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**Integrating chemical fate and population-level effect models for pesticides on the
landscape scale: new options for risk assessment**

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Abstract

When aiming for more ecological realism, the challenge for ecological risk assessment of chemicals is to integrate different aspects of the chemical and the species of concern, like spatial scales of emissions, chemical exposure patterns in space and time, species population growth dynamics and dispersal behaviour in landscapes. These aspects are not contained in the current scheme for risk assessment, but risk assessors and managers express increasing interest in understanding more about the occurrence and the effects of chemicals on the landscape level.

In this study, we introduce an extension of the spatially explicit MASTEP model approach for simulating population dynamics and effects of pesticides on aquatic species within a spatially realistic landscape. We applied the MASTEPregional approach in a case study which simulated the effects of concentrations of the insecticide λ -cyhalothrin on the water louse *Asellus aquaticus* for a typical Dutch landscape of about 10 km² size containing 137 waterbodies with a total length of about 65 km and different degrees of connection. Pesticide treatments used in potato crop were assumed to result in spray drift input of 5% (non-mitigated) and 1% (mitigated) of 15 applications of 0.005 kg/ha of λ -cyhalothrin into parts of the water course network. These scenarios resulted in highly variable exposure patterns both in space and time. Downstream transport of the pesticide led to exposure of water courses that did not directly receive spray drift input, even though of λ -cyhalothrin was assumed to dissipate rapidly from water (DT50=1 day). The effect simulations show a proof of concept of the chosen modelling approach to assess the risks of pesticide exposure to aquatic organisms in a spatially realistic landscape context. The observed differences in effect and recovery patterns ranged between no observable effects for the low spray-drift and a low sensitivity scenario and severe reduction of abundances for the high spray-drift and a high sensitivity scenario. These results illustrate the sensitivity of our modelling approach, but also shows the necessity of precise calculations of pesticide inputs and model parameterisation.

This study demonstrates the possibilities of using this model approach to address some concerns of pesticide regulators. Modelling can deliver more realistic simulations of pesticide fate and effects than can be provided by edge-of-field approaches. Coupled fate-and effect modelling offers the potential to explore scenarios like multiple pesticides resulting from one crop or from more crops
5 grown in a landscape, or to extrapolate fate and effect simulations to different climate regions. Spatial realism of the landscape ensures the realistic consideration of population growth and dispersal as the two main recovery mechanisms. Further options for a landscape-scale simulation approach could involve exploring the effects of mitigation measures on the risk estimates on the landscape scale and hence a step towards risk management, or supporting field monitoring studies
10 with spatially realistic simulations.

1. Introduction

The function of environmental risk assessment (ERA), a part of the regulatory registration process for chemicals, is to protect the environment from unacceptable effects that chemicals such as pesticides may have on the environment (Hommen et al., 2010, SANCO 2002). The term “unacceptable effects” is often interpreted as meaning that recovery of affected populations does not occur in a given time period after effect. Identifying factors that determine population effects and recovery in a prospective way is a key issue in this context.

Pesticides are applied to protect crops from diseases and to optimize the productivity of crop farming. Applications usually take place on the spatial scale of crop fields and landscapes. However, research on the impact of pesticides on populations is still focussing on the edge-of-field scale in ERA. This may be caused in part by the intrinsic complexity that accompanies the integration between chemical pollution and ecosystem function and population dynamics (Cairns and Niederlehner, 1996, Van den Brink, 2008). While the effects of chemicals are mostly measured on the level of individuals in the ERA procedures, in terms of environmental protection it is crucial to analyse and understand chemical effects on the spatial scale of the application, i.e. on the landscape scale. Additionally, the exposure of water organisms to pesticides is known to be highly variable in space and time, as considered for example by the FOCUS surface water scenarios (FOCUS 2001), thus it appears to be necessary to assess exposure and effect patterns on spatially explicit scales (Schwarzenbach et al., 2006). Both the extrapolation problem, from individuals to populations (Forbes et al., 2008), and the demand for spatially explicit exposure assessment pose a challenge for ecological research in the field or ERA of pesticides.

