

TRACE document

This is a TRACE document (“TRANSPARENT and Comprehensive model Evaluation”) which provides supporting evidence that our model presented in:

Focks A, ter Horst M, Van den Berg E, Baveco H, Van den Brink PJ. 2014. Integrating chemical fate and population-level effect models for pesticides on the landscape scale: new options for risk assessment. *Ecological Modelling* (in press, DOI: 10.1016/j.ecolmodel.2013.09.023)

was thoughtfully designed, correctly implemented, thoroughly tested, well understood, and appropriately used for its intended purpose.

The rationale of this document follows:

Schmolke A, Thorbek P, DeAngelis DL, Grimm V. 2010. Ecological modelling supporting environmental decision making: a strategy for the future. *Trends in Ecology and Evolution* 25: 479-486.

and uses the updated standard terminology and document structure in:

Grimm V, Augusiak J, Focks A, Frank B, Gabsi F, Johnston ASA, Kułakowska K, Liu C, Martin BT, Meli M, Radchuk V, Schmolke A, Thorbek P, Railsback SF. 2014. Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. *Ecological Modelling*

and

Augusiak J, Van den Brink PJ, Grimm V. 2014. Merging validation and evaluation of ecological models to ‘evaluation’: a review of terminology and a practical approach. *Ecological Modelling*.

If this document include **hyperlinks**, navigation back and forth along previously chosen links works via “ALT” + “←” or “ALT” + “→”.

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1 Problem formulation

This TRACE element provides supporting information on: The decision-making context in which the model will be used; the types of model clients or stakeholders addressed; a precise specification of the question(s) that should be answered with the model, including a specification of necessary model outputs; and a statement of the domain of applicability of the model, including the extent of acceptable extrapolations.

Summary:

The MASTEP-regional model will be used by risk managers and scientists who are interested in effects of pesticides at the landscape scale. The model provides the possibility to assess the effects of multiple applications of a pesticide in space and time, as being typical for agricultural landscapes, on the population dynamics of aquatic species. The approach does not provide yet endpoints that are immediately operational for environmental risk assessment. Further research about what new indicators could look like is recommended. Extrapolations to other species and landscapes are intended and supported by the model.

When aiming for more ecological realism in the ERA of pesticides, the challenge is to integrate different aspects of the risk assessment: spatial scale of the emission, the chemical exposure patterns in space and time, and population growth dynamics and dispersal behaviour in landscapes. To face this challenge, spatially explicit population models including population effects and recovery are ideal candidates. However, spatially explicit population models are rarely used in risk assessment. In a recent review, only 5 of 68 reviewed population-level ecological models took space explicitly into account and touched upon the extrapolation of population recovery after stress events (Galic et al., 2010).

The simulation approach that we use strives for connecting spatio-temporal exposure patterns of chemicals with an ecological model that describes the population dynamics of an aquatic macroinvertebrate species on the landscape scale including the most relevant life-history species traits. It integrates about chemical fate and population dynamics as well as landscape structures and hence provides the means for extrapolations of pesticide effects from small scale observations to the field scale.

The approach provides new possibilities for the simulation of pesticide effects on aquatic macroinvertebrates on a landscape scale. Risk assessors can use integrated simulation frameworks like the one proposed in this study for the aquatic environment to add information about possible effects of a substance in realistic landscapes, under realistic application schemes. Such simulation studies could be very useful to prepare and accompany field monitoring studies. Moreover, they could answer some of their most pressing questions like “What if the compound is applied several times in different places?”, “What if not only this compound but also others are applied in the same region?”, or “What if the species already suffer from other stress factors such as drought?”. Questions like these are not contained in the current scheme for risk assessment, and it is not certain if they ever will be part of it. However, these are exactly some of the questions risk assessors and managers are interested in, because pesticides are not used in isolation and with single applications in the real world. Additionally, researchers in aquatic toxicology being interested in field-scale assessments and coupling between exposure and population effects might be interested to utilize the modelling approach for research questions or the planning of monitoring campaigns.

The generality of our framework (Fig.1) enables future simulation studies where chemical exposure patterns as calculated with an arbitrary fate simulation tool can be used as input for an interchangeable local population model for different species; simulations are then

Our approach does not provide yet endpoints that are immediately operational for environmental risk assessment. Further research about what new indicators could look like

and how they could be integrated into the current ERA framework is recommended before applying the modelling approach in higher tier registration procedures.

The model results show the seasonal population dynamics of the aquatic organisms in the ditch network, and at the times of pesticide exposures spatio-temporal mortality patterns are used with a spatial resolution of 10 m. The model provides insights in the spatial extent of pesticide mortalities as caused in water bodies receiving direct spray-drift input as well as in water bodies affected by transport of pesticide loads downstream in the ditch network. This information can be used for the calculation of indicators quantifying the area where population densities are affected by pesticide applications.

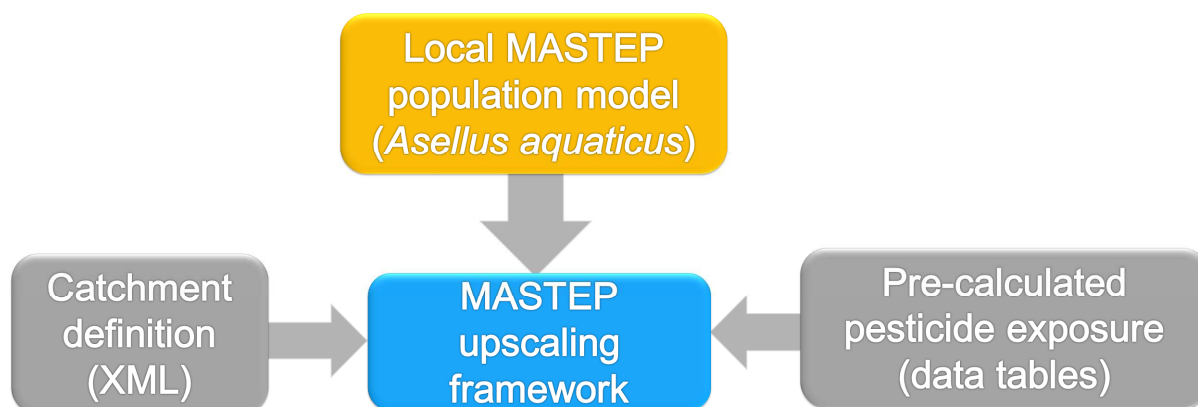


Figure 1: Overview about the building blocks of the upscaling framework.

2 Model description

This TRACE element provides supporting information on: The model. Provide a detailed written model description. For individual/agent-based and other simulation models, the ODD protocol is recommended as standard format. For complex submodels it should include concise explanations of the underlying rationale. Model users should learn what the model is, how it works, and what guided its design.

Summary:

The MASTEP-regional model is described in detail. The model provides a framework, that compiles the [definition of a landscape structure](#), [pesticide exposure time series](#) and a [population model](#) (ODD format) into landscape-scale simulations. Concrete examples for the subparts of the MASTEP-regional approach are given. An [overview](#) about the modelling approach is given at first.

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Overview

The model setup in terms of landscape structure definition is very flexible and designed to represent any given landscape structure in terms of a water body network. As an application example, a landscape definition for a typical Dutch landscape structure in terms of a network of drainage ditches in an agricultural landscape is given. Semi-realism of the landscape setup is provided by abstracting the number, connections and concrete lengths and widths of the ditches from an existing landscape. The spatial scale of the simulated landscape is approximately 10 km², the total length of simulated water bodies comprises 65 km. All ditches are simulated with a spatial resolution of 10m. An overview about the landscape definition is given in Figure 2.

Pesticides exposure concentrations are provided to the simulation model as calculated with an external simulation software (see [Exposure model](#)). For the current example, the CASCADE-TOXSWA software (Kruijne et al., 2008) was utilised to provide pesticide concentrations in water in daily time steps for each of the 10 meter segments of the water course network. The rationale for choosing the given pesticide exposure was to assume typical treatment schemes for the crops in the landscape, in this case of the insecticide λ -cyhalothrin for potato, and to calculate the fate dynamics of the pesticide in water following spray-drift input. Information on typical pesticide application patterns in potato was extracted from literature (Arts et al., 2006), and the product label for the product Karate Zeon that contains λ -cyhalothrin as active ingredient (<http://www.fytostat.nl/>, Dutch product label).

Local population dynamics within the upscaling framework can be simulated with any NetLogo population model that follows a small number of conventions (see [Local population model](#)). For the current example, the population dynamics of the water louse is simulated using an adapted version of the MASTEP model for *Asellus aquaticus* (Galic et al., 2012; Van den Brink et al., 2007). The model simulates water louse populations in northern European countries, that show typically bivoltine populations dynamics over a year. Population ecology in the MASTEP approach combines a species traits-based approach with empirical descriptions of reproductive periods. Species traits being considered for population dynamics are e.g. dispersal behaviour or number of offspring. The model is formulating growth in length and emergence of juveniles as functions of time, so the dynamical description is not driven by first principles like nutrient uptake or temperature.

