ODD-protocol

The model description follows the ODD (Overview, Design concepts, Details) protocol for describing individual- and agent-based models (Grimm et al., 2010, 2006). The IBCgrassGUI is based on the grassland community model IBC-grass (Körner et al., 2014; May et al., 2009; Reeg et al. 2017; Weiss et al., 2014). This ODD-protocol is based on the version by Reeg et al (2017), modified processes and extensions are marked in bold.

# Purpose

This extended version of IBC-grass is designed to analyse potential impacts on a local plant community adjacent to arable fields induced by herbicide drift.

# Entities, state variables and scales

Table 1 summarizes the state variables of IBC-grass. The model simulates plant community processes within a local approx. 3 m² patch designed as a grid of x\*x grid cells, i.e. one grid cell represents 1cm². The size of a patch can vary between 100\*100 cm² and 173\*173 cm². Each grid cell can comprise several seeds and not more than one individual plant. Each seed is described with the state variable of its specific location on the grid and moreover its age and mass. An individual plant can either be a ramet of a clonal plant type or a non-clonal plant. Each plant individual is described by its specific position on the grid, the duration of resource stress exposure, the shoot, root and reproductive mass and the presence of growing spacers in case of clonal plant types. Plant individuals are categorized into plant functional types (PFT), which differ in their characteristics of 12 selected trait parameters (see Table 2). Plant individuals have circular area around their stem, the ‘zone-of-influence’ (ZOI). Within this area, plants acquire and compete for resources in the case of overlapping ZOIs. Two compartments (layers) are distinguished: above- and belowground. ZOIs are determined by the specific above- and belowground biomasses of the individual plant. As plants grow, the ZOI areas increase over time. One simulated time step represents one week; in each year 30 weeks of the vegetation period are simulated.

**Resources are homogenously distributed over the grid. Aboveground and belowground resource levels can be determined separately. For aboveground resources, seasonal variation can be included by defining the amplitude of the assumed sine curve. This function is based on the day length (and thus duration of light) over the year, which follows a sine distribution.**

**Resources [week] = (amplitude\*sin(2\*pi/365)\*(((week+11)\*7)-80))+0.73)\*resource\_level**

**Week is the current week of the growing season, resource\_level is the basic resource level.**

Table 1: Main state variables of IBC-grass including a short explanation and the unit

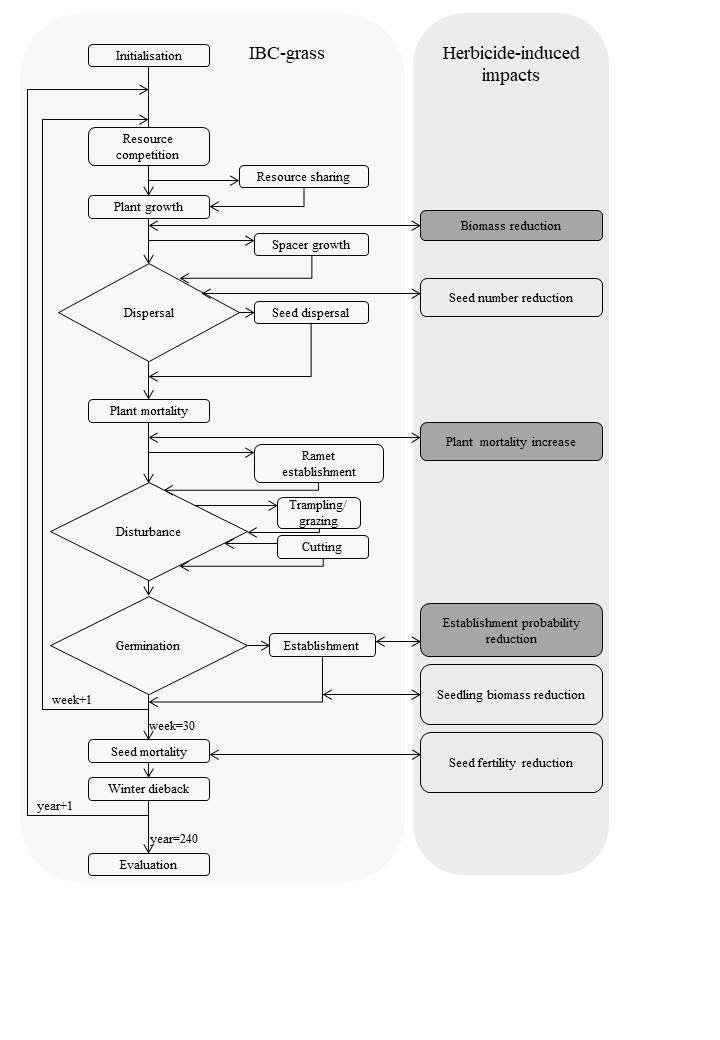
|  |  |  |
| --- | --- | --- |
| **State variable** | **Explanation** | **Unit** |
| xcoord, ycoord | location of the plant's stem on the grid |  |
| age | age of the plant | years |
| mshoot/root/repro | shoot/root/reproductive mass | mg dry mass |
| wstress | consecutive weeks of stress (i.e. lack of resources) | weeks |
| SpacerLength | current spacer length | cm |
| Spacerdirection | spacer direction |  |
| ResA/B/cell | Above- , belowground and cell resources per cm² | Resource units |
| nPFT | number of neighbouring PFTs |  |
| current\_abundance | current abundance of a PFT |  |