Ecological modelling approaches can serve as a tool to extrapolate from individual to population effects of chemicals (Galic et al., 2010; Thorbek et al., 2010). They provide means to translate individual mortality to the sustainability of populations. Especially combining population modelling with explicit representation of space has a high potential to integrate chemical exposure with

resulting effects on population dynamics and ecosystem functioning. An individual-based modelling (IBM) approach can easily deal with the demand for a spatially explicit environment, and at the same time incorporate species processes such as density dependence of growth and mortality, individual movement and also individual variations in life-history parameters (Grimm and Railsback, 2006).

5 Macroinvertebrate species have important functions in aquatic ecosystems with respect to energy and nutrient cycling (Bellisario et al., 2012; Dangles et al., 2002; Lecerf and Richardson, 2010). Species such as the detritivore *Asellus aquaticus* for instance consume decaying vegetation, protozoa or algae, and invertebrate animals, thereby making energy available for higher trophic levels. Often arthropod macroinvertebrates appear to be sensitive towards insecticide loads (Maltby et al., 2005).

10 Regular exposure to pesticide loads resulting from crop treatments may cause effects on sensitive macroinvertebrate species in terms of reduced abundances as reported in some semi-field studies (Arts et al., 2006; Van Wijngaarden et al., 2004). To assess factors influencing the ecotoxicological effects on populations, the population vulnerability concept of Van Straalen (1994) is useful. It describes the vulnerability of populations in three categories: external exposure, intrinsic sensitivity,

15 and population sustainability. While external exposure is determined by pesticide applications and the following dissipation and distribution dynamics, and intrinsic sensitivity is related to the effect of chemicals on the individual level, population sustainability describes the potential of a population to recover from any toxic effect by demographic dynamics and by recolonisation. The reproductive strategy of a species plays an important role in this respect, because species with a high reproductive

20 output and/or number of generations per year have a higher potential to compensate for pesticide mortality than those with lower ones (Niemi et al., 1990). The second factor determining the recovery is the potential immigration into affected patches, influenced by the dispersal behaviour of the species and the presence of other (source) populations in the neighbourhood. To take into account potential population recovery from pesticide exposure, effects of pesticides have to be

25 assessed in a spatially-explicit environment.

In an example for such a spatially-explicit model from the aquatic domain, Van den Brink et al. (2007) used the IBM approach to simulate the response of *Asellus aquaticus* to pesticide stress in aquatic systems mimicking exposure scenarios already in use for the registration of pesticides in the EU (FOCUS, 2001).. An adapted version of the MASTEP model was used to assess the influence of the
5 timing of pesticide stress during the year and landscape connectivity on recovery times of *A. aquaticus* (Galic et al., 2012). In this study, we introduce an extension of the spatially-explicit MASTEP model approach for simulating population dynamics and effects of pesticides on aquatic species within a virtual, but spatially-realistic landscape. The MASTEPregional modelling approach allows for the free definition of water course networks, the assignment of previously calculated
10 concentration time series to single water courses, and for the simulation of population dynamics, effects and recovery based on an existing NetLogo population model. It thus provides a flexible platform for performing spatially realistic integrated risk analyses on the landscape scale.

We applied the MASTEPregional approach in a case study where effects of concentrations of the insecticide λ -cyhalothrin, as calculated with the chemical fate model CASCADE-TOXSWA on the water
15 louse *A. aquaticus*, were simulated for a typical Dutch landscape of about 10 km² size. The intention of this case study was not to perform a risk assessment for this specific compound. The primary objective of this study was instead to show the applicability of the landscape-scale simulation approach, the proof of concept that the MASTEPregional approach is able to detect effects when that is appropriate and also to show no effect when no risk can be expected and finally to discuss the
20 potential of such approaches for being used in higher tier environmental risk assessment in the future.

2. Material & Methods

The information provided in this section gives an overview about rationale and most important parts of our modelling approach. A more detailed model description in the ODD format and more information about model development and testing in the TRACE format (Schmolke et al., 2010) is available in the supporting information.