Local exposure concentrations in the water network are linked to individual mortalities per day via a dose-response relationship (see [Linking exposure with effects](#)).

MASTEP regional consists of a Java-coded framework for the upscaling of the population dynamics simulations and the coupling to landscape-scale exposure patterns (see also [Landscape-scale and implementation](#)). A landscape definition file that contains the main components of the landscape definition, i.e. sections and nodes of the water bodies, is read into the software. For each section being defined in the landscape definition, a local MASTEP model is initialised. Pre-calculated concentration time series that provide one concentration value per day and segment are imported from data files and assigned to each local model. The framework controls the simulations of all local models and synchronizes the exchange of individuals across the section borders. A flow diagram depicts the structure of the landscape-scale simulation steps (Fig. 3). All programs and scripts required to run MASTEP regional are available at <http://cream-itn.eu/projects/wp-1/scales-4>.

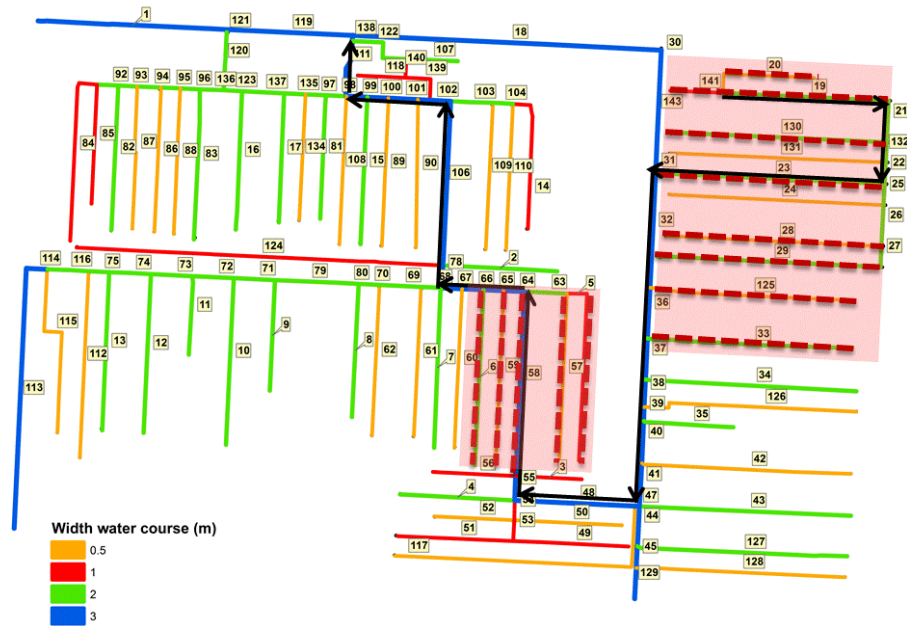


Figure 2: Overview of the simulated water course network. The colours of the water courses indicate different widths (see legend bottom left corner). The sections that received spray drift input are displayed in red dashed lines (----) and are located in the red dyed boxes, the corresponding section numbers are 33, 125, 29, 28, 23, 130, 19, 141, 20 and 6, 59, 58, 57, 5 (black numbers in the picture). Analyses of exposure and effects of the pesticide are shown for the transect from section 19 to 111, as indicated by the black arrows in the network, that give also the flow direction of these water courses (downstream transect consists of sections 19,21, 132, 22, 23, 32, 36, 37, 38, 40, 41, 47, 55, 58, 64, 65, 66, 67, 77, 106, 102, 101, 100, 99, 111) .

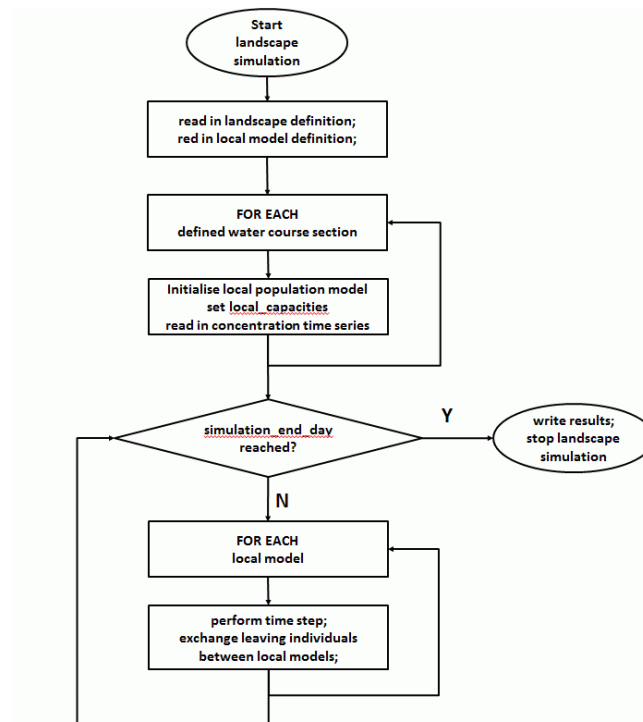


Figure 3: Flow chart of the upscaling framework.

Exposure model

Spatio-temporal explicit exposure concentrations in the ditches were simulated using the CASCADE-TOXSWA model. The CASCADE-TOXSWA model has been developed to assess the fate of pesticides in an interconnected system of watercourses with variable hydrological characteristics. It is based on TOXSWA, a model for the simulation of pesticide fate in water and sediment systems (Adriaanse, 1996; Beltman et al., 2006). The TOXSWA model is used in the registration procedure of plant protection products at the national level of the Netherlands and the EU level (FOCUS, 2001).

The catchment consists of seven water management subareas in which the water level is controlled by weirs and pumps. The CASCADE catchment has one outlet point and the hydrology in this catchment has been described using the SWQN model (Smit and Siderius, 2007). SWQN is a simple hydraulic model (kinematic wave) which computes flows and water levels in a network of nodes and segments on a daily basis. Input on drainage into the water courses and infiltration via the sediment is calculated with the SWAP model (Kroes et al., 2008). The hydrology in the catchment of Klazienaveen-Zwartemeer has been calibrated using measured hydrological data from the study region (Kruijne et al., 2008).

The present version of the CASCADE-TOXSWA model only considers the water layer in the system of watercourses. So far, no sediment compartment has been implemented. The included transport processes are advection and dispersion. The transfer of the pesticide from one watercourse to a receiving watercourse depends on the water discharge at the end of the watercourse and the pesticide concentration in this water flow. Dispersion is not yet taken into account at junctions. Other watercourses discharging into the same receiving watercourse may dilute the pesticide concentration in the receiving watercourse or add to the mass entering this watercourse. Sorption of the pesticide to suspended solids in the water layer is described using a Freundlich sorption isotherm. The transformation of the pesticide in water is described using first-order kinetics. The volatilisation of substance from the water layer is described using the concept of Liss and Slater (1974). The mass conservation equation for the transport of substance in the watercourse is solved using the explicit integration method described by Adriaanse (1996) for the single watercourse model TOXSWA. The entry pathway of the pesticide in this study was deposition due to spray drift. Multiple spray drift loading events have been specified for the watercourses.

Local population model

The local model was adapted from the NetLogo (Wilensky, 1999) source code of Galic et al. (2012). Small changes were necessary to enable the use of this model as a building block for the landscape-scale simulations. An overview about the simulation steps in the local model is provided in form of a flow chart (Figure 4).

In the following, a detailed model description following the ODD protocol for describing individual- and agent-based models is provided (Grimm et al., 2006; Grimm et al., 2010). All information in the following refers to the local population model only and does not relate to the landscape scale.

Purpose

The main purpose of the model is to simulate population dynamics of the water louse, *Asellus aquaticus* in a water body in daily time steps.

Entities, state variables, and scales

Entities in the model are water louse individual females and square cells comprising the habitat. For individual females we distinguish between juvenile and adult stage.

Individual state variables are age [days], size [length in mm], hatching date [day in the calendar year], lifespan [days] and location [continuous X and Y coordinates] in the local model. Adults, i.e. individuals older than 44 days, have in addition the variable reproductive status which takes on the value of either 0 (= not yet reproduced) or 1 (= reproduced).

The state variables of cells are the carrying capacity and the local mortality of *Asellus* induced by pesticides and by the density of individuals in the patch. Additionally, each cells contains a number that refers to the ID of the water body number in the water network.



Figure 4: Flow chart for the local model. $\text{rand}(1)$ are uniformly distributed random numbers between 0 and 1.

