Supplement of**:**

**Crop growth and soil water fluxes at erosion-affected arable sites: Using weighing lysimeter data for model inter-comparison**

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Supplement data:

Table S 1: Physical and chemical soil characteristics of soil from Grünow (Gr), Dedelow (Dd), and Holzendorf (Hd), including soil horizon, horizon thickness, bulk density, gravel, sand, silt, clay, calcium carbonate (CaCO3), soil organic carbon (SOC); total nitrogen (Nt), ratio between carbon and nitrogen ration (C/N), and pH in CaCl2.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Soil | Horizon | Upper depth | Lower depth | Bulk density | Gravel | Sand | Silt | Clay | CaCO3 | SOC | Nt | C/N | pHCaCl2 |
|  |  | m | m | g/cm³ | wt.-% | % | % | % | % | % | % |  |  |
| Gr\_K | eAp | 0.00 | 0.27 | 1.67 | 4 | 55 | 28 | 17 | 6 | 0.91 | 0.096 | 10 | 7.63 |
|  | Sd-elCc | 0.27 | 0.70 | 1.86 | 5 | 53 | 30 | 17 | 14 | 0.19 | 0.023 | 8 | 7.79 |
|  | elCc | 0.70 | 1.50 | 1.89 | 5 | 57 | 29 | 14 | 13 | 0.10 | 0.015 | 7 | 7.85 |
| Dd\_5 | Ap | 0.00 | 0.30 | 1.50 | 3 | 47 | 37 | 16 | 0 | 0.75 | 0.088 | 9 | 6.64 |
|  | Bt | 0.30 | 0.65 | 1.52 | 3 | 50 | 24 | 26 | 0 | 0.47 | 0.06 | 7 | 7.15 |
|  | elCcv1 | 0.65 | 1.15 | 1.69 | 4 | 66 | 24 | 11 | 13 | 0.06 | 0.02 | 4 | 7.79 |
|  | elCcv2 | 1.15 | 1.50 | 1.79 | 3 | 61 | 27 | 12 | 13 | 0.05 | 0.01 | 4 | 7.82 |
| Dd\_1 | Ap | 0.00 | 0.30 | 1.43 | 2 | 54 | 31 | 15 | 0 | 0.73 | 0.091 | 8 | 7.0 |
|  | Al+Bt | 0.30 | 0.42 | 1.55 | 2 | 51 | 34 | 15 | 0 | 0.42 | 0.063 | 7 | 6.5 |
|  | Bt | 0.42 | 0.80 | 1.59 | 4 | 52 | 23 | 25 | 0 | 0.31 | 0.050 | 6 | 7.0 |
|  | elCcv | 0.80 | 1.50 | 1.60 | 6 | 59 | 29 | 12 | 12 | 0.06 | 0.012 | 5 | 7.8 |
| Hd\_S | Ap | 0.00 | 0.28 | 1.55 | 1.6 | 70 | 20 | 10 | 0.1 | 1.08 | 0.104 | 10 | 7.01 |
|  | Go-M | 0.28 | 0.50 | 1.60 | 2.4 | 63 | 26 | 11 | 0.2 | 0.82 | 0.085 | 10 | 7.23 |
|  | Go-ejC | 0.50 | 0.55 | 1.55 | 0.3 | 60 | 29 | 12 | 1.9 | 0.50 | 0.055 | 9 | 7.54 |
|  | Go-fAh | 0.55 | 0.65 | 1.45 | 0.2 | 21 | 52 | 27 | 0.2 | 1.37 | 0.150 | 9 | 7.42 |
|  | Gor-M | 0.65 | 0.80 | 1.46 | 1.0 | 72 | 22 | 6 | 0.2 | 0.60 | 0.050 | 12 | 7.54 |
|  | Gr | 0.80 | 1.10 | 1.65 | 1.1 | 74 | 21 | 5 | 0.2 | 0.18 | 0.016 | 11 | 7.35 |
|  | Gr-fAh | 1.10 | 1.30 | 1.86 | 0.7 | 77 | 18 | 5 | 0.0 | 0.36 | 0.025 | 14 | 7.20 |
|  | Gr | 1.30 | 1.50 | 1.68 | 0.1 | 86 | 13 | 1 | 0.0 | 0.17 | 0.011 | 15 | 7.22 |