2.2 Modelled landscape

The selected catchment for our case study represents a typical Dutch agricultural area in the north-east of the Netherlands in the region of Klazinaveen-Zwartemeer. The area of approximately 10 km² is drained by a network of open drainage ditches with bottom widths between 0.5 and 3 m and a total length of 65 km (Kruijne et al., 2008, figure 2). The modelled water network consisted of 137 sections.

A typical crop grown in the area is potato. An insecticide typically used in potato crops is λ -cyhalothrin, a pyrethroid compound with relatively low application rates but also high aquatic toxicity (Van Wijngaarden et al., 2006). For two subareas in the total area, we assumed a treatment of potatoes with λ -cyhalothrin resulting in a spray drift input into the water courses. The respective section numbers were for area 1: 33, 125, 29, 28, 23, 130, 19, 141, 20; and for area 2: 6, 59, 58, 57, 5 (indicated by red dashed lines in figure 2). We simulated two spray drift intensities, being 1% and 5% of the applied mass. The application rate was, following the label information, set at 0.005 kg/ha, and 15 applications to the same fields were simulated, starting at day 121 with intervals of 7 days in between. Applications were only simulated for the first year; in the second and third year of effect simulations no pesticide applications were assumed.

2.3 Simulated exposure concentrations

2.3.1 Exposure model

Spatio-temporal explicit exposure concentrations in the ditches were simulated using the CASCADE-TOXSWA model (Van den Berg et al. 2011). 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 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.

2.3.2 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-live 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. The concentration in the water as resulting from CASCADE-TOXSWA are given in hourly time steps per segment.

2.4 Local population model

2.4.1 Population dynamics

The individual-based model simulates growth, reproduction, mortality and movement for a population of individuals in a section of the water course network. We used the MASTEP model for the water louse *A. aquaticus* (Galic et al. 2012) in an adapted version for the simulation of the local populations. We give a short overview about processes and entities of the model here. For a more detailed description we refer to the ODD model documentation in the supporting information. A TRACE document with information about model development and testing is also available in the supporting information.

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 . The local carrying capacities were used for calculating density-dependent growth and mortalities. The central entity in the individual-based model was the female water louse individual simulated as juveniles or adults which have unique individual age (days), size (length in mm), hatching date (days), lifespan (days) and location (x

and y coordinates). Size increment was density dependent and restricted by a maximum size. Individual size at the hatching day determined the brood size (number of offspring). Mortality probability was implemented as the result of background mortality, due to density dependence and due to pesticide stress. In order to mimic the bivoltine reproduction pattern being frequently
5 observed in north-west Europe (Van den Brink et al., 2007), two reproduction periods per year were assumed, starting in the beginning of May (around day 120) and mid-July (around day 200). A flow chart depicts the steps in the local population model (Fig. 3).

2.4.2 Linking exposure with effects

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

$$m_{chem} = 100 / (1 + \exp (-slope \cdot (\ln(C(t,i)) - \ln(EC_{50})))) \quad (\text{eq. 1})$$

The actual exposure concentration at time t in segment i , $C(t,i)$ (mg/L), and the constants EC_{50} (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
15 randomly chosen individuals from the local segment. For each new simulation day, the mortality probability was imposed to the total of the remaining population. This corresponds to the stochastic death approach (Jager et al., 2011).

The dose-response relationship for λ -cyhalothrin was parameterised from the literature (Schroer et al., 2004). The slope was calculated from the reported EC50 and EC10 concentrations to 2.341 (-); for
20 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 which the EC50 value was obtained; thus we also evaluated the scenarios using 48 ng/L as the EC50.

5 2.5 Simulation scenarios and analysis

Simulation runs are performed as control and treatments. Based on the definition of the water course network, local population models were defined for each section of the water course network with a given length, area, and capacity for each of the segments within the section. The population models were initialised at 10% of their segment's carrying capacity, which was 5 individuals/m² for our case study. The population dynamics were simulated for 3 years with 365 days each, in daily time steps. The simulation period was set to 3 years to balance between ecological relevance and computational effort. Ecological relevance would have meant to continue the simulations until recovery was observed in all treatments, but the computational effort was already in the range of several days on a high performance cluster for the given simulation period. The control scenario was simulated using the population model without pesticide-induced mortality. On each simulation day, background and density-dependent mortality probabilities, growth in size, reproduction and movement were calculated in the local models.