Table 2: PFT Trait parameter and the corresponsing plant trait data bases

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Trait/trait syndrome and attributes** | **Trait parameters** | | | | **Database** |
| **Growth form** | **fleaf** |  |  |  | *BiolFlor- rosette attribute* |
| Rosette | 1 |  |  |  | rosette |
| Intermediate | 0.75 |  |  |  | Semi-rosette |
| Erect | 0.5 |  |  |  | erect |
| **Maximum plant size** | **mmax** | **mseed** | **meandisp** | **stddisp** | *LEDA - seed releasing height* |
| Large | 5000 mg | 1 mg | 0.1 m | 0.1 m | >0.87m |
| Medium | 2000 mg | 0.3 mg | 0.3 m | 0.3 m | 0.42-0.87m |
| Small | 1000 mg | 0.1 mg | 0.6 m | 0.6 m | <0.42m |
| **Resource response** | **rumax** | **survmax** |  |  | *BiolFlor - plant strategy type* |
| Competitor | 60 resource units | 2 weeks |  |  | c, cr |
| Intermediate | 40 resource units | 4 weeks |  |  | csr, r |
| Stress-tolerator | 20 resource units | 6 weeks |  |  | sr, cs, s |
| **Grazing response** | **palat** | **cshoot** |  |  | *BiolFlor – indicator values grazing tolerance* |
| Tolerator | 1 | 1 |  |  | 4-6 |
| Intermediate | 0.5 | 0.75 |  |  | 1-3 |
| Avoider | 0.25 | 0.5 |  |  | 7-9 |
| **Herbicide susceptibility** | **Sens** |  |  |  | *Randomly distributed* |
| 0-1 |
| **Clonal integration** | **Resshare** |  |  |  | *cloPla3 – persistence of connection* |
| Integrator | 1 |  |  |  | >=2 years |
| Splitter | 0 |  |  |  | <2 years |
| **Lateral spread** | **SpacerL** | **stdSpacerL** |  |  | *cloPla3 – lateral spread* |
| Short | 2.5 cm | 2.5 cm |  |  | <0.01 m/y |
| Long | 17.5 cm | 12.5 cm |  |  | 0.01-0.25 m/y and longer |

# Process overview and scheduling

The schedule of the simulated processes is shown in Figure 1. All processes except for seed dispersal, seedling establishment and cutting are executed each week. Seed dispersal, seedling establishment and cutting are limited to certain weeks within the year. Winter dieback of aboveground biomass and seed mortality is considered once at the end of each year. The plant’s functional traits determine all processes. The state variable mass and age are synchronously updated each week and year after all model entities have been processed.