Table S 2: Parameter for the soil water retention characteristic and unsaturated hydraulic conductivity function of the Mualem-van Genuchten model. Model parameters were obtained with the evaporation method using HYPROP technique.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Soil | Soil horizon | Upper depth | Lower depth | θs | θr | α | n | Ks | nFK | FK | PWP |
|  |  | m | m | cm3 cm-3 | cm3 cm-3 | cm-1 | - | cm d-1 | Vol. % | Vol. % | Vol. % |
| Gr\_K | eAp | 0.00 | 0.27 | 0.329 | 0.043 | 0.0251 | 1.296 | *34.0* | 17.7 | 26.80 | 9.11 |
|  | Sd-elCc | 0.27 | 0.70 | 0.330 | 0.029 | 0.0267 | 1.219 | *54.5* | 16.8 | 27.69 | 10.86 |
|  | elCc | 0.70 | 1.50 | 0.312 | 0.047 | 0.0199 | 1.372 | *25.9* | 17.8 | 25.58 | 7.80 |
| Dd\_5 | Ap | 0.00 | 0.30 | 0.381 | 0.000 | 0.0529 | 1.241 | *413.2* | 19.8 | 27.32 | 7.49 |
|  | Bt | 0.30 | 0.65 | 0.384 | 0.000 | 0.0546 | 1.225 | *92.9* | 19.6 | 27.91 | 8.35 |
|  | elCcv1 | 0.65 | 1.15 | 0.335 | 0.000 | 0.0136 | 1.257 | *7.3* | 21.2 | 29.58 | 8.41 |
|  | elCcv2 | 1.15 | 1.50 | 0.294 | 0.000 | 0.0204 | 1.264 | *124.7* | 18.1 | 24.44 | 6.36 |
| Dd\_1 | Ap | 0.00 | 0.30 | 0.419 | 0.019 | 0.0361 | 1.312 | 442.9 | 21.3 | 32.062 | 10.7 |
|  | Al+Bt | 0.30 | 0.42 | 0.364 | 0.028 | 0.0255 | 1.311 | 179.7 | 18.7 | 29.564 | 10.9 |
|  | Bt | 0.42 | 0.80 | 0.376 | 0.045 | 0.0717 | 1.280 | 278.1 | 15.7 | 27.275 | 11.6 |
|  | elCcv | 0.80 | 1.50 | 0.337 | 0.004 | 0.0276 | 1.329 | 112.2 | 18.6 | 26.343 | 7.8 |
| Hd\_S | Ap | 0.00 | 0.28 | 0.383 | 0.000 | 0.0306 | 1.268 | *57.8* | 22.4 | 29.61 | 7.25 |
|  | Go-M | 0.28 | 0.50 | 0.348 | 0.000 | 0.0447 | 1.242 | *239.3* | 18.7 | 25.71 | 7.05 |
|  | Go-ejC | 0.50 | 0.55 | 0.349 | 0.000 | 0.0254 | 1.261 | *14.5* | 20.8 | 28.06 | 7.26 |
|  | Go-fAh | 0.55 | 0.65 | 0.465 | 0.070 | 0.0300 | 1.200 | *35.2* | 21.1 | 39.54 | 18.47 |
|  | Gor-M | 0.65 | 0.80 | 0.385 | 0.085 | 0.0200 | 1.550 | *117.0* | 20.5 | 30.24 | 9.75 |
|  | Gr | 0.80 | 1.10 | 0.315 | 0.040 | 0.0210 | 1.500 | *104.0* | 18.6 | 24.08 | 5.49 |
|  | Gr-fAh | 1.10 | 1.30 | 0.300 | 0.020 | 0.0160 | 1.500 | *27.9* | 20.3 | 24.06 | 3.74 |
|  | Gr | 1.30 | 1.50 | 0.340 | 0.020 | 0.0160 | 1.550 | *60.0* | 23.3 | 26.80 | 3.51 |

Table S 3: Management information on crops, sowing and harvesting date, duration, seed density, and on the application of different fertilizer.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Crop | Sowing | Harvest | Duration [days] | Seed density  [seed m-2] | Nitrogen-fertilizer [kg N ha-1] | Kieserit [kg ha-1] | Liquid mangan [l ha-1] | P40 [kg ha-1] |
| Winter wheat | 2014/ 09/17 | 2015/ 07/23 | 309 | 260 | 160 | 100 | 0 | 0 |
| Winter rye | 2015/ 10/02 | 2016/ 07/27 | 299 | 280 | 200 | 100 | 1 | 0 |
| Winter wheat | 2016/ 10/06 | 2017/ 08/02 | 300 | 200 | 100 | 100 | 0 | 0 |
| Winter rye | 2017/ 10/20 | 2018/ 04/11 | 173 | 280 | 0 | 0 | 0 | 0 |
| Oat | 2018/ 04/11 | 2018/ 07/27 | 107 | 350 | 100 | 100 | 0 | 22 |