The CASCADE-TOXSWA model was used to simulate the fate dynamics of λ -cyhalothrin in the water courses of the catchment following two pesticide application scenarios with 1% and 5% spray drift input. Resulting pesticide water concentrations (see Figure 4 as an example) were used as input for population effect and recovery simulations on the landscape scale. Two effect scenarios were simulated for each of those two exposure scenarios using EC50 values of 24 ng/L and 48 ng/L, to calculate mortality probabilities (eq. 1). In total, four scenarios resulted with combinations of high (5%) or low spray drift input (1%) and high (EC50 = 24 ng/L) or low species sensitivities (EC50 = 48 ng/L), respectively.

All simulations were performed in 10 replicates. This number of replicates ensured in our experience in general a reasonable variance of the population dynamics (see also section 2 of the TRACE documentation). In the pesticide exposed scenarios, pesticide mortality was imposed following the log-logistic dose-response relationship (eq. 1). On each day, the number of adult and juvenile Asselids were recorded for all segments. The effects of the pesticide applications were evaluated as the reduction of the abundances in the treatment simulations compared to the control simulations. Relative abundances were calculated for the pesticide treatments by dividing the mean of the 10 replicates of a specific pesticide scenario by the mean of the 10 replicates of the control scenario for each 10 m segment of the water course network. A relative abundance of zero means that the population is absent in that particular segment in that pesticide exposure scenario.

The reduction of the relative abundances was calculated per segment of the water course network. For each segment, the 10th percentile of the relative abundance time series over the years (p_{10}) was calculated, i.e. on 10% of the days the relative abundances in that segment were lower than this value. For sections 19, 23 and 58 and separately for the remainder of the downstream transect (“remote areas”, compare Figure 2), the number of segments was calculated for which the 10th percentile of the relative abundances was below 90%. As an indicator for the extent of the affected area $P_{\text{aff_area}}$ (%) we define

$$P_{\text{aff_area}} = 100 \cdot (n_{p10<0.9} / n_{\text{tot}}) \quad (\text{eq. 2})$$

where $n_{p10<0.9}$ is the number of segments in the respective part of the water courses for which 10% of the daily relative abundance values within the time period of three years were below 90% and n_{tot} is the total number of segments in the respective part of the water courses.

For the calculation of recovery times, absolute abundances of the water louse from each pesticide scenario replicate run (10 in total) were divided by the respective abundances from each control scenario replicate run (10 in total), resulting in 100 relative abundances for each segment over time. The median over these 100 relative abundances over time per segment was calculated. Recovery

times were estimated by calculating how many days after the last application day (220) were needed until the median relative abundance was larger than 90 % on 5 out of 10 consecutive days (see Galic et al., 2012).

3. Results

5 3.1 Concentration dynamics

The downstream transect from section 19 to section 111 (see black arrows in Figure 2) was comprised of 28 sections, with three sections that directly received spray drift input, i.e. sections 19, 23 and 58. The concentration levels in sections 19 and 23 were comparable on all application days, however, in section 58 the concentrations were slightly lower (Figure 4). Along the whole
10 downstream transect, fast pesticide dissipation from the water phase resulted in water concentrations near zero before the next application, for all applications. Compared over simulation time, the most obvious difference between the different sections was the length of the exposed downstream sections. For example, the transportation of pesticide loads from section 23 (approx., 1330 m downstream) to section 32, led to different parts of section 32 being contaminated over the
15 application period (Figure 4). In the first seven weeks of treatment, that is from Julian day 121 until 170, concentrations of λ -cyhalothrin were higher than 10 ng/L up to the middle of section 32. In the summer months of July and August, water levels and also flow velocities (Table 3) were much lower and consequently there was nearly no downstream transport visible in section 32.

