

The dry matter is supplied by an additional amount of H_2O, according to the average water content of the plant (in our case 0.682).

The synthesized biomass is divided between the leaves, roots and product state elements of the plant, according to the plant-specific ratios that also depend on the phenological condition of the model. Furthermore, different stoichiometries can be used by the various parts of the plant.

In addition to the increase in the amount of synthesized biomass, a given proportion of that which is stored in the short term is utilized to meet the energy demand supplied by respiration for the synthesis of plant biomass according to Eqs. 8-10.

4.4 Solar energy-driven "natural demand logistics" of water and nutrient uptake

Considering the "natural demand logistics," the solar energy facilitates the uptake of water and dissolved nutrients from the soil as well as of H_2O and CO_2, the by-products of respiration. The respective evapotranspiration is calculated according to the Penman-Monteith combination equation [22] as well by Eqs. 6-7. The related subprocesses of the plant model are denoted in red lines in Fig. 1.

Depending on the meteorological conditions, the H_2O and CO_2 content of the uptaken material to be stored is emitted into the atmosphere by the process of evapotranspiration. Simultaneously, the by-products of respiration, namely H_2O and CO_2, accumulate here, moreover, the necessary amounts of H_2O as well as of dissolved nitrogen and phosphorus are utilized for photosynthesis from this store. In the knowledge of the resultant actual conditions with regard to the uptaken material to be stored, the uptake is controlled by demand-determined pull actions according to the concentration bounds and uptake rules as follows:

Lower and upper bounds for H_2O as well as N and P atoms are known. The rule that is applied is the following:

if Actual $\leq$ Lower, then
Demand = $\min$((Upper-Actual), Available),
otherwise Demand = 0, where
Actual = actual amount of uptaken material
to be stored,
Lower = lower bound,

Upper = upper bound,
Demand = quantity to be uptaken,
Available = available amount in the topsoil.

4.5 Generation and simulation of the PPS model

The files describing the respective model are found in the "Plant" directory of a Mendeley database [31].

The process network of the example model is defined in the text file named Plant_N.pl. The initial conditions (mass, biomass, components, etc.) and parameters (coefficients of equations, bounds, etc.) are described in the text file entitled Plant_D.pl, which was derived using an appropriately configured MS Excel spreadsheet. Starting from these case-specific files and the general definition of state and transition meta-prototypes, the general-purpose kernel program generates the editable graphical model Plant_G.graphml.

In parallel, by utilizing the meta-prototypes-based templates, modeling experts have to prepare the local programs for the respective elements of the prototypes. The locally executable programs of the prototypes are described in the file entitled Plant_G_prot.graphml.

In the knowledge of the prototype elements, the second generating algorithm of the PPS kernel prepares the dynamic databases of the simulation, namely

- Plant_Exp.pl containing the declaration of the Prolog clauses describing the local programs; and
- Plant_Use.pl containing the declaration of the Prolog facts describing the case-specific elements of the model along with their initial values and parameters.

The actually selected simulation results are saved in the file named Plant_Out.csv, while the data can be visualized using a case-specific MS Excel spreadsheet.

Some examples of the simulated results are illustrated in Figs. 2-5.

Fig. 2 shows the change in the total amount of biomass produced over one hectare during consecutive half days in the simulation. Time = 0 indicates when the land was sowed. Biomass begins to be produced following germination and stops at the end of the vegetation period. Fluctuations in biomass production indicate that its rate is higher during the daytime compared to at nighttime.

In Fig. 3, water that evaporated from the plant (blue) and from the land (red) are illustrated. Evaporation from the land follows the weather conditions much more closely and dominates during the early stages of the growing season, particularly when the leaves develop. Similarly to the production of biomass, evaporation rates are also higher in this simulation during the daytime.

In Fig. 4, the biomass of the parts of one plant (leaves, stem, roots, products) can be seen. The leaves, stem and roots begin to develop at the point of germination, while products appear later on. Although the leaves, stem and products are removed at harvest time, the roots are transformed into residues as a result of ploughing. Of course,