Spatial heterogeneity, e.g. the linking between chemical exposure and population dynamics, is done in segments. A segment is a 10m long part of a water course section, for that a specific area (m^2) and pesticide exposure concentration per day (mg/L) is given. The area (m^2) and the corresponding local capacity (individuals/segment) for each of the segments were calculated assuming a carrying capacity of 50 individuals/ m^2 . A segment is assumed to be build up from 10 NetLogo patches. Each patch is initialised with the tenth part of the capacity (individuals per segment). The patch carrying capacities are used for calculating density-dependent growth and mortalities.

The boundary conditions of the local model are specifically defined. The vertical boundaries, that are the riversides, are periodic so that individuals could just move. The horizontal boundaries of the local model, mimicking the interfaces to other local models or water body-junctions, are defined in a way, that if an individual would make a move out of the local model, it is recorded in an "exchange table" and removed from a local model. This exchange table is then used by the upscaling framework to put that leaving individual into an appropriate other local model. The individual object is deep copied, that means with all current lifetime characteristics.

The basic time step in the model is one day. There are 365 days in a year. Simulations start on day 0 (Jan 1) and go for 3 years or until there are no surviving individuals left.

The table with all parameters and their distributions is provided in Table 1.

Process overview and scheduling

Every time step (day), the following processes, or submodels, are scheduled for all individuals in a randomized sequence for each process; state variables are updated immediately (asynchronous updating). A flow diagram of the local model is given in fig 4.:

```
Aging (Increase age of individuals by one time step)
If Mortality (background and density-dependent)
    Delete from the population
Else
    Move - same for all, individuals leaving the local model
           put into the exchange table
    Grow - both juveniles and adults until they reach maximum
           size
    Mature - when juvenile reaches 45 days, it becomes adult
             and can reproduce
    Reproduce - once per each individual adult,
                2 generations in 1 year
    Pesticide mortality
```

Design Concepts

Basic principles. The model relies locally on a phenomenological representation of density-dependent effects. Another principle explored is the effect of movement on recovery, and of metapopulation and rescue effects, i.e. of individuals immigrating other areas.

Emergence. Population dynamics and in particular the response of the population to pesticide-induced mortality arise from individual behaviour (movement) and local, within-cell density-dependent effects.

Interaction. Individuals interact indirectly via local density-dependent effects on growth, reproduction, and mortality. In individuals that have not reached their maximal size, daily growth increment is hampered by increasing density in their local environment (single cell), and the size at reproduction time determines the final clutch size. Probability of dying increases with increasing density of individuals in a patch.

Stochasticity. Values of most parameters are drawn from probability distributions obtained from literature data to represent natural variability observed in asellid populations. All parameter values and distributions are shown in Table 1.

Observation. For each patch, the density of adult and juvenile asellids are observed.

Initialization

The initial population of adult individuals is set according to the area of the local model, each individual with a given size, drawn from a normal distribution (mean 3 mm, SD 0.2, based on Chambers, 1977). Individuals are randomly distributed within their aquatic habitat and have their variables defined at the start of the simulation.

The following pseudo-code gives an overview of the initialization process:

```
initialize all cells:
set carrying capacity
assign pesticide exposure to patch
initialize Asellus individuals within the cell
    set size
    set age
    set location ...
```

Input data

The model does only include external input for pesticide exposure concentrations. Other environmental drivers of system behaviour such as temperature, rainfall etc. are not imported.

The pesticide exposure data is organised in a table that provides for each patch and for each simulation day one concentration value (can also be zero). This table is read from the given files and transferred to the local NetLogo model by the upscaling framework.

Submodels

There are four submodels in MASTEP for *Asellus aquaticus*: mortality, dispersal, growth and reproduction.

MORTALITY

Individuals suffer from three types of mortality: background, density-dependent and pesticide induced. Mortalities and their probabilities are sequential, and not summed up.

First is the background or natural mortality, based on the lifespan of *A. aquaticus* in NW Europe (up to 600 days in (Vitagliano G et al., 1991)). Natural mortality is related to age, reproductive status, predation, and we assume juveniles experience a higher mortality rate than adults (Van Den Brink et al., 2007). Under this assumption, we assign each individual a lifespan from an exponential distribution with a mean 90, resulting in less than 1% of individuals surviving longer than 400 days. Once the number of time steps in the simulation reaches an individual's lifespan, it will die and be erased from the population.

Including density-dependent mortality is an indirect way of modeling resource competition, because we do not model resource dynamics. Even though exact mechanisms of density dependence are not clear, it is known that populations of *A. aquaticus* are regulated to a certain level by their densities see e.g. (Adcock, 1979; Iversen and Thorup, 1988; Van Den Brink et al., 2007)); we follow the mortality based on local densities from van den Brink et al. (2007), where

$$\mu_{dd} = \mu_1 \cdot N \quad (\text{eq. 1})$$

where μ_1 is a parameter governing the steepness of the density dependence ($\text{m}^2/\text{ind} \cdot \text{d}$) and N is the local density (ind/m^2). Density-dependent mortality is cell based, so all individuals in one cell have the same probability of dying due to overcrowding.

Eq. 1 is the simplest assumption on effects of density, where each individual has a certain effect on each of its conspecifics within 1 cell. We chose to use this relation over, for instance, a logistic density dependent function which has very little effect at very low densities (thus, not very regulating), but after a certain threshold, the mortality is 100%. In previous test runs, this resulted in the mortality of all individuals in 1 cell after reproductive events.

Pesticide- induced daily mortality risk m_{chem} (%) was calculated from predicted exposure concentrations for each segment (see [Linking exposure with effects](#)).

DISPERSAL

Very little data exists on movement patterns and dispersal speed of *A.aquaticus* individuals. Van den Brink et al. (2007) calculate the mean residence time of individuals in one cell to be 51 minutes, where they move one third, and rest for 2 thirds of their time. (Englund and Hambäck, 2004) showed a step length frequency distribution of individuals of *A. aquaticus*, where the majority of steps fall between 0 and 4 cm, both downstream and upstream. Yet, no estimations are made on the daily step frequency.

Active dispersal in the ditch

In this model, we assume that individuals move one step per minute, and that they move 480 minutes of the day (1/3 of 1440 minutes in 24 hours). As the exact details on *Asellus* dispersal are unknown, we assume they follow the correlated random walk (CRW) rules where each new orientation of an individual depends probabilistically on the previous orientation, i.e. there is a preference to continue in a similar direction, depending on the defined angle of a circular distribution. This approach seems to work for many animal species where exact movement patterns were analysed.

We used the von Mises probability distribution, a normal distribution on the circle, given by the following equation

$$f(x) = \frac{e^{\kappa \cdot \cos(x-\mu)}}{2\pi \cdot I_0(\kappa)} \quad (\text{eq. 2})$$

where $I_0(\kappa)$ is the modified Bessel function of order 0. μ is the mean of the distribution, while the variance is defined by κ . The smaller κ , the more diffused the distribution is and resembles a uniform distribution at value 0. The larger values of κ are, the distribution centers more around the mean, which means that if used in CRW procedure, the movement will be very directed. For our purposes, both μ and κ are estimated from experiments (unpublished data, see Table 1 in the TRACE documentation).

Once the new turning angle is drawn from the afore defined distribution, each individual moves the distance of the chosen step length.

Because small, individual movement is on a very fine time scale (in minutes), while the basic time step in the model is 1 day, we chose to simulate the fine dispersal separately and include only the distances covered after 24 hours in the population model.

For that, we simulated dispersal of 100 000 individuals in a ditch, all starting from the same position in one cell, counted the number of individuals in each of the cells after the simulation and from that, estimated the probability distribution of distances each individual is expected to cover in one time step (fig. 5).

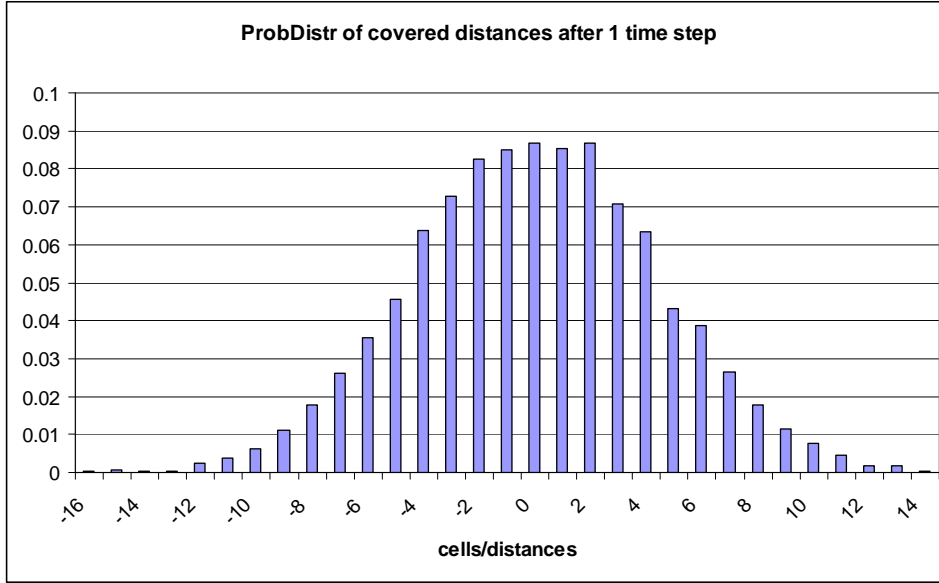


Figure 5. Distribution of distances covered from cell 0, movement 1/3 of one day (480 minutes).