Local exposure to 10 ng/L corresponds to 2.5 and 11 % mortality for EC50 values of 48 and 24 ng/L,
20 respectively (eq. 1). As a result of downstream transport, pesticide concentrations were present in sections 64 till 67 and 77 and partially also in section 106 above a concentration of 10 ng/L. This input was caused by downstream transport from section 58, and also the outflow from the treated sections 59, 6, 60 and the treated sections 57 and 5 via untreated section 63 entered this part of the ditch network (compare water network setup in Figure. 2). Similar as described before, the

downstream transport was far more pronounced in the weeks of May and June, whereas the applications in July and August were subject to a lower amount of downstream transport. In some cases, pesticide loads were visible in the downstream transect that resulted from pesticide loads from side ditches, e.g. the first part of section 36 was polluted by the output of section 125 (Figure 4). The concentrations as simulated for the 1-percent spray-drift scenario showed exactly the same patterns in space and time, only the absolute height of the pesticide water concentrations was lower by approximately a factor of 5 (results not shown).

The maximum predicted environmental concentrations (PECs) in surface water in the affected ditches were 11.03 ng/L and 55.01 ng/L for the 1% and 5% drift scenarios, respectively. A lower tier PEC simulation was performed with FOCUS TOXSWA (potato crop, D3 scenario), and the maximum concentration found there was 9.05 ng/L.

3.2 Control population dynamics

Local control population dynamics showed a bivoltine time course with an early year peak at the end of April and a second, higher peak in mid-July (see TRACE documentation in the supporting information). Since the ditch network was, with the exception of chemical exposure, defined spatially homogeneously in the sense of habitat conditions, the population dynamics in the whole catchment showed the same pattern.

3.3 Population effects and recovery

Population effects were simulated using the two different intensities of spray-drift input and two different sensitivities. In the 5% spray drift input and the lower sensitivity scenario, decreased abundances were observed in the three input sections in the downstream transect after the simulated spray-drift events (sections 19, 23 and 58, Figure 5, top). The reductions showed different intensities in the three sections with direct pesticide input. Whereas in sections 19 and 23 the extent of the affected area (i.e. the number of segments for which the 10th percentile of relative

abundances over 3 years was below 90%) reached 100 % (Table 2), in section 58 the exposure concentrations were lower and so the reduction of the abundance of the water louse was less severe. However, still an extent of the affected area of 98 % was calculated. The spatial extent of the reduction of the abundances appeared quite constant throughout the sections with direct spray drift input. At the day of the last pesticide input, the whole of sections 19 and 23 showed relative abundances of nearly zero, while in section 58 a relative abundance of approximately 30% was recorded (Figure 5, top). Remote effects, which are defined as a reduction of the relative abundance to less than 90% in sections that were not subject to direct spray drift input, were observed in 13 % of all segments in the downstream transect (Table 2). Clearly reduced abundances as a result of downstream pesticide transport or pollution from tributaries were observable in e.g. sections 32, 64 and 65 (Figure 5, top).

Between the last day of pesticide input, i.e. Julian day 228, and the day of the first population peak in the second simulated year (Julian day 485), the reduction of the spatial extent of the pesticide effect proceeded only slowly. In this time period there was no reproduction of the Asellids, so the recovery at the edges of sections 19 and 23 (Figure 5, top) were caused by recolonisation of affected areas from undisturbed parts of neighbouring ditches. The second population peak in the second simulated year (Julian day 565) initiated a quick recovery of the population abundances. In section 58 the recovery was already complete at this time, and in sections 19 and 23, the abundances recovered to more than 50 % of the controls. These recovery patterns resulted in mean recovery times of 211 days for section 58, and 429 and 456 days for sections 19 and 23, respectively (Table 2).

The simulations resulting from the 5% spray-drift input and the higher sensitivity value scenario showed similar effect patterns as described for the lower sensitivity scenario during the period of spray drift input between day 121 and day 221. In comparison with the lower sensitivity simulations, section 58 showed a more severe impact and remote effects were far more pronounced (Figure 5, bottom). About the first half of section 32 and the complete sections 64, 65, 67 and 77 showed

reductions of the relative abundances to values below 50%. This pattern translated into extents of affected areas of 100% for sections 19,23 and 58 and of 23% for the remote sections (Table 2). Hence, the higher sensitivity led to an enlargement of the area with observed downstream mortality, in about one quarter of the sections that were not subject to direct pesticide input the water louse abundances were reduced to values below 90 % of the control.