Table S 4: Observed phenological stages for each soil profiles at the lysimeter station in Dedelow, Germany.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Time | Gr\_K (BBCH) | Dd\_5 (BBCH) | Dd\_1 (BBCH) | Hd\_S (BBCH) |
| 2015-07-23 | 89 | 89 | 89 | 87-89 |
| 2016-04-21. | 30 | 30 | 30 | 30 |
| 2016-05-03 | 30-31 | 31 | 31 | 30 |
| 2016-05-12 | 32 | 32 | 33 | 33 |
| 2016-05-18 | 37 | 33 | 33-37 | 37 |
| 2016-05-25 | 45 | 51 | 51 | 45 |
| 2016-06-02 | 55-59 | 55-59 | 59 | 55-59 |
| 2016-06-16 | 71-75 | 71-75 | 71-75 | 71-75 |
| 2016-06-23 | 75 | 75 | 75 | 75 |
| 2016-06-30 | 75 | 75 | 75 | 75 |
| 2016-07-07 | 80 | 80 | 80 | 80 |
| 2016-07-19 | 89 | 89 | 89 | 89 |
| 2016-07-27 | 92 | 92 | 92 | 92 |
| 2017-06-09 | 59 | 59 | 59 | 59 |
| 2017-06-21 | 71 | 71 | 71 | 71 |
| 2017-06-27 | 75 | 75 | 75 | 75 |
| 2017-07-05 | 85 | 85 | 85 | 85 |
| 2017-07-11 | 85 | 85 | 85 | 85 |
| 2017-07-18 | 87 | 87 | 87 | 87 |
| 2017-07-31 | 89-92 | 89-92 | 89-92 | 89-92 |
| 2017-10-25 | 10 | 10 | 10 | 10 |
| 2017-11-14 | 12 | 12 | 12 | 12 |
| 2018-02-20 | 23-24 | 23-24 | 23-24 | 23-24 |
| 2018-04-23 | 11 | 11 | 11 | 11 |
| 2018-05-02 | 13 | 13 | 13 | 13 |
| 2018-05-07 | 13-21 | 13-21 | 13-21 | 13-21 |
| 2018-05-14 | 21-22 | 21-22 | 21-22 | 21-22 |
| 2018-05-22 | 30-31 | 30-31 | 30-31 | 30-31 |
| 2018-05-28 | 39-43 | 39-43 | 39-43 | 39-43 |
| 2018-06-01 | 47-55 | 47-55 | 47-55 | 47-55 |
| 2018-06-07 | 59 | 59 | 59 | 59 |
| 2018-06-12 | 69 | 69 | 69 | 69 |
| 2018-06-18 | 71-73 | 71-73 | 71-73 | 71-73 |
| 2018-06-25 | 73-75 | 73-75 | 73-75 | 73-75 |
| 2018-07-04 | 77-87 | 77-87 | 77-87 | 77-87 |
| 2018-07-16 | 87-89 | 87-89 | 87-89 | 87-89 |
| 2018-07-27 | 89-92 | 89-92 | 89-92 | 89-92 |

Supplement: Model description

**AgroC:**

**General description**

AgroC was designed to estimate the net ecosystem carbon fluxes in agroecosystems. The model essentially is a coupling of three modules. The model core is the SoilCO2 module (Šimůnek and Suarez, 1993), which is a numerical model for the simulation of the 1-dimensional flow of heat, water and CO2 in soils. The second module consists of a 1-dimensional implementation of RothC (Coleman and Jenkinson, 2005), a model to describe soil carbon turnover. The coupling of these two modules has already been validated in several studies. The third module is the dynamic plant growth module SUCROS (Spitters, van Keulen, et al., 1989). SUCROS simulates water stress dependent photosynthesis, phenology-based distribution of assimilates to plant organs and respiration. The combination of these subprograms enables a closed carbon balance of agricultural ecosystems at an hourly or daily time step. A special feature of the model is the consideration of root exudation and dying roots, as well as the effect of both processes on heterotrophic soil respiration.

AgroC thus enables the estimation of carbon balances in agricultural stands depending on environmental factors such as temperature, precipitation or atmospheric CO2 concentration. The overall model has also been validated in several case studies. Input data for the model are meteorological information, irradiation, potential evapotranspiration, soil hydraulic and thermal properties and plant parameters. The latter are available as standard parameter sets for cereals, sugar beet, rape, maize, potatoes and grassland. Model results include gross primary production (GPP), respiration, net carbon fluxes (NEE), crop yield, biomass, leaf area index, soil moisture and soil temperature.

**Model set-up and protocol**

For setting up the model all available data (initial profile information in water content, soil layering, soil hydraulic parameters (van Genuchten parameters), atmospheric forcing (precipitation, provided reference ET (ET0, Penman-Monteith), radiation, min and max air temperature), lower boundary condition in terms of pressure applied, and management data (seeding density, day of emergence, harvest dates, rooting depth)) were used. Provided BBCH stages were converted to development stages (DVS) according to Wang and Engel (1998) as AgroC will provide DVS. For the calibration of the development stages all provided BBCH stages (or in detail DVS stages) were used for all lysimeters and the corresponding crop. Hereby, the calibration was performed using the automatic search algorithm SCE-UA (Shuffled Complex Evolution University of Arizona) as described by Duan, Sorooshian, et al. (1992) and Duan, Sorooshian, et al. (1994), whereby the mismatch between observed and simulated development stage was minimized using the sum of squared residuals in the cost function. The calibration routine was written in Matlab and the entire system was run on a LINUX cluster. For the calibration, three parameters were estimated scaling the start temperature for plant growth (C\*day) (TEMPSTART) and two tables in the plant growth routine, namely, the table describing the ‘Daily average temperature against development rate, if DVS < 1 (RATDVS)' and the table describing the ‘Daily average temperature against development rate, if DVS > 1 (RATDVS)'. The three parameters were chosen as they directly impact predicted phenology. Additionally, the parameters describing the potential CO2-assimilation rate of a unit leaf area for light saturation (kg CO2/ha leaf/h) (AMX) as well as the initial light use efficiency (kg CO2/ha leaf/h) (EFF) were adapted by trial and error to match mean regional yields. Here, it has to be noted that for the two different winter wheat cultivars (Julius and Pionier) only one single parameter set was optimized.