In the population model, all of the individuals of the initial population and their subsequent offspring are positioned randomly within a cell. In each time step, each individual will be assigned a random number from the simulated distribution and will change its x coordinate accordingly, by summing it up with the drawn number. In that way, individuals during their lifetime do not change the position in the cell itself, but move from cell to cell. Since we do not include any heterogeneity nor are any processes different within cells, changing the exact position of individuals within cells is irrelevant.

Passive dispersal

In the current version passive dispersal (e.g. via drift) is not considered.

GROWTH

Individuals grow following the von Bertalanffy growth equation, leading to a logistic growth curve which is observed in most isomorphs under constant food conditions:

$$l(a) = l_{\max} \cdot (1 - e^{-\kappa a}) \quad (\text{eq. 3})$$

where l_{\max} is the maximal length an individual can reach, κ is the daily growth rate and a is age (days). The maximum size of individuals varies depending on the region, between 11 and 12 mm in the publication by (Økland, 1978), 9 mm (Chambers, 1977), around 12 mm (Arakelova, 2001) and up to 12 mm (Marcus JH et al., 1978).

The newly hatched individuals get their sizes assigned to them from normal distributions, 1 mm with 0.2 mm SD (Adcock, 1979). Following the growth function (with a growth rate as in table 1), an individual starting with 1 mm length needs 145 days to reach 95% of the maximum given size, i.e. 11.4 mm.

Daily growth increment is then the derivative of eq.3

$$\frac{dl}{da} = \kappa \cdot l \cdot \left(\frac{l_{\max}}{l} - 1 \right) \quad (\text{eq. 4})$$

We assume that growth is density dependent, and decreases exponentially with high densities in a patch (fig. 6). The density dependent factor is expressed as

$$DDG(density) = e^{-y/K} * density \quad (\text{eq. 5})$$

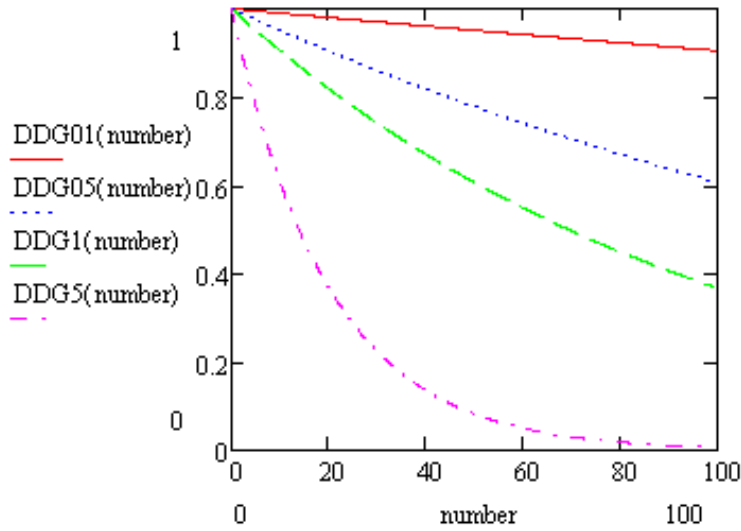


Figure 6. The strength of individual growth dependence on local densities (eq. 5) is expressed with a scaling parameter. The carrying capacity in this figure is 100 individuals, and 4 different values are depicted, namely 0.1, 0.5, 1 (the default value) and 5.

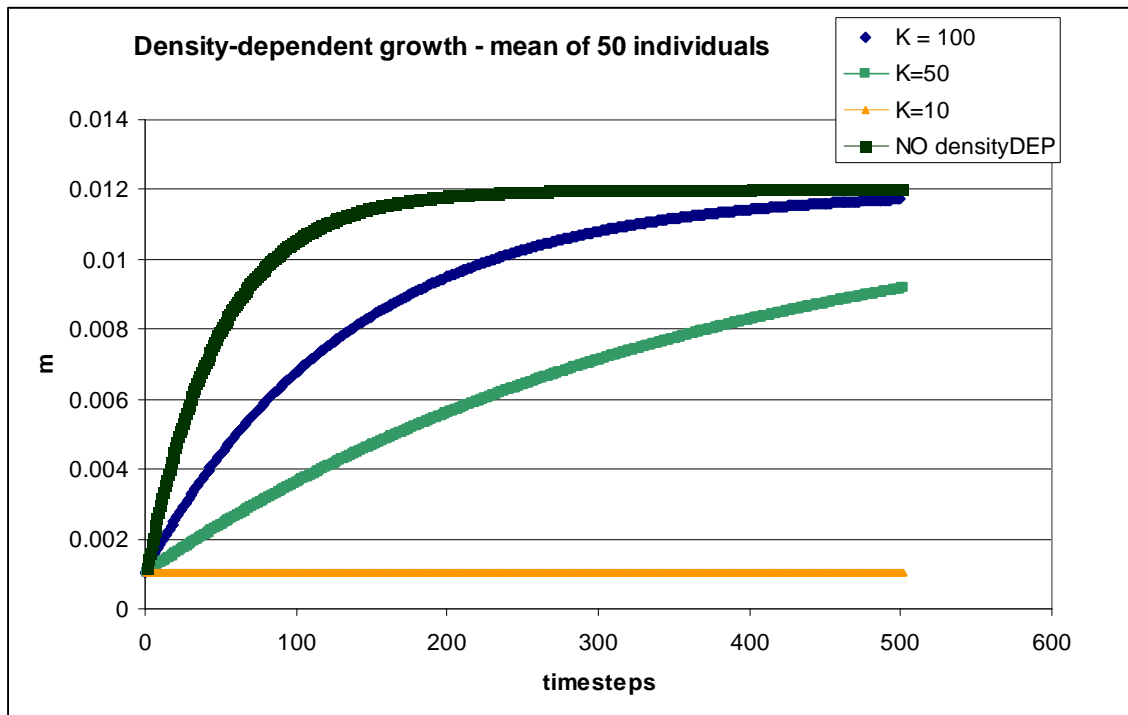


Figure 7. Average values of individual growth trajectories of populations under different densities. m is the size in meters, and “timesteps” are in days. There are 50 individuals in this population (that only go through the growth procedure), their growth is modeled under no density-dependent effects, and under set K of 10, 50 and 100.

where y is the scaling factor of the function, and K is the local (single cell) carrying capacity.

The reasoning behind it is the publication of Marcus et al. (1978) who show a hampered growth when individuals are fed on less preferred substrate. Similarly, (Hynes and Williams, 1965) experimentally showed that water louse populations produce more offspring when housed in larger jars; even though the amount of food in their experiments was the same, the lower productivity indicates certain effects of, possibly interference, competition resulting in lowered production.

We approximate the effect of less preferred habitat or scarce resource by including the effects of density on daily size increments, in such a way that when the density in a cell reaches the assigned carrying capacity, each individual has a decrease in its size increment of 60% (green line in fig. 6). The model output is analyzed with respect to the density dependent scaling parameter y .

Figure 7 shows (mean individual) growth trajectories in dependence of the (constant) density of the population (density dependent scaling parameter is set to 1, there are 50 individuals in the population), where overall carrying capacity varies. With no density dependent effects, individuals reach their maximal size by day 200.

It takes the asellids around 300 days longer in case when the density is half of the set carrying capacity, and much longer in case the population is at its K . If the density exceeds carrying capacity by 5x (K is 10, fig. 7) individuals almost stop growing.

REPRODUCTION

When they hatch, juveniles get the date when they are going to reproduce. Once individuals reach an age of 45 days, they become adults, so maturation is age-dependent, and they can reproduce. The onsets of reproduction in the model are days 120 (April/May) and 200 (July) (adapted from van den Brink et al. 2007), which mimic the typical months when the water louse reproduces in NW Europe.

Individuals are given 3 weeks in the spring and 5 weeks in the summer, during which they reproduce. This means that each individual gets a number (drawn from a normal distribution) that signifies the day after the reproductive onset (d 120 or 200) at which it will release its offspring. E.g. an individual will draw number 12 and if it is in the overwintering population, it will release its young at day 132 (onset 120 + 12).