A considerable difference between the low and high sensitivity simulations was visible in the spatial dynamics of the affected area over time. In the high sensitivity scenario, all three affected parts of the downstream transect showed relative abundances near zero over time (Figure 5, bottom). The fraction of survivors from pesticide stress for the low sensitivity simulations was between 1 and 10 % for sections 19 and 23 and at about 60% for section 58, whereas in the high sensitivity scenario in sections 19 and 23 no survivors were observed (Figure 7). The corresponding recovery times for the three input sections were in line with these observations and considerably larger for the higher sensitivity scenario, as recovery to 90% of the control took more than two years after the last pesticide input (Table 2). In the remote part of the downstream transect, the mean recovery time was 67 days for the high sensitivity scenario. This is remarkable, because it is an average value and for many of the downstream segments there was no pesticide-induced mortality at all.

The 1% spray drift input scenario resulted in five times lower peak pesticide concentrations in water as compared to the 5% spray drift scenario. Using these lower concentration values for population effect simulations, much smaller effects on the simulated abundances were observed for the lower species sensitivity scenario compared to the same scenario receiving 5% spray drift. In the space-time plot (Figure 6, top), the impact of the pesticide input is hardly distinguishable from the simulation variability caused by the stochasticity of the simulations. In about one quarter of the segments of sections 19 and 23, the relative abundances dropped below 90% for 10% of the simulation days. Similarly, for section 58 the affected area was 15%. For the remote regions, the

affected area was calculated to be 2.6 %. The median of the relative abundances in the respective areas did not fall below 90%, so recovery times were not calculated.

Using the 1% spray-drift scenario concentrations and the higher species sensitivity scenario, the reduction of relative abundances was clearer in the space-time plot (Figure 6, bottom). The affected area in the input sections 19 and 23 was 100%, and 12.4 % in section 58 (Table 2). After the last input of pesticides, recovery took 14 and 20 days in sections 19 and 23, respectively, whereas in section 58 and the remote parts of the downstream transect no recovery times were calculated since median relative abundance values did not drop below 90%.

4. Discussion

4.1 Validity and realism of the simulations

4.1.1 Modelling approach

In this study a realistic representation of an agricultural landscape with respect to the water course network structure and to the respective hydrology was used for simulating effects on water louse populations and the subsequent population recovery. The modelling approach used a combination of different modules and was not validated as a whole. Following the rationale of “compare like with like”, no comparison of simulated pesticide concentrations or population dynamics with experimental or field data was possible because we were not aware of any available dataset on the landscape scale at the necessary temporal and spatial resolution. The framework could, however, be evaluated and validated in parts (e.g. the reproduction part of the ecological model) and for different sources of uncertainty using the recommendations by Augusiak et al. (Subm., this issue).

4.1.1.1 Fate simulations

Exposure patterns of the pesticide have been calculated using the CASCADE-TOXSWA model. 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 uses the theory implemented in TOXSWA, which was in turn tested with a number of chemical concentration measurements (FOCUS, 2001). A critical issue in the use of CASCADE is that it is simplified compared to TOXSWA as a sediment compartment is missing, and TOXSWA itself is already simplified in some important aspects, e.g. all degradation processes in the water column are lumped into one half-life and pH is assumed constant. Given these simplifications, the fate simulations that we produced cannot claim to give realistic results as could be expected from a mechanistic fate model that explicitly considers substance flows between water and sediment, that separates between different dissipation processes in water such as hydrolysis, photolysis, and microbial degradation in the sediment, and that considers variation in environmental conditions such as in pH. As a consequence of missing diffusion fluxes between water and sediment, CASCADE simulations will probably underestimate long-term low-level exposure, because it can be expected that the sediment acts like a buffer from where low levels of chemicals flow back into the water. For the case of λ -cyhalothrin, however, previous studies reported that transformation rates in water seem to be too fast to allow substantial fractions of the dose to build up in plant and sediment (Leistra et al., 2003). In addition, low levels of the compound have virtually no acute toxic effect at all. In this respect, we assume that the lack of a sediment compartment has not influenced the quality of the simulations of the peak water concentrations and of the coupled acute effect estimations significantly. Finally, we parameterised the half-life in water taking into account the missing sediment compartment (see next section).