**Figure 1: Flow chart of the processes within IBC-grass. Dark grey boxes mark plant attributes currently tested in ecotoxicological standard studies.**

# Design concepts

## Basic principles

The model simulates local competition by using the zone-of-influence approach in two layers: above ground and below ground. Thereby, it distinguishes between symmetric (below ground) and asymmetric (above ground) competition. Competition among individuals of the same functional type (i.e. intra-PFT competition) is assumed to be higher than competition between individuals of different PFTs (i.e. inter-PFT competition) (Berendse, 1983). In this model version, density-dependent mortality is included.

## Emergence

Endpoints on population and community level, e.g. PFT abundance, diversity or total biomass, emerge from individual plant-plant interactions, resource levels, disturbance events like trampling, grazing and cutting and herbicide exposure effects.

## Adaptation

Plants balance the uptake of above- and belowground resources by adapting the allocation of resources to shoot and root growth.

## Interactions

Plants compete for resources and space by the ZOI approach.

## Stochasticity

Demographic noise is included by modelling seed dispersal, seedling establishment, seed mortality and plant mortality stochastically. In addition, grazing and trampling occur randomly on the simulated grid. The plant’s individual probability to be grazed is determined by its specific plant traits.

# Initialization

Initially, ten seeds per PFT of the regional PFT pool are randomly distributed over the grid. Their germination probability is set to 100% in order to have equal initial population sizes of all PFTs. Above- as well as below ground resources are distributed spatially and temporally homogenous.

# Input

The model needs the information about the available PFT pool and the trait characteristics of the respective PFTs. In addition, herbicide effects are introduced either via dose-response data of ecotoxicological standard studies or via a .txt file which includes the effect per year per attribute (see sub-model “herbicide exposure effects”).

# Sub-models

Most sub-models are adopted from the model version described by Weiß et al ( 2014). New and modified sub-models are marked in bold.

## Competition

Following the ZOI approach, plants compete for resources in a circular area around their central location point. To relate plant mass to the area covered (Ashoot), the allometric relation by Weiner et al. (2001) is used.

**** Eq. (1)

Where cshoot is a constant ratio between leaf mass and ZOI area and mshoot is vegetative shoot mass. The factor fleaf is introduced to describe different shoot geometries and is defined as the ratio between photosynthetic active (leaf) and inactive (stem) tissue. Only the former is considered for the calculation of the ZOI size. These circular areas are projected onto a grid of discrete cells. Grid cells thus contain the information by which plants they are covered, so that resource competition can be calculated cell by cell. The resources within a cell are shared among plants according to their relative competition coefficients (βi). The resource uptake (∆res) of plant i from a cell with resource availability (Rescell) covered by n plants is thus calculated as

**.**  Eq. (2)

Calculating βi in different ways allows including different modes of competition, i.e. symmetric or asymmetric (Weiner et al., 2001). We assume that the relative competitive ability of a plant is correlated with its maximum growth rate in the absence of resource competition. Therefore βi is proportional to maximum resource utilization per unit area covered (rumax, seeSub-model “Plant growth and mortality”). In the case of size-symmetric competition, βi simply equals rumax:

**.**  Eq. (3)

In the case of partially size-asymmetric competition βi is a function of plant mass and shoot geometry:

**.** Eq. (4)

The inverse of fleaf is used, because plants with a lower fraction of leaf tissue are considered to be higher and thus show a higher competitive ability by overtopping other plants. In this way, plants with equal rumax receive equal amounts of resources from one unit of area irrespective of their mass or height in the case of size-symmetric competition, while larger and higher plants receive a higher share of resources in proportion to their shoot geometry in the case of partially asymmetric competition (Schwinning and Parsons, 1999; Weiner et al., 2001). The resource uptake of a plant within one week can then be determined by summing the results of Eq. (2) over all cells covered by the plant.