Individuals are allowed to reproduce only once in their lifetime, as this is most common (Chambers 1977). The number of offspring (egg production) is size-dependent and is positively correlated with size (Chambers 1977), see figure 8.

$$N_{\text{offspring}} = \text{current_size} / \text{max_size} \cdot \text{max_clutch_size} \quad (\text{eq. 6})$$

Each adult, thus, gives birth to a different number of juveniles and dies shortly after. Females from the winter generation are bigger and will have more offspring per female, but are fewer to start with; summer females are smaller, as by the time they start reproducing (after around 80 days and less), they will be maximum 9 mm long (according to (Økland, 1978), summer females are up to 7 mm in length).

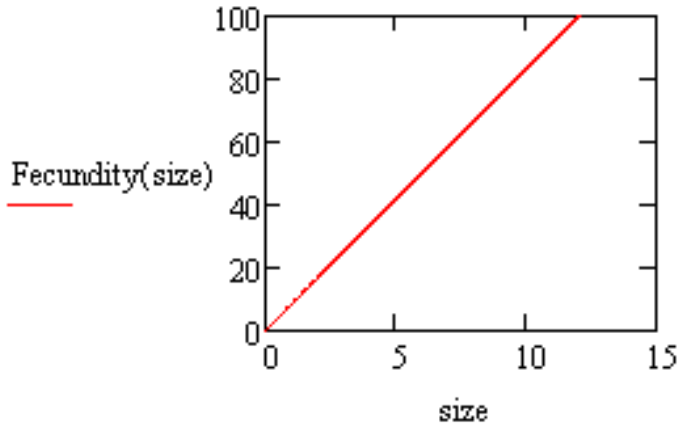


Figure 8. Relationship between size and number of offspring each female releases in 1 reproductive cycle.

Linking exposure with effects

Pesticide-induced daily mortality risk m_{chem} (%) was calculated from predicted exposure concentrations for each segment applying the dose response equation:

$$m_{chem} = 100 / (1 + \exp (-\text{slope} \cdot (\ln(C(t,i)) - \ln(EC50)))) \quad (\text{eq. 7})$$

The actual exposure concentration at time t in segment i , $C(t,i)$ (mg/L), and the constants $EC50$ (mg/L) and slope (-) thus scale the specific toxicity of the simulated pesticide. The calculated mortality probability for a given pesticide concentration was implemented by removing a respective fraction of randomly chosen individuals from the local segment. For each new simulation day, the mortality probability was imposed to the total 100% of the remaining population, corresponding to the stochastic death approach (Jager et al., 2011).

Landscape-scale and implementation

A modelled landscape consists of connected linear watercourses called sections, that together make up a water course network (example in Fig. 2). Each section in the catchment has defined widths at the upstream and downstream boundaries, a defined section length and an associated length of internal segments. The internal segments can be of a variable length, but in the case study we fixed it to 10m. Each segment has a specific associated area (m^2), capacity (# individuals), and concentration time series (for each day one concentration value in mg/L). The internal segments are the central elements for linking exposure concentration and population dynamics. The linking between exposure and effects can be implemented flexible in the population model. More details about linking the exposure of λ -cyhalothrin to effects in the case study are given below.

TRACE document: Focks et al., Effect models for pesticides at landscape scale.

Table 1: Key parameters, values and references

Category	Name (meaning)	Value (distribution)	Unit	Reference
Population model				
Habitat	Local_capacity	50 ^a	Individuals/m ²	Following Galic et al. (2012)
Mortality	Lifespan	90 (Exponential)	-	Galic et al. (2012), Vitagliano et al. (1991) therein
	Steepness_DDmort (Steepness of mortality function)	0.05	-	Galic et al. (2012),
	Repro_date_1 (Age at reproduction 1 st period)	120	day	Galic et al. (2012)
Reproduction	Repro_date_2 (Age at reproduction 2 nd period)	200	day	Galic et al. (2012)
	Max_offspring (Maximum offspring number)	100	individuals	Galic et al. (2012)
	Repro_len_1 (Length of 1 st reproduction period)	1 to 28 (uniform)	day	Galic et al. (2012), Chambers (1977) therein
Growth	Repro_len_2 (Length of 2 nd reproduction period)	1 to 45 (uniform)	day	Galic et al. (2012), Chambers (1977) therein
	Max_size (Maximum size)	12	mm	Galic et al. (2012), references therein
	Min_size (Minimum size)	Mean 1, SD 0.2 (Normal)	mm	Galic et al. (2012), Adcock (1979) therein
Movement	K (Size growth rate constant)	0.02	1/day	Galic et al. (2012)
	Mat_age (Age at maturity)	45	day	Galic et al. (2012)
	Step_size	Mean 0.004, SD 4.44 (Normal)	m	Following van den Brink et al. (2007)
Population model forcing functions	Prob_DD_mort (Probability density dependent mortality)	Prob_DD_mort = individuals(patch)/local_capacity x steepness_DDmort	%	Galic et al. (2012)
	Length (Body size)	Len (age)= Max_size x (1-exp(-k x age))	mm	Galic et al. (2012)
	N_offsp (Number of offspring)	N_offsp = Len/Max_size x Max_offspring	individuals	Galic et al. (2012)
Pesticide fate model				
	Molar mass	449.9		
	Solubility in water	0.005 (at 20 °C)	mg/L	
	DegT50 in water	1 (at 20 °C)	day	
	K _{om} soil, sediment, suspended solids	138820	L kg ⁻¹	
	1/n (Freundlich exponent)	0.9	-	
	Saturated vapour pressure	2Exp(-7) (20 °C)	Pa	
	Molar enthalpy of vaporisation	95	kJ/mol	
	Molar enthalpy of dissolution	27	kJ/mol	
	Concentration suspended solids	11	g/m ³	Typical value for Dutch surface waters; refer to Tiktak et al. (2012)
	Mass fraction of organic matter in suspended solids	0.09	kg/kg	FOCUS (2001)

^a: specific values per segment were calculated according to the segment area

The single water courses (sections) in the landscape are directed in the sense that they have defined flow directions and open boundaries, so that simulated individuals can move across one of the boundaries to a different section. Each section has one or none downstream section and none, one, or more upstream sections. Sections without a connected upstream section are closed in the upstream boundary for individual movement. In the section without a downstream section the very last boundary is open, meaning that moving individuals and transported chemicals leave the catchment at this point.

The upscaling framework was implemented in Java (Java SE Development Kit 6 u25, Oracle). The program flow in the upscaling framework is as follows. A definition file is read into the software at the beginning (for a typical example see table 2). The definition file contains mandatory a working path, a landscape definition file, the name of a NetLogo model being used as population model, the path to the pesticide scenario, where concentration data files are accessible, and two values defining the simulation end day and the local capacity per m². The main components of the landscape definition are sections and nodes of the water courses, both defined as entries in an XML data structure. For each section as defined in the landscape definition, a local MASTEP model is initialised using the NetLogo-Java bridge (object `org.nlogo.headless.HeadlessWorkspace`) and the given filename. Pre-calculated concentration time series are read in from the given directory, checked for consistency, and assigned to the given local models, resulting in one concentration value per day and segment. The framework controls the simulations of all local models and synchronizes the exchange of individuals across the section borders (flow chart in figure 3). The source code of the upscaling framework and the used NetLogo model for the population dynamics of *Asellus aquaticus* is accessible online at <http://www.cream-itn.eu/projects/wp-1/scales-4>.

Table 2: Typical content of a definition file for the upscaling framework

```
workingPath = "D:\test-scen2\"
catchmentDefinitionFileName= "D:\workspace\MASTEP-regional\catchment-
definitions\Klazinaveen-real.xml"
netLogoFileName = "D:\workspace\MASTEP-
regional\NetLogoCode\Asellus_v3\Asellus-UPSCALE-v2.nlogo"
pesticideScenarioPath = "D:\workspace\MASTEP-
regional\pest_scenarios\appDay105\V1D2\"
simulationEndDay = 1090
capacity = 50
// COMMANDS being submitted to all local netLogo models BEFORE the
invocation of their setup method-----
commands = "set fraction_of_exposed 1"
commands = "set initDensity 0.1"
commands = "set LC50 0.1"
commands = "set flow_velocity 0.001"
commands = "set steepness_DDmort 0.05"
...
```

3 Data evaluation

This TRACE element provides supporting information on: The quality and sources of numerical and qualitative data used to parameterize the model, both directly and inversely via calibration, and of the observed patterns that were used to design the overall model structure. This critical evaluation will allow model users to assess the scope and the uncertainty of the data and knowledge on which the model is based.

Summary:

The model was not calibrated to experimental data. Overall, the available data for parameterization of the model parts was taken from peer-reviewed literature.

For the parameterization of the pesticide fate model, several scientific publications were evaluated. The population model was parameterized based on a number of scientific publications that focused, however, primarily on size and fecundity related aspects. Previous applications of the population model indicate its reasonability. However, information on density dependence and dispersal parameters are scarce. The link between exposure and effects was parameterized based on an appropriate scientific publication.