The strong point of CASCADE fate simulations is obviously the spatial precision of the calculation of exposure concentrations and the consideration of hydrological influences such as dilution by changing volumes over time and by untreated side tributaries.

4.1.1.2 Population modelling at the field scale

The MASTEP model that was used as a building block in the upscaling framework was not validated as a whole. Some of the submodels and parameters are taken from accurate reports in the scientific literature, for example those for mortality, breeding, and size structure (Adcock, 1979; Arakelova, 2001; Chambers, 1977; Hynes and Williams, 1965; Iversen and Thorup, 1988; Marcus, 1990; Marcus JH et al., 1978; Økland, 1978; Vitagliano et al., 1991). This is, however, not the case for the density dependence of growth and mortality and for dispersal. We are aware of only one study on the movement of *Asellus aquaticus*, from which the parameterisation of the movement is derived (Van den Brink et al., 2007). The consequences of the uncertainty in the parameterisation of density dependence and movement for the quality of the simulations of population effects and recovery are not clear. More research on this is definitely needed, and until more information is available population dynamics, effects and recovery simulations should be considered to be showing an idealised or generic case, and not claim to produce realistic numbers that can be found in the field.

Given these uncertainties, it may not appear logical to perform simulations of the population dynamics on the landscape scale, because the coupling of chemical concentrations and populations can also be done on the edge-of-field-scale. However, two severe constraints make the coupling within a spatially-realistic landscape setting more reliable than in an edge-of-field situation: 1) At the edge-of-field scale simulations of the population dynamics are not spatially realistic, because often such studies work with periodic boundary conditions in the IBM, meaning that if an individual leaves the model region downstream it re-enters it upstream in the next time step (Van den Brink et al., 2007, Galic et al., 2012). This may result in artefacts in the results of such simulations. 2) Downstream transport of chemical input may transport effective concentrations to remote areas. Going from edge-of-field scales to landscapes, the potential of chemicals to affect remote areas is automatically considered.

4.1.2 Parameterisation of the scenarios

4.1.2.1 Comparison with lower tier values

The application scenarios were selected with the objective to show drastic effects for the high spray drift scenario and only slight to no effects for the lower spray drift scenario. The exposure concentrations in the high spray drift scenario are based on unmitigated application scenarios and worst-case assumptions considering spray drift, so they will be lower in the “real world” where mitigation is common practice (FOCUS, 2007) and climatic conditions such as wind speed or wind direction will have an effect on spray drift. We calculated maximum PEC values for the FOCUS surface water scenario (potato crop, D3 water body) to quantify the difference between the scenarios that we used and a lower tier risk assessment. The maximum PEC in surface water in the FOCUS D3 ditch was 9.05 ng/L, while the spray drift scenarios in this study resulted in maximum PECs of 11.03 ng/L and 55.01 ng/L for 1% and 5% spray drift scenarios. The maximum concentrations in the non-mitigated scenario (5% spray drift) overestimated realistic worst-case concentrations by a factor of more than five. Since we parameterised the dose-response relationship with EC50 values instead of LC50 values, thereby increasing the sensitivity of the *A. aquaticus* and adding more conservatism to the simulations, and concentrations in the 5% spray drift scenario were quite high, effects as shown by these simulations are not likely to occur in the environment. Exposure simulations with CASCADE for the scenario with 1% spray drift input yields in contrast a maximum PEC value of 11.03 ng/L, which is comparable to the maximum PEC of 9.05 ng/L as obtained by the FOCUS surface water scenario D3 simulation. In the simulations we found almost no effects for the 1% spray drift scenario, even for the conservative parameterisation of the dose-response relationship.