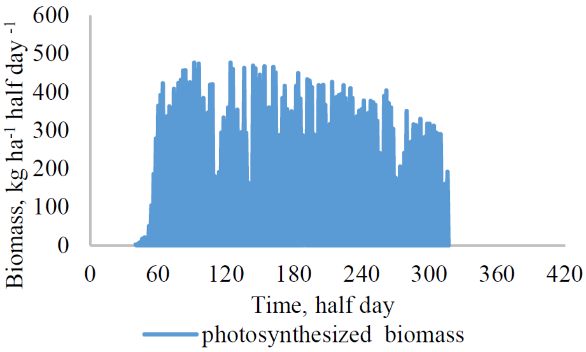

Figure 2: Total amount of photosynthesized biomass per hectare

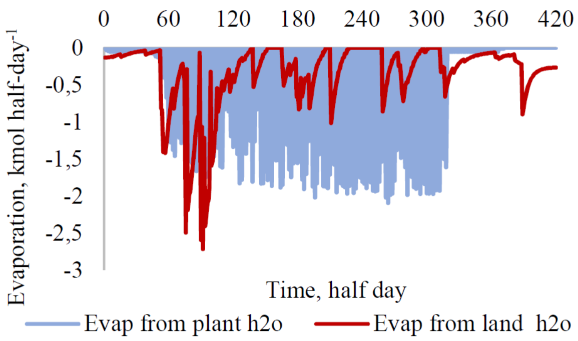

Figure 3: Dynamic changes in the evaporation rate of H_2O from plants and the surface of the land

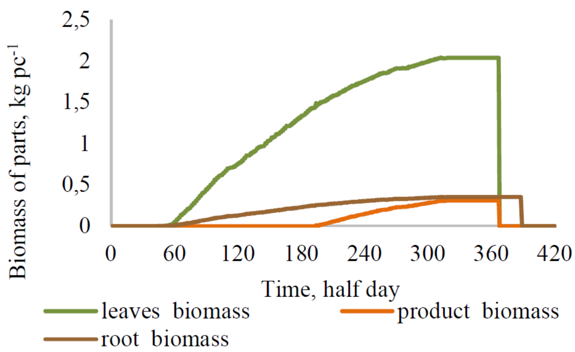

Figure 4: Biomass of plant parts throughout the growing season

the stepwise increase in biomass is insignificant in this integrated illustration.

Fig. 5 shows the sequestrated CO_2 over one hectare during consecutive half days of the simulation. The negative values refer to the reduction in its concentration in the surrounding atmosphere.

5. Conclusion

Although detailed plant models for well-defined important crops are available that require hundreds of parame-

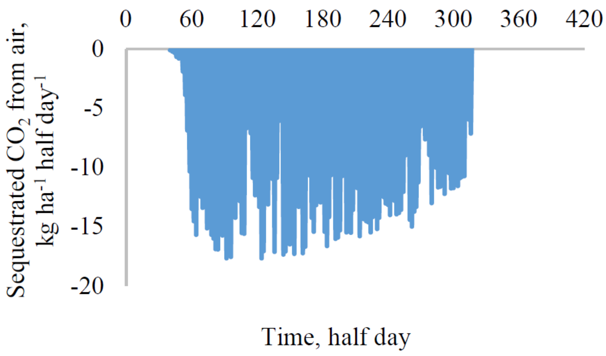

Figure 5: Amount of sequestrated CO_2

ters to be identified, the increasing complexity of agricultural systems within the broader context of the bio-based circular carbon economy requires simplified and unified plant models, which can describe the primary production of biomass. The suggested conceptual framework and its experimental implementation show how the chemical process engineering principles of process units, stoichiometric conservational processes, process networks, driving force-controlled functionalities and supply/demand processes can result in a reduced, unified plant model.

The structure of the model can be generated from the process net of the underlying state and transition elements. The model contains two special state elements for the short-term storage of the synthesized biomass to be distributed amongst the state elements of the plant as well as for the short-term storage of the uptaken aqueous nutrients required for evapotranspiration and photosynthesis. These two forms of logistical storage used represent the roles of phloem and xylem in detailed biophysical models.

The transition-related dynamic models follow the essential causalities and balances of natural self-control. Solar radiation-driven photosynthesis produces a stoichiometric composition of biomass that, as a result of the downflow of products to be stored in the short term, increases the biomass in the various plant elements. Moreover, solar radiation-driven evapotranspiration forces water and dissolved nutrients to be uptaken through the upflow of products to be stored in the short term, which increases the amount of water and the additional resources for photosynthesis required, as well as removes the by-products of energy-producing respiration. The natural self-control of plant life is organized by the solar radiation-driven push logistics of downflow as well as by the solar radiation-driven pull logistics of upflow.

The suggested stoichiometric approach underlines the increasing importance of elemental analysis with regard to agriculture-related raw materials and products.

The experimental PPS implementation of a simple example model illustrates the possible application of the reduced plant model prepared according to the suggested principles inspired by process systems engineering.

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