Parameterisation of fate dynamics

The fate of λ -cyhalothrin in water is rather complex with the dominant processes being sorption to sediment and dissolved organic matter and alkaline hydrolysis. The latter processes will depend on surface water conditions, primarily season, mass of macrophytes and changes in pH. However, in general the dissipation of λ -cyhalothrin from water proceeds rather fast. From three microcosm studies, the dissipation time of the pyrethroid was estimated to be less than one day ($DT_{50} < 1d$, Leistra et al., 2003). In the same study, the authors came to the conclusion that transformation rates in water seem to be too fast to allow substantial fractions of initial doses to build up in plant and sediment. In this respect, we disregarded the sediment compartment and parameterised the dissipation rate from water with a half-life of 1 day. Dissipation times in the range of 1 day have also been reported from other studies (Arts et al., 2006, Schroer et al., 2004).

The hydrological regime was calculated for the years 1994 - 1996. Other parameter values used for the numerical simulation of chemical fate are shown in table 1.

Population model

Most model parameters were taken from the publication of Galic and colleagues (2012); the values we used are summarised in table 1. Stochasticity in the life history of the individuals was introduced into the model by the assignment of an individual life span and an individual time to reproduction at the simulated birth of each individual. Respective values were drawn from statistical distributions. Details on the parameterisation of the submodels are given in [Submodels](#).

Applications of the local population model have been performed and analysed and the meaningfulness of the simulation results have been assessed. Van den Brink et al. (2007) used the IBM approach to simulate the response of *A. aquaticus* to pesticide stress in aquatic systems mimicking exposure scenarios already in use for the registration of pesticides in the EU (FOCUS, 2001). In the MASTEP model (Van den Brink et al., 2007), exposure to a hypothetical, rapidly disappearing pesticide and resulting individual mortalities was simulated spatially explicit within a single ditch, stream or pond. The authors showed that the type of water body used influenced population effects and recovery. In streams, for instance, individual drift led to faster population recovery in the exposed part of the stream compared to recovery observed without drift, while in unexposed parts of the stream populations became affected, i.e. drift initiated action at distance. An adapted version of the MASTEP model was used to assess the influence of the timing of pesticide stress during the year and landscape connectivity on recovery times of *A. aquaticus* (Galic et al., 2012). The simulation results indicated that population recovery is mainly driven by reproductive periods and that high habitat connectivity leads to faster recovery. The concept of the local population model can, based on the two publications with analyses therein (Van den Brink et al., 2007 and Galic et al., 2012), be considered to be evaluated.

Linking exposure and effects

The concentration time series, as given by the CASCADE simulations (see [Exposure model](#)), were transformed in a post-processing step to serve as input for the population effect simulations. Concentrations were aggregated over time by taking the maximum value over 24 hours. Aggregation was necessary because the population model uses daily steps to convert exposure concentrations to mortality probabilities. We took the maximum concentration over 24 hours rather than the average due to the setup of the experimental study that we used to parameterise the effect simulations. In the experiments of Schroer and co-workers, the initial concentrations were measured at the start of the lab experiments (Schroer et al., 2004). Over 24 hours, the initial concentrations dropped to values between 31 and 51 % of the initial concentration. Hence, taking the maximum value over 24 hours for the quantification of effects in the simulations resembles the setup of these experiments, because in both cases the effect on the water louse is evaluated 24 hours after the maximum concentration appeared in the water. Concentration values for each simulation day were assigned to the segments of the population model.

The dose-response relationship for λ -cyhalothrin (eq. 7) was parameterised from the literature (Schroer et al., 2004). The slope was calculated from the reported EC50 and EC10 concentrations to 2.341 (-), for the toxicity parameter we used the 48h-EC50 value of 24 ng/L. We chose the effective concentration for immobility (EC50) rather than the lethal concentration (LC50) because immobility of individuals is in practice often leading to mortality, either by predation of immobile individuals or because detoxification is not efficient enough to lead to individual recovery.

There is a mismatch between the exposure periods of 48 hours in the experiments and 24 hours in the simulations. The exposure time in the simulations was shorter compared to the experiments from that the EC50 value was obtained, thus we also evaluated the scenarios using 48 ng/L as the EC50.

4 Conceptual model evaluation

This TRACE element provides supporting information on: The simplifying assumptions underlying a model's design, both with regard to empirical knowledge and general, basic principles. This critical evaluation allows model users to understand that model design was not ad hoc but based on carefully scrutinized considerations.

Summary:

The MASTEP-regional model builds on existing models whose model concepts make quite some simplifying assumptions. These simplifying assumptions are not discussed in this document. The concept for the landscape-scaled approach of the MASTEP-regional follows from embedding an already existing model into a spatially-realistic landscape. Only a few simplifying assumptions had to be made and are discussed.

For the current model application, we assume the population of water louses to live in spatially continuous and connected ditches in the simulated landscape. Following pesticide introduction, individuals living in the downstream part of the network are exposed to pesticide concentrations.

On the level of the upscaling to the scale of agricultural landscapes, the model combines landscape definition, spatio-temporal exposure profiles and ecological population model as building blocks (Figure 1). Because the main focus of the upscaling approach is to assess the spatial aspect of population effects of pesticides and of the recovery processes, the model framework is based on a spatially explicit description. The landscape is defined in terms of a water network with sections and nodes, where each section has a defined width and length,

and the sections are connected in the nodes with other sections. The sections are internally organised in 10m long segments. This is the spatial unit where the area and so the local density dependence, the pesticide exposure and the local population dynamics are linked. The nodes between the sections are interfaces for the dispersal of individuals from one section into another one. The level of the landscape introduces a given complexity into the modelled system by the definition of the network, however, still the segments of the water bodies within the network are of the same quality. Considering heterogeneous or patchy habitat qualities would introduce an additional level of complexity into the upscaling framework, but is not considered to be relevant for the basic understanding and the answers to the main questions.

The most important model assumptions for the upscaling, landscape level are that the simulated individuals are assumed to live only inside the water bodies throughout their whole life cycle. Emergence of insects from aquatic to flying life stages cannot be taken into account on the landscape level. Individual movement is assumed to occur only within the water courses. This assumption is valid for the water louse, and for other species with pure aquatic life-cycles.

The second main simplification concerning the landscape level is that, as mentioned above already, the habitat quality of all positions within the water network is assumed to be equal, so that spatially heterogeneity is just given by the network structure and by the pesticide exposure. This simplification is justified for the area that is subject for the current study, because drainage ditch networks in agricultural landscapes provide rather uniform conditions, because they are artificially constructed. Another reason for neglecting spatially heterogeneous habitat qualities was to concentrate our research on the influence of spatially explicit pesticide exposure patterns. To consider the latter is already a challenge with respect to model evaluation, so in order to focus on the research questions and to avoid the model results being too complex we chose the described representation of spatial heterogeneity.

Time (CTR):134											
model no. 1	bal=	0	lc(t+1)= 79927	lc(t)= 78780	bc = 4861	dc = 3765	leave = 34	(0)	incoming = 85		
model no. 2	bal=	0	lc(t+1)= 33522	lc(t)= 32910	bc = 2198	dc = 1622	leave = 10	(0)	incoming = 46		
model no. 3	bal=	0	lc(t+1)= 9459	lc(t)= 9480	bc = 457	dc = 488	leave = 20	(0)	incoming = 30		
model no. 4	bal=	0	lc(t+1)= 30608	lc(t)= 30299	bc = 1738	dc = 1470	leave = 16	(0)	incoming = 57		
model no. 5	bal=	0	lc(t+1)= 22903	lc(t)= 22029	bc = 2019	dc = 1160	leave = 26	(0)	incoming = 41		
model no. 6	bal=	0	lc(t+1)= 48135	lc(t)= 46058	bc = 4408	dc = 2324	leave = 26	(0)	incoming = 19		
model no. 7	bal=	0	lc(t+1)= 43455	lc(t)= 42196	bc = 3310	dc = 2068	leave = 13	(0)	incoming = 30		
model no. 8	bal=	0	lc(t+1)= 34863	lc(t)= 34715	bc = 1745	dc = 1616	leave = 30	(0)	incoming = 49		
model no. 9	bal=	0	lc(t+1)= 28258	lc(t)= 27823	bc = 1747	dc = 1324	leave = 9	(0)	incoming = 21		
model no. 10	bal=	0	lc(t+1)= 45486	lc(t)= 44665	bc = 2938	dc = 2150	leave = 9	(0)	incoming = 42		
model no. 11	bal=	0	lc(t+1)= 21623	lc(t)= 21245	bc = 1467	dc = 1084	leave = 40	(0)	incoming = 35		
model no. 12	bal=	0	lc(t+1)= 43972	lc(t)= 43454	bc = 2670	dc = 2162	leave = 25	(0)	incoming = 35		
model no. 13	bal=	0	lc(t+1)= 43566	lc(t)= 41270	bc = 4505	dc = 2227	leave = 39	(0)	incoming = 57		
model no. 14	bal=	0	lc(t+1)= 18082	lc(t)= 18245	bc = 640	dc = 828	leave = 17	(0)	incoming = 42		
model no. 15	bal=	0	lc(t+1)= 41876	lc(t)= 41164	bc = 2757	dc = 2070	leave = 35	(0)	incoming = 60		
model no. 16	bal=	0	lc(t+1)= 37297	lc(t)= 36326	bc = 2667	dc = 1718	leave = 122	(0)	incoming = 144		

Figure 9: Example balance of individuals as performed by the simulation software. lc(t+1): life count of individuals in the local model i in the next time step, lc(t): life count at time t , bc: birth count, dc: death count, leave: individuals leaving the local model i to an adjacent model, incoming: individuals incoming from adjacent models to local model i .