**DailyDayCent:**

**General description**

The model DailyDayCent is a biogeochemical model, which includes a crop growth routine based on radiation use efficiency (Fitton, Datta, et al., 2014). The crop growth routine is implemented in modules describing the carbon and nitrogen dynamics. Growth is based on a genetic growth potential and is adjusted due to environmental conditions and is limited by water or nutrient limitations. The water balance is simulated by a tipping bucket model for soil water content and by Penman for the ET0 (Parton, Hartman, et al., 1998). The model runs on daily time steps.

**Model set-up and protocol**

DailyDayCent results presented in this work are from single forward simulations, one for each lysimeter (no calibration). Crop parameters were used from the available crop-files, which contain data from former calibrations. The runs were without spin-up and initial values for carbon were distributed to the different carbon pools according to the DailyDayCent protocol.

**Daisy:**

**General description**

DAISY is a physically based and dynamic numerical agro-ecosystem 1D/2D model which describes the coupled processes governing water fluxes, nitrogen/carbon turnover and transport, crop growth, and solute transport in the soil-plant atmosphere system (Hansen, Abrahamsen, et al., 2012; Daisy.ku.dk). It is continuously developed and has been applied to various studies , with a focus on the environmental fate of agrochemicals in agro- ecosystems (Hansen, Abrahamsen, et al., 2012, Rasmussen, Abrahamsen, et al., 2015), with an emphasis on nitrogen and pesticides dynamics in soils. The main processes implemented in DAISY are water and heat flow, nitrogen and general solute transport, carbon dynamics and crop growth under different agronomic practices. In the soil matrix, water flow is described by the Richards equation and in the macro-pore domain by a simple mass-balance approach. Root water uptake is simulated based on the single root concept (microscopic approach) and is a function of the pressure potential at the root surface and the root density. Solute transport is described by the advection-dispersion equation. The Carbon module assumes that the organic carbon is part of crops, litter, organic fertilizers and soil organic matter. Crop development is monitored by the development stage and is a function of temperature. Crop growth is driven by photosynthesis, which is depended on a light response curve. A potential photosynthesis rate can be reduced due to plant water and nitrogen stress. In Daisy, conversion of development stage to BBCH-stage was conducted based on user defined conversion tables. For this study, conversion tables for Winter Wheat (and Winter Rye) and Spring Barley were derived from comparison between simulations and data from a large number of field studies in Denmark.

**Model set-up and protocol**

Daisy results presented in this work are from single forward simulations, one for each lysimeter (no calibration). Daily values of ET0 and precipitation were used for setting up the upper boundary condition. For the lower boundary condition, daily values of depth to groundwater were used. Soil hydraulic properties were described by the van Genuchten-Mualem model (van Genuchten, 1980) and parameters were provided based on the evaporation method, as mentioned. For Winter Wheat and Winter Rye, two different parametrisations for the DAISY crop model were used. Both parametrizations are solely based on studies in Denmark. Due to a missing default Oat parametrisation, we chose to parameterise Oat as Spring Barley.

**Expert-N:**

**General description**

Expert-N is a development system for nitrogen (N) turnover models to simulate the N cycle in arable agriculture (Priesack, Gayler, et al., 2006). The system consists of modular model components for soil water flow, for soil heat and N transport and for crop growth. These components are composed of different standardized model units representing each a single process. For example, model units exist for a model component such as N mineralization as part of the N transport model or the root water uptake model as sub-model of the crop growth model.

The modular structure allows an easy exchange of model units to compare different sub-models or model algorithms describing the same process. For each model component and model unit several distinct interchangeable sub-models are available. Additional user defined models can be easily implemented by the supported use of dynamic link libraries. This enables the user to analyse the impact of different or new modelling approaches on the simulation results component by component.

By the modular structure of Expert-N is also an extremely flexible simulation model for N dynamics in soil-plant systems, which can be easily adapted to the actual simulation purpose including management or research, to the specific site conditions involving crop, soil and agricultural practice and to the quality and availability of data.

Several different vegetation growth models exist to simulate agricultural crops, but also forest and grassland growth models are part of the Expert-N framework. Each of these models are newly reprogrammed in the programming language C to fit to the Expert-N program structure and to support the coupling with exchangeable model units of soil water flow and soil solution transport or soil carbon and nitrogen turnover models.