To include differences between intra- and interspecific competition, individuals of the same PFT are considered as con-specifics and those of different PFTs as hetero-specifics. The relative competitive ability βi of one plant is then determined as a decreasing function of the number of plants belonging to the same PFT (nPFT) and covering the same cell:

**.** Eq. (5)

Eq. (5) is used for size-symmetric competition instead of Eq. (3). In the case of size asymmetry, plant mass and geometry are taken into consideration according to Eq. (4). This approach represents a situation where intra-PFT competition is increased relatively to inter-PFT competition and therefore implicitly includes niche differentiation of resource competition at the cell scale, which has been known as an important factor for species coexistence (Chesson, 2000; Silvertown, 2004).

## Plant growth and mortality

Plant growth only depends on the resources (∆res) that the plant acquired during the current time step. In the absence of competition, plants show sigmoid growth. Therefore the growth equation used by Weiner et al. (2001) was adapted to the description of plant geometry used here:

**,** Eq. (6)

where *g* is a constant conversion rate between resource units and plant biomass and *m*max is the maximum mass of shoot and root, respectively. In addition, the maximum amount of resources that is allocated to growth each week is limited by a maximum resource utilization rate given by rumax [resource units/cm²] multiplied by ZOI area [cm²]. If Eq. (6) yields a negative result, ∆m is set to zero and thus negative growth is prohibited. Lateral plant growth is simulated by considering clonality of plants (see *Growth, dispersal and establishment of spacers of clonal plant types*).

Growth of generative reproductive mass is restricted to the time between weeks 1-5 for early flowering PFTs and 16 – 20 for late flowering PFTs. In this period, a constant fraction of the resources (5 % for all PFTs) is allocated to growth of reproductive mass (Schippers et al., 2001), and reproductive mass is limited to 5 % of shoot mass in total. The same resource conversion rate, *g*, is used for reproductive and vegetative biomass.

Eqs. (1) – (6) are applied to shoot and root ZOIs independently, with the difference that for root growth the factor fleaf is always one. We assume that the minimum uptake of above- and below-ground resources limits plant growth (Lehsten and Kleyer, 2007) and introduced adaptive shoot-root allocation in a way that more resources are allocated to the growth of the plant compartment that harvests the limiting resource (Weiner, 2004). For resource partitioning, we adopt the model of Johnson (1985) which assumes that the fraction of resources allocated to shoot growth is calculated as

**,**  Eq. (7)

where ∆resA is above-ground and ∆resB is below-ground resource uptake.

Plants suffer resource stress if their resource uptake (in any layer) is below a fixed threshold fraction (thrres) of their optimal uptake, which is calculated as maximum resource utilization times ZOI area. That means each week the condition

∆res < thrres ∙Ashoot/root∙rumax

is evaluated and if it is true either for shoot or root the plant is considered as stress exposed during this week, and the state variable “duration of stress exposure”, wstress, is incremented. Consecutive weeks of resource stress linearly increase the probability of death

**,** Eq. (8)

where survmax is the maximum number of weeks a plant can survive under stress exposure and pbase is the stress independent background mortality of 0.7 % per week corresponding to an annual mortality rate of 20 % (Schippers et al., 2001). In order to increase the mean number of PFTs, we extended plant mortality by introducing density dependent background mortality. We multiplied pbase by a density dependent factor:

Eq. (9)

Current abundance is the number of individuals of a PFT existing in the current time step; maximal abundance the potential number of full-grown individuals on the patch in monoculture. A factor of 5 was selected by pattern oriented modelling. Lower factors did not lead to the desired effect of slightly increasing the coexistence/mean number of frequent PFT; higher factors resulted in too strong effects on mortality. Without this extension, plant communities consisted only of 5-6 dominant PFTs. By expert judgement, one would expect a higher number of PFTs in such highly disturbed and nutrient rich environments. By adding that density dependent mortality, mean PFT number increased to 10 frequent PFTs.

Dead plants do not grow and reproduce anymore, but they still can shade others and are therefore still considered for above-ground competition. Each week the mass of all dead plants is reduced by 50 % and they are removed from the grid completely as soon as their total mass decreases below 10 mg.