5 Implementation verification

This TRACE element provides supporting information on: (1) whether the computer code implementing the model has been thoroughly tested for programming errors, (2) whether the implemented model performs as indicated by the model description, and (3) how the software has been designed and documented to provide necessary usability tools (interfaces, automation of experiments, etc.) and to facilitate future installation, modification, and maintenance.

Summary:

In addition to standard verification tests such as code check being performed for compilation, two main approaches were followed to ensure a correct implementation of the MASTEP-regional upscaling approach. A species balance calculation is performed for each time step to ensure that individual processes are correctly linked to the upscaling framework. Specific test simulations using manipulated code ensured further integrity of the model code.

We report some basic tests that were performed with the upscaling framework. As first point, the upscaling framework performs and prints out a complete balance of all individuals within all local models for each simulation time step (for an example see fig. 9). In case there are errors in the mass balance, the software stops the simulations and gives out an error. This check ensures that the exchange of individuals at the nodes as elements connecting the single sections of the water network is implemented correctly, and that mortality and hatching events are implemented properly.

A second check of the implementation of the upscaling framework, and of the population model was performed by commenting out the mortality and reproduction parts of the main loop of the population model in the respective NetLogo file. As a result, the population dynamics was checked if it remains constant over the whole simulated time period.

A verification in relation to the main objective of the model, being the simulation of pesticide mortality and recovery, was performed as part of the [Model analysis](#).

Software

The local model, MASTEP, has been implemented in NetLogo (Wilensky 1999), a free software platform. The program is available at <http://cream-itn.eu/projects/wp-1/scales-4>. After installing NetLogo, which is available for all major operating systems, users can run our model and use the graphical user interface and an integrated tool to perform simulation experiments (“BehaviorSpace”, Wilensky and Shargel, 2002). The developers of NetLogo always provide transition guides to new version of NetLogo, and keep old versions for download. Modifications of the program require knowledge of NetLogo.

Information on how to install and run MASTEP regional are provided in the section [Landscape-scale and implementation](#).

6 Model output verification

This TRACE element provides supporting information on: (1) how well model output matches observations and (2) how much calibration and effects of environmental drivers were involved in obtaining good fits of model output and data.

Summary:

In this study, no calibration of model parameters was executed in the sense of optimizing parameters to a given data set. Information on how well model simulations match observations are presented in [Model output corroboration](#).

7 Model analysis

This TRACE elements provides supporting information on: (1) how sensitive model output is to changes in model parameters (sensitivity analysis), and (2) how well the emergence of model output has been understood.

Summary:

A comprehensive sensitivity analysis of the MASTEP-regional model is due to the relatively high computation times not possible. However, the sensitivity of the model outcomes was evaluated in a set of simulations covering a wide range of

pesticide toxicity and persistence. The simulation results indicate a reasonable and meaningful response of the model.

The sensitivity of model outcomes in terms of population effects and recovery times has been tested for a few sets of model parameters. A sensitivity analysis in a more comprehensive, technical sense is impossible to perform with the whole upscaling framework, because the computation times are too high. Hence, the contribution of single model parameters to the model outcome is not known quantitatively.

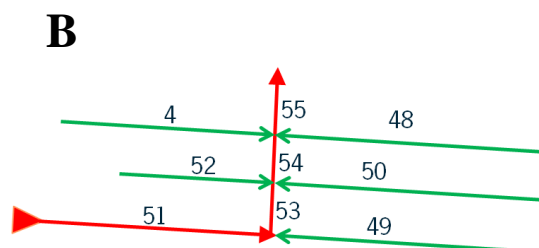
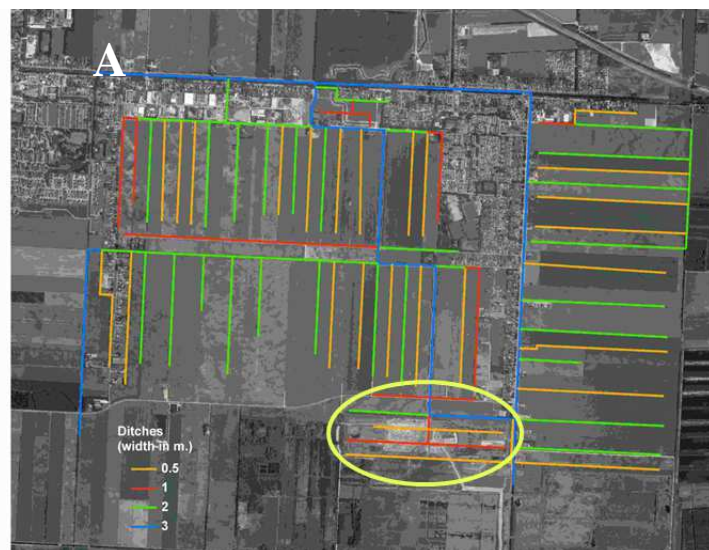


Figure 10: (panel A) Overview about the test area, showing a typical Dutch agricultural area with a dense network of drainage ditches. The subarea in the yellow ellipse in the upper panel is the subcatchment used for sensitivity studies Sketch of the simulated networks. (B) Water flow is indicated by arrows. Pesticide input was always in the beginning of section 51. Numbers are section IDs. Downstream length (red part of network) has length of 878 m. Total uncontaminated section length (green) is 2575 m.

To have a basic picture of the sensitivity of population effects and recovery times, we performed simulations with changing parameter values for pesticide toxicity and chemical dissipation from the water phase. Respective simulations were performed in a subcatchment of the Klazinaveen Zwartemeer area (see figure 10). Combinations of LC50 values ($T1 = 10\text{ mg/L}$, $T2 = 1\text{ mg/L}$ and $T3 = 0.1\text{ mg/L}$) and DT50 times ($DT50 = 1, 2, 3\text{ days}$) were used to simulate population effects and recoveries in the downstream area (see Figure 10B).

The results of these simulations show recovery times indicating reasonable responses to changes in both the dissipation times and toxicities (Figure 11) in reaction to an input of 10 mg/L of a pesticide into about 10% of the total downstream area.

The parameter values used for this sensitivity study comprised a reasonable parameter range, as dissipation of pesticides from the water phase is known to proceed within a few days after input. The toxicity of the compound (or inherently the sensitivity of the water louse) was varied over three orders of magnitude.