**Model set-up and protocol**

In this study Expert-N is applied in a forward simulation using the Richards equation approach to simulate soil water flow similar to the Hydrus model (Simunek, Huang, et al., 1998), the N-turnover and N-transport following the approach of the LEACHM model (Hutson and Wagenet, 1992). The van Genuchten-Mualem parameterization was used to represent the hydraulic properties based on the prescribed parameter values. To simulate crop growth each of the growth model components of the models CERES, SPASS, SUCROS and GECROS are applied also in a forward way, keeping the other components representing the soil fixed. For the different crop species wheat, rye and oat, that were grown on the lysimeters, the available standard parametrisations are used. No parameter fitting was performed, even not to minimize differences between simulated and the given measured development stages.

**Expert-N CERES**

**General description**

Crop development is calculated by development stages depending on sums of daily average air temperatures (Ritchie, 1991). The growth component of the CERES model consists of a canopy-scale photosynthesis model assuming a big leaf model based on radiation use efficiency and applying an empirical light extinction function depending on canopy depth and leaf area. Growth and respiration are considered for each plant organ (root, stem, leaf, and fruit) modelled by specific growth and respiration rates depending on temperature, water and nitrogen availability. Nitrogen demands are simulated using empirical optimal nitrogen concentrations for each plant organ and each development stage. Assimilate allocation is described by partitioning coefficients and efficiency factors (Priesack and Gayler, 2009).

**Expert-N SUCROS:**

**General description**

A simple scheme to simulate phenological development is used based on phenological rates that depend on mean daily air temperatures and reached development stage. A more mechanistic approach to model the canopy photosynthesis is applied by the SUCROS model. The two-leaf approach integrates leaf photosynthesis over different leaf layer from the top of the canopy to the soil surface. Sunlit and shaded leaves are distinguished and leaf angle distributions are taken into account. Assimilates are distributed to the different plant organs by fixed partitioning and carbon use efficiency factors, also growth and maintenance respiration are considered. For the Expert-N version of the growth model additionally potential and actual N-uptake are described including limitations of photosynthesis and growth, if the crop demand cannot be fulfilled by the available soil nitrogen.

**Expert-N SPASS:**

**General description**

The Expert-N specific crop model SPASS is built up from components of the models CERES and SUCROS. Simulation of development stages are based on the BBCH scale (Wang and Engel, 1998) but otherwise follow the CERES approach. Photosynthesis is modelled using the two-leaf approach of the SUCROS model, also description of assimilate partitioning, growth and respiration follows the SUCROS model approach but additionally accounting for impacts of plant organ nitrogen contents. Root growth, soil water and soil nitrogen uptake and plant internal nitrogen allocations are similar to corresponding process models of the CERES model.

**Expert-N GECROS:**

**General description**

The model GECROS was designed to better address the genotype by environment interactions thereby giving the growth model a better model structure and a minimal set of input parameters (Yin and van Laar, 2005). The GECROS model describes the phenological development similar to the SUCROS model. Leaf photosynthesis is simulated in case of C3 plants based on the approach of Farquhar, von Caemmerer, et al. (1980) and in case of C4 plants according to Yin and Struik (2009). Similar to the SUCROS model also sunlit and shaded leaves are considered following the two-leaf concept. But now the concept is combined with leaf energy balance calculations for each leaf type to simulate the impact of stomatal conductivity on both leaf photosynthesis and leaf transpiration (Wang and Leuning, 1998). For the assimilate partitioning between shoot and roots the model GECROS assumes a functional balance, hence N acquisition by roots is assumed to be proportional to the C gain by shoots. The within-shoot C partitioning is determined by the strengths of growing organs as sinks for the available C and by assuming a priority scheme between the plant organs. Growth and respiration of plant organs is then simulated in dependence of soil water and soil nitrogen availability.