## Growth, dispersal and establishment of spacers of clonal plant types

For each individual (i.e. ramet) one spacer can grow at a time step. Analogously to generative reproduction, but in each week except for weeks of generative reproduction, 5% of resources acquired by the individual (∆*res*) are allocated to the growth of the spacer. First, the direction and distance of spacer growth is determined. The direction in which the spacer grows is chosen randomly from a uniform distribution. The distance of spacer growth is randomly chosen from a normal distribution, but the mean distance (SpacerL) is type-specific. The actual distance a spacer grows per week is calculated following:

**** Eq. (10)

where *g* is a constant conversion rate between resource units and plant biomass (see above) and mSpacer is a type unspecific spacer mass of 70 mg per cm; this value was derived as mean of spacer masses of *Phragmites australis* (Granéli et al., 1992) and different sea grass species (Marbà et al., 2002). If the determined distance the spacer has to grow is reached and the respective cell is not the centre of another individual, spacer growth stops and the new ramet can establish with a fixed probability (pram) (see sub-model “Seed production, dispersal, and establishment” below). If the reached cell is occupied by the centre of a different plant, spacer growth continues randomly within a radius of two cells.

## Resource sharing

Clonal plants of the integrator-type (sensu Oborny et al., 2000) share resources throughout the whole genet. Thereby each ramet provides above- and below-ground resources that are not essential for its own survival. The minimum resources (Resmin) a ramet needs for survival are calculated as a fixed threshold fraction (thrres) of the ramet´s optimal uptake analogously to the threshold fraction which determines resource stress (see above *Plant growth and mortality*).

Resmin = thrres ∙Ashoot/root ∙ rumax.  Eq. (11)

Surplus resources are added for all ramets of the genet and hence equally shared among ramets. Ramets of non-integrator clonal plant types behave like non-clonal plant individuals in this respect, i.e. they do not share resources.

## Seed production, dispersal and establishment

Early flowering plants disperse their seeds in week 6 each year, late flowering plants in week 21 each year. Seed number is determined by dividing reproductive mass by the average mass of one seed (Lehsten and Kleyer, 2007; Schippers et al., 2001). For each seed, dispersal distance is drawn from a log-normal, and direction from a uniform distribution (Stoyan and Wagner, 2001). Note that to avoid edge effects periodic boundary conditions are used.

Germination and seedling establishment are limited to four weeks in autumn directly after dispersal and four weeks in spring of the next year for all PFTs. In between, a winter mortality of 50 % of seeds is assumed and all seeds which did not germinate in these two seasons are removed.

Seedling recruitment is separated in two consecutive processes: (i) Seed germination and (ii) seedling competition. Germination is only allowed in grid cells that are not covered by any plant or its above-ground ZOI. In such cells, seeds germinate with a fixed probability (pgerm) and are converted to seedlings. In each cell only a single plant is allowed to establish. Seedling competition is modelled as a weighted lottery, using seed mass as a measure of competitive ability between seedlings (Chesson and Warner, 1981; Schippers et al., 2001). The seedling that is chosen for establishment is converted into a plant with a shoot and root mass equal to seed mass. All other seedlings, which germinated within the cell, die and are removed from the grid.

At the end of the vegetation period all growing spacers of clonal individuals establish with a fixed probability (pram) unless the cell they have reached by the time is occupied by the centre of a different individual already. If this is the case, the spacer is removed from the grid.

## Disturbances

### (1) Grazing

Grazing is modelled as partial removal of an individual’s above-ground biomass. The frequency of grazing is specified by a constant weekly probability (pgraz) of a grazing event. Grazing is a process that acts selectively towards trait attributes such as shoot size and tissue properties. Therefore, for each plant the susceptibility to grazing (sgraz) is calculated as a function of shoot size, geometry and PFT-specific palatability (palat).