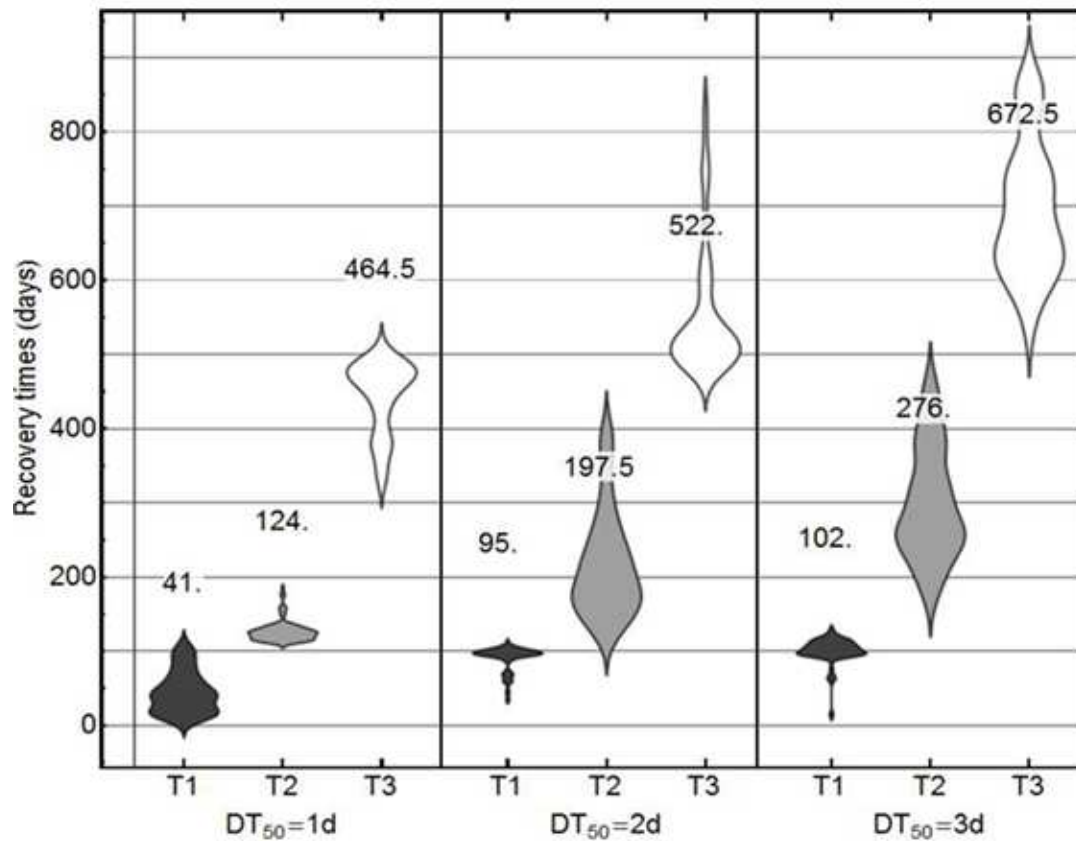


Figure 11: Violin plots (i.e. density distribution plots) of the recovery times of the populations for the treatments as given by the labels at the x-axis. Numbers in the insets give the median values of the respective recovery time distributions. T1 indicates $LC_{50}=10$ mg/L, T2 $LC_{50}=1$ mg/L, and T3 $LC_{50}=0.1$ mg/L.

Uncertainties concerning parameter values are addressed in the population model by two means. At first, some of the parameters of the local models are drawn from probability distributions (see Table 1). Every time when an individual is “born”, reproduces or moves within the model, random values from the probability distributions are drawn and cover in this way the uncertainty of these processes.

The second means is basically that for the calculation of the density dependent and the pesticide-induced mortalities the respective threshold values (compare Figure 3 and equations in Table 1) were compared to uniform random variables between 0 and 1. That results in a certain level of stochasticity, e.g. when a pesticide concentration is translated into a mortality probability of 75% for a given patch at a specific time, the realised population mortality at this patch will not exactly be 75%. In this sense, each model simulation is a realisation of a random experiment.

Because we performed all simulation runs in 10 replicates, we can aggregate about these 10 replicates and on this way have an idea of the variability in the model outcome. Figure 11 (top) shows median values and 10- and 90-percentile of 10 replicates for a simulation run in the subcatchment (Figure 10). It can be seen that the absolute population abundances show low variability. For the presentation of results from the model application example (figure 9 and 10), relative abundances were used, being defined as the ratio of the abundances in a pesticide exposure scenario and the abundances in the control simulation in a given region of the water network.

For the evaluation of the abundances over time, we divided 10 pesticide exposed replicates by 10 control replicates and so ended up with 10 relative abundances. Plotted the median and 10- and 90-percentile over time, the variability appears higher (figure 11 (bottom)). However, the 10- and 90-percentiles are most of the simulation times in a range of about 10% of the relative abundance, only around the times of the population peaks, the variability increases drastically.

8 Model output corroboration

This TRACE element provides supporting information on: How model predictions compare to independent data and patterns that were not used, and preferably not even known, while the model was developed, parameterized, and verified. By documenting model output corroboration, model users learn about evidence which, in addition to model output verification, indicates that the model is structurally realistic so that its predictions can be trusted to some degree.

Summary:

Given the spatial dimension and resolution of the landscape-scale simulations, data that can be used to corroborate model results is hard to find. We used data from field monitoring campaigns in the Netherlands to corroborate at least the undisturbed population dynamics as simulated with a local MASTEP population model.

The modelling approach uses a combination of different modules and has not been validated as a whole. Following the rationale of “compare like with like”, no comparison of simulated population dynamics with data is possible because we are not aware of a dataset being available on the landscape scale in the necessary temporal and spatial resolution.

We found, however, one data source that seems to be appropriate to be compared to model simulation outcomes of at least the local MASTEP population model. The website www.limnodata.nl provides data on the status of Dutch water bodies. It is maintained by STOWA (Stichting toegepast onderzoek waterbeheer), a Dutch public organization that collects information from a large number of stakeholders in the area of water quality. We downloaded a data set on the abundances of *Asellus aquaticus* from all possible locations in the Netherlands and all available sampling times (n=19651). We selected the abundances that were collected in edge-of-field ditches concerning to the simulated landscape (n=4519) and grouped the abundances by the day in the year. Figure 12 shows a comparison of this data set with the average of 10 replicates of simulations of the local population model in a 100 m water body. It is obvious that the data itself does not show very pronounced bivoltine population dynamics as it can be observed in the results of the population model. However, the order of magnitude of the abundances in the field data is surprisingly well matched by the non-calibrated modelling results. In this sense, the comparison of model and data shows that the model produces somewhat idealized results. These results are relating to real-world data to a satisfactory degree.

Exposure patterns for the pesticide have been calculated using the CASCADE-TOXSWA software. The hydrological part of this model approach was validated against measured hydrological data from the study region (Kruijne et al., 2008). The chemical fate description in CASCADE is using the theory being implemented in TOXSWA, which was in turn validated basically against a small number of chemical concentration measurements.

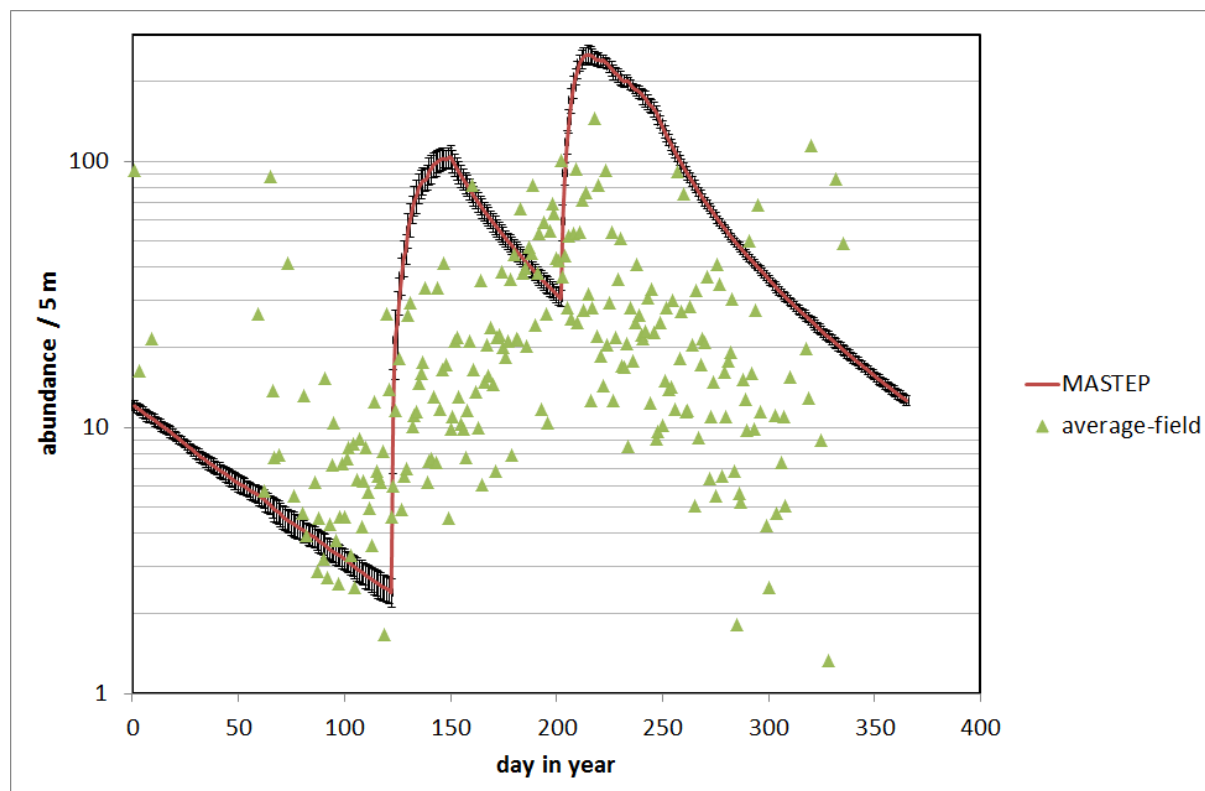


Figure 12: Comparison of field monitoring data and model simulations. Data basis: Field abundances as retrieved from www.limnodata.nl (water type: Sloop, n=4519). Presented are the average values per day-in-year. MASTEP model simulations have been performed with the parameterization as described above in 10 replicates.

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