**HERMES:**

**General description**

The process-oriented functional model HERMES was designed to simulate crop-growth, water, and nitrogen dynamics for arable land. It was originally developed for practical use (e.g., irrigation and fertilisation recommendation). Hence, relatively simple and robust model approaches were implemented to simulate crop growth, yield performance, water and nitrogen uptake, and the soil nitrogen dynamics. The crop growth module was built on the basis of the SUCROS model (Van Keulen, Penning, et al., 1982) following a generic approach which is able to simulate different crops using external crop parameter files. Crop growth is simulated by the daily net dry matter production as a result of gross photosynthesis minus respiration; the processes are driven by global radiation and temperature. In dependence on the simulated crop development stages, initialised by stage dependent temperature sums, partitioning of dry matter production to crop organs is modelled. The crop-specific potential evapotranspiration is calculated from daily weather data (cf. Table). HERMES has implemented different ET models ranging from an empirical approach following Haude (1955) to more physically based calculations of Turc-Wendling (Wendling, Schellin, et al., 1991), Priestley-Taylor (Priestley and Taylor, 1972), and Penman-Monteith (Allen, Pereira, et al., 1998). The effect of changing atmospheric CO2 concentrations is considered in HERMES by a dynamic calculation of the stomatal conductance controlling crop transpiration within the Penman-Monteith equation according to Yu, Goudriaan, et al. (2001). Transpiration is further controlled by root water uptake which depends on the root length density and the available water in the soil. In case of a water deficit in upper soil layers root water uptake shifts to lower layers whereas this relocation depends on the effective rooting depth of the soil profile. Soil water dynamics are described by using a capacity approach and the corresponding parameters are consistent with the German soil texture classification and related capacity parameters (Ad-hoc-Arbeitsgruppe-Boden, 2005). Parameters are modified by soil organic matter content, bulk density classes, and groundwater level. These default parameters can be inactivated if site-specific parameters are available. Capillary rise from shallow groundwater was implemented to account for a daily steady state water flux to the deepest soil layer where the critical water content for depletion amounts to 70% of available water. Daily fluxes are estimated depending on soil texture and the distance between the layer and the groundwater level based on characteristic values of Ad-hoc-Arbeitsgruppe-Boden (2005). In the HERMES model crop growth is limited by water and nitrogen stress. Water stress is induced by a crop development stage dependent ratio of potential to actual transpiration and nitrogen shortage is considered by applying the concept of critical N concentrations in plants (Greenwood, Lemaire, et al., 1990).

**Model set-up and protocol**

According to the present study model set-up included all available input data (e.g., initial values, soil parameters, weather and management data). Calculation of ET0 was inactivated as it was provided uniformly to all modellers. A previous year’s winter wheat yield of 3.5 t ha-1 was included in the crop rotation in order to enable the model to calculate the input of crop residues as a start value at the beginning of the simulation period. As mentioned above data for model validation and subsequent calibration included time series of crop phenology (BBCH) per each soil profile and the crop-specific yield range observed at the test site. HERMES itself comprises of in total six crop development phases which have been translated into the BBCH scale as follows: sowing till emergence (BBCH 1 to 10), emergence till double ridge (BBCH 11 to 20), double ridge till ear emergence (BBCH 21 to 51), ear emergence till flowering (BBCH 51 to 61), grain filling (BBCH 62 to 91), and senescence (BBCH 92). The updating of the BBCH stages within the HERMES development phases takes place depending on the respective vernalisation demand and the fulfilment of the temperature sum. The following table shows how the respective crop parameters were calibrated with the aim of a good match of observed and simulated phenotype. The yields simulated in this way are within the specified observed range for all crops.

Table S 5: Overview of selected crop parameters for oats, winter rye, and winter wheat and their calibration for the present blind forward simulation with HERMES model

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter oat** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| Amax | kg CO2 ha-1 h-1 | maximum assimilation rate | match yield range | 37 | na | na | 45 |
| Tsum2 | °C | temperature sum phase 2 | match BBCH | 250 | na | na | 214 |
| Tsum3 | °C | temperature sum phase 3 | match BBCH | 280 | na | na | 250 |
| Tsum4 | °C | temperature sum phase 4 | match BBCH | 180 | na | na | 100 |
| Tsum5 | °C | temperature sum phase 5 | match BBCH | 350 | na | na | 480 |
| **Parameter winter rye** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| Tsum1 | °C | temperature sum phase 1 | match BBCH | 120 | na | na | 130 |
| Tsum3 | °C | temperature sum phase 3 | match BBCH | 420 | na | na | 300 |
| kc2 | - | kc-factor phase 2 | match yield range | 1.1 | na | na | 1.0 |
| kc3 | - | kc-factor phase 3 | match yield range | 1.5 | na | na | 1.1 |
| **Parameter winter wheat** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| Partleaves | kg DM ha-1 | partitioning leaves (phase 3) | match yield range | 0.25 | na | na | 0.33 |
| Partstem | kg DM ha-1 | partitioning stem (phase 3) | match yield range | 0.62 | na | na | 0.54 |

In total, the selected crop parameters are known to significantly influence the simulation of crop development, especially phenology and yield performance. The different number of selected parameters per crop results from a quite diverse crop-specific calibration history. For example the calibration for winter wheat is the most advanced as wheat was the first crop defined in HERMES and has been validated and adapted throughout a huge number of model inter-comparisons. The calibration procedure was carried out using expert knowledge regarding the impact of crop parameters on phenology and yield output and the effect of calibration was assessed visually by plotting the simulations against the observed values. In the present blind forward simulation parameter uncertainty and/or resulting prediction uncertainty was not evaluated.