**** Eq. (12)

The probability for each plant to be grazed within one a grazing event is derived by dividing individual susceptibilities by the current maximum individual susceptibility of all plants. All plants are checked for grazing in random order. In case a plant is grazed, 50 % of its shoot mass and its complete reproductive mass are removed. The random choice of plants is repeated for all other plants until 50 % of the total (aboveground) biomass on the whole grid has been removed. When all plants have been checked for grazing once, but less than 50% of the total above-ground biomass has been removed, grazing probabilities for all individuals are calculated once more based on Eq. (12) and the whole procedure is repeated until 50% of aboveground biomass has been removed or until a residual biomass is reached which is considered not grazable. This fraction is set to 15 g/m² following Schwinning and Parsons (1999). This allows a plant individual to be grazed never or several times during one week with a grazing event.

In addition to stochastic grazing, each year at the end of the vegetation period 50 % of the above-ground mass of all plant individuals is removed to mimic vegetation dieback in winter.

### (2) Trampling

Trampling is integrated to account for effects of crossing vehicles, pedestrians or larger animals. Disturbances related to trampling are subdivided in small patches of 10x10 cm² that are randomly distributed on the overall grid. Each week a given percentage of the total area is prone to trampling and plant individuals from the disturbed patches are removed.

### (3) Cutting

Depending on the management regime, cutting events are simulated one to three times during the vegetation period. During a week of simulated cutting, aboveground biomass of a plant individual is reduced to a PFT specific cutting mass. Accounting for different growth forms, and thus different plant heights, the shoot mass left after a cutting event (*mshoot\_left*) depends on the growth form *fleaf* :

*mshoot\_left*=*cutmass*\**fleaf*² Eq. (13)

*Cutmass* (500 mg) is a reference for PFTs with a rosette growth form (*fleaf*=1.0). Cutting occurs either in autumn (1 cutting event per year), spring and autumn (2 cutting events per year) or in spring, summer and autumn (3 cutting events per year).

### (4) Herbicide effects

**To include effects of herbicide exposure on plant individuals in IBC-grass, toxicological sub-processes are included. Several processes are potentially influenced by an herbicide effect: Mortality of plants, biomass of seedlings and plants, establishment of seedlings, seed production and seed fertility (i.e. sterility).**

* **Plants suffer from an additional, herbicide-induced mortality probability. The strength of effect *(pherb)* is determined by the specific effect intensity and is added after the density-dependent mortality.**
* **The biomass of seedlings and biomass gain of plants is reduced according to the specific effect intensity (*growthFac*).**
* **The establishment probability of seedlings is reduced by the specific effect intensity (*survFac)*.**
* **The resources available for seed production are reduced by the specific effect intensity (*AllocSeedFac*). The PFT specific seed weight is kept constant, resulting in a lower number of produced seeds.**
* **Seed sterility is increased by adding an herbicide-induced seed mortality probability** **according to the specific effect intensity (*survFacSE)*, which is comparable to seed fertility.**

**Effect intensities can be either based on dose-response data calculated from standardized ecotoxicological experiments or set as a discrete effect for each attribute. Plant sensitivities can be assigned randomly or specifically.**

**If the effect intensity is based on ecotoxicological data, either a random dose-response function, which is within the range of those of the tested species, or a specific dose response of one of the tested species, or no dose response (i.e. not impacted) can be assigned for each PFT in order to cover for different sensitivities.**

**If the effect intensities are based on discrete values, the sensitivity can be set to either random (0-1), full (1), high (0.65-1), medium (0.35-0.65), low (0.1-0.35) or not affected (0). The effect intensity is multiplied with the sensitivity value in order to include different sensitivities.**

**Herbicide application is simulated in a specific week of each simulated year, bearing in mind that only the growing season starting in spring is simulated in IBC-grass. In this week, the individual herbicide effect profile based on the scenario settings is assigned to the individual plants and seeds. However, each of the herbicide-induced effects appears only within the first week of the specific process (e.g. seed production is simulated only in week 6 or 21, depending on the flowering type, therefore the herbicide effect on seed production occurs within this week).**

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