**MONICA:**

**General description**

Monica (the Model for Nitrogen and Carbon dynamics in Agro-ecosystems) is a daily-based one-dimensional model designed to simulate crop growth, water and nitrogen uptake, and the soil organic carbon dynamics in soil. The model has been extended from the HERMES model to simulate carbon cycle in soil and plant. It also simulates the impact of CO2 on crop growths. MONICA has been adapted for various crops using crop-specific parameters describing crop physiology and development. Crop growth development has been divided into 5 to 6 phenological stages (depending on the crop) from emergence to senescence. The stages based temperature sum is the key parameter specifying the phenological stage of crop.

**Model set-up and protocol**

For model set-up, we included all available input data (e.g. initial values, soil parameters, and weather and management data). The provided ET0 was assimilated into the model and its calculation was inactivated. The model was validated using the provided information on crop phenology for each growing season and each crop. Similar to HERMES, MONICA itself comprises of in total six crop development stages which have been translated into the BBCH scale as follows: sowing till emergence (BBCH 1 to 10), emergence till double ridge (BBCH 11 to 20), double ridge till ear emergence (BBCH 21 to 51), ear emergence till flowering (BBCH 51 to 61), grain filling (BBCH 62 to 91), and senescence (BBCH 92).

Table S 6: Overview of selected crop parameters for oats, winter rye, and winter wheat and their calibration for the present blind forward simulation with MONICA model.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Parameter oat** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| MaxAssRate | kg CO2 ha-1 h-1 | maximum assimilation rate | match yield range | 32 | na | na | 45 |
| SLA5 | ha kg-1 | Specific leaf area stage 5 | match yield range | 0.0015 | na | na | 0.002 |
| AssParCoeff | - | Assimilation partitioning coefficient organ 1 stage 2 | Match BBCH and yield | 0.25 | na | na | 0.2 |
| AssParCoeff | - | Assimilation partitioning coefficient organ 2 stage 2 | Match BBCH and yield | 0.50 | na | na | 0.5999 |
| AssParCoeff | - | Assimilation partitioning coefficient organ 3 stage 2 | Match BBCH and yield | 0.25 | na | na | 0.2 |
| **Parameter winter rye** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| SLA1 | ha kg-1 | Specific leaf area stage 1 | match yield range | 0.0014 | na | na | 0.002 |
| SLA2 | ha kg-1 | Specific leaf area stage 2 | match yield range | 0.0013 | na | na | 0.002 |
| SLA3 | ha kg-1 | Specific leaf area stage 3 | match yield range | 0.0013 | na | na | 0.002 |
| SLA4 | ha kg-1 | Specific leaf area stage 4 | match yield range | 0.0015 | na | na | 0.002 |
| SLA5 | ha kg-1 | Specific leaf area stage 5 | match yield range | 0.0015 | na | na | 0.002 |
| **Parameter winter wheat** | | | | | | | previous simulation |
| abbr. | unit | description | choice (why) | opt. value | range-min | range-max | value |
| MaxAssRate | kg CO2 ha-1 h-1 | maximum assimilation rate | match yield range | 40 | na | na | 30 |
| Tsum2 | °C | temperature sum stage 2 | match BBCH | 384 | na | na | 284 |
| Tsum3 | °C | temperature sum stage 3 | match BBCH | 440 | na | na | 380 |
| Tsum5 | °C | temperature sum stage 5 | match BBCH | 420 | na | na | 380 |

The transition from one stage to another stage will be controlled using the defined temperature sum for each step. Table S 6 represented the assigned values for different crop parameters.

**THESEUS:**

**General description**

This model is combination of the generic crop growth model WOFOST7.1 using a modified Penman-approach for the calculation of potential evapotranspiration and the soil water flux model SAWAH. WOFOST7.1 is a mechanistic crop growth model that describes plant growth using light interception and CO2 assimilation as growth driving processes, and crop phenological development as a growth controlling process. SAWAH is a Simulation Algorithm for Water flow in Aquic Habitats. It simulates one-dimensional vertical movement of water in soil, and describes on a field scale the dynamics of soil water content, water potential, and water flux at different depths in the soil profile, i.e. between the soil surface and a lower boundary at a user-specified depth. SAWAH is a deterministic model, based on standard physical soil characteristics (moisture retention curve, hydraulic conductivity curve), measured groundwater levels, and meteorological conditions. It solves the general flow equation numerically; under given boundary conditions and root sink strength, and keeps an account of the soil water balance. The model operates on daily time step. Inputs are meteorological data, soil water retention parameters, soil profile data and seeding and harvest date. Crop growth is only limited by water and temperature stress, limitation due to nutrient stress is not simulated. In the actual state of the model, up to nine different crop types can be simulated and thus total crop rotations can be calculated. More information can be obtained from e.g. Wegehenkel, Luzi, et al. (2019).

**Model set-up and protocol**

For the model set-up we used all available input data such as initial soil water contents, soil parameters, weather, lower boundary conditions and crop management data such as seeding and harvest). Daily rainfall rates were used as upper and measured values of depth to groundwater as lower boundary condition. Soil hydraulic properties were described by the van Genuchten-Mualem model, corresponding parameters for all lysimeter soils were provided by the organizers of the workshop (Workshop: Calibration and Validation data for the coupled modeling of agronomic and environmental variables in the soil-plant-atmosphere system, H. H. Gerke, J. Groh, Berlin, 2018-10-15). For the calibration of the crop growth model we used time series of observed crop phenology (BBCH). The crop growth model WOFOST7.1 used three crop development stages: emergence, anthesis and maturity. These three stages have been transformed into the BBCH scale as follows: sowing till emergence (BBCH 1 to 10), anthesis (BBCH 55 to 60), and maturity (BBCH 92). For calibration of the BBCH stages, we used the temperature approach implemented in WOFOST7.1 using two temperature sums (Table S7).

Table S 7: Overview of selected crop parameters for oat, winter rye, and winter wheat and their calibration for the present blind forward simulation with THESEUS model.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Parameter winter wheat | | | | | | | Previous simulation |
| abbr | unit | description | choice | Calibrated value | Min | Max | Value |
| TSUM1 | C | Temperature sum from emergence to anthesis | sensitive | 1700 | - | - | 1700 |
| TSUM2 | C | Temperature sum from anthesis to maturity | sensitive | 900 | - | - | 600 |
| Parameter winter rye | | | | | | |  |
| TSUM1 | C | Temperature sum from emergence to anthesis | sensitive | 1700 | - | - | 1700 |
| TSUM2 | C | Temperature sum from anthesis to maturity | sensitive | 700 | - | - | 600 |
| Parameter Oat | | | | | | |  |
| TSUM1 | C | Temperature sum from emergence to anthesis | sensitive | 800 | - | - | New estimated |
| TSUM2 | C | Temperature sum from anthesis to maturity | sensitive | 750 | - | - | “ |

The calibration was based on expert knowledge regarding crop parameters for phenology. The impact of calibration was checked by comparing simulated and observed BBCH-stages. Due to the forward simulation procedure with limited calibration information, parameter uncertainty and resulting prediction uncertainty were not evaluated.

**Hydrus-1D:**

**General description**

The HYDRUS program numerically solves the Richard’s equation for variably-saturated water flow and advection-dispersion type equations for heat and solute transport (Šimůnek, Šejna, et al., 2013). The water flow equation includes a sink term for the calculation of root water uptake by plant. The heat transport equation considers transport due to conduction and convection with flowing water. Coupled water, vapour, and energy transport can be considered as well. The water flow part can deal with prescribed head and flux boundaries, boundaries controlled by atmospheric conditions, as well as free drainage boundary conditions. The governing flow and transport equations are solved numerically using Galerkin-type linear finite element schemes.

**Model set-up and protocol**

For the model set-up we used initial soil water contents values, soil parameters, weather data, and lower boundary conditions. Daily measured rainfall rates, as well as daily reference ET, LAI and rooting depth simulated by THESEUS were used as upper and measured values of depth to groundwater as lower boundary condition. Soil hydraulic properties were described by the van Genuchten-Mualem model, corresponding parameters for all lysimeters soils were provided by the organizers of the workshop. Parameter uncertainty and resulting prediction uncertainty were not evaluated.

**HydroGeoSphere:**

**General description**

HydroGeoSphere is a process-based hydrological model. The code solves the fully-integrated surface and subsurface water flow and solute transport problems in variably saturated media using a control-volume finite element method (AQUANTY, 2013, Brunner and Simmons, 2012). Further the 2D diffusive-wave equation and the 3D form of Richards’ equation are solved simultaneously by using a globally-implicit approach. Interception and comprehensive evapotranspiration(Panday and Huyakorn, 2004) are solved as mechanistic processes governed by plant and climatic conditions as noted by Kristensen and Jensen (1975), and Wigmosta, Vail, et al. (1994).

**Model set-up and protocol**

For each lysimeter its area was mapped in the model by a cell of 3 nodes. This cell was placed on top of each other at a distance of 1 centimetre to the thickness of the lysimeter. This resulted in a mesh of 450 nodes. The boundary condition at the upper end was hourly height of the precipitation and the potential evapotranspiration and at the lower end specified head, which came as variable pressure head from the corresponding lysimeter. The lateral boundaries were impermeable.

Each node was assigned the soil properties of the corresponding lysimeter in the form of van Genuchten values. The upper soil layer was assigned the respective plant properties for the evapotranspiration model, such as canopy storage, transpiration fitting parameters (Kristensen and Jensen, 1975), transpiration and evaporation limiting pressure heads (Feddes, Kowalik, et al., 1978) and evaporation and root depth function as quadratic decay. In addition, the time series of leaf area indices and root depths calculated by THESEUS/ WOFOST7.1 for each corresponding lysimeter were assigned.

The transpiration fitting parameters was fitted at the measured evapotranspiration of the corresponding lysimeter using transpiration and evaporation limiting pressure heads in the style of Wesseling, Elbers, et al. (1991), canopy storage from experiences and leaf area indices and root depths.

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