4.1.2.2 Fate model parameters

As discussed in the previous section, the fate simulations with CASCADE-TOXSWA require one lumped rate constant that quantifies the dissipation of the substance from water. We used a half-life of one day to parameterise dissipation, based on a study of Leistra et al. (2003). Additional studies confirm the dissipation time of λ -cyhalothrin from water to be in the range of 1 day. In microcosm experiments the dissipation time of λ -cyhalothrin was checked roughly by measuring remaining

concentrations in water 24 and 48 hours after the start of the experiments. The concentrations dropped to values between 39 and 51% of the initial concentration within 24 hours, which indicates similar dissipation dynamics as those seen in fate and effect studies in more complex systems (Schroer et al., 2004). Results from mesocosm experiments reported DT50 values for λ -cyhalothrin in semi-natural ditch systems with sediment and macrophytes in the range of 0.7 – 2.7 days; the average was 1.2 days (n=6) (Arts et al., 2006). In the environment, there will certainly be some variation over space and time in the dissipation of the pyrethroid from water, but the dissipation rate constant itself is confirmed by more than one study, especially also by a study that was performed under semi-field conditions (Arts et al., 2006).

10 ***4.2 Influencing factors and processes for effect and recovery patterns of water louse populations***

4.2.1 Exposure patterns

The spatial extent of the effects in the simulations is governed by exposure and species sensitivity. The exposure pattern itself was influenced by a number of factors, starting with the application scenario (application rates, amount of spray-drift, locations and frequency) that led to the initial water concentrations. Dissipation from the water phase, as summarised by the DT50, transport of pesticide loads with the water flow and pollution and dilution processes within the water network, resulted in the simulated exposure patterns in space and time (Figure 4). These processes occurred on very different temporal and spatial scales; the water flow in this regulated drainage ditch system for instance happens at the speed of tens or hundreds of meters per day, whereas diffusion into sediment occurs at the molecular scale at the range of millimetres to centimetres per day. The variability of the exposure patterns in space and time would be even larger in real landscapes than in this simplified simulation example, because not only spray drift, but also mobilisation of soil-bound residues by surface runoff (Doppler et al., 2012) and/or leaching by drain flow (Tiktak et al., 2012) introduce pesticide loads into surface water.

As a consequence, any attempt to introduce more realism into the assessment of effects of chemicals in the aquatic environment should consider whether exposure has been included into the assessment at an appropriate spatial and temporal resolution. FOCUS surface water scenarios result in pesticide concentration profiles which are highly variable in time, but not at an explicit spatial scale (FOCUS, 2001). Since the results show that the spatial heterogeneity also influences recovery patterns at the landscape scale, we consider that for a comprehensive integration of chemical exposure and effects dynamics on landscape scales it is crucial to account for any heterogeneity in the habitat conditions for *A. aquaticus* at least by taking into account the chemical environmental conditions.

4.2.2 Species sensitivity and link between exposure and effect

Species sensitivity as defined in the species vulnerability concept (Van Straalen, 1994) can be used to connect exposure patterns with effects. In general, the sensitivity of aquatic species towards pesticide exposures in the environment is mechanistically determined by uptake and excretion of pesticides by the organism and by the toxic effect dynamics inside that lead to lethal or sublethal effects. For λ -cyhalothrin, we linked concentrations in the water layer to effects, hence we assumed complete mixing of the chemical in the water phase, so that the PEC in surface water would also be appropriate at the lower layer of the water column. It is straightforward to relate the external concentration to the effect on survival because this was done in the same way in the toxicity experiments that we used for parameterisation. It is of course possible to consider additional routes of uptake for the chemical. For example, adsorbed masses of the chemical could enter the organisms via food uptake. While this is an interesting aspect, we did not consider this uptake route in our simulations in order not to increase further the complexity of the simulations.

Based on the setup of the toxicity experiments by Schroer and co-workers (2004) we used maximum exposure concentrations over 24 hours and linked them to effects in the form of the log-logistic

dose-response relationship. We decided to proceed in this way because the information on toxicity of the compound towards *Asellus aquaticus* was available.

It would have been preferable to use a mechanistic modelling approach such as toxicokinetics-toxicodynamics (TKTD) (Jager et al., 2011) for the linking of exposure and effects, because then it would have been possible to link hourly exposures to internal concentrations and from there to lethality. However, TKTD parameters for λ -cyhalothrin and *A. aquaticus* were not available. This is the same for the majority of species-chemical combinations, hence often dose-response relationships are used to assign effects to a certain exposure level. Since these dose-response relationships are established empirically rather than mechanistically like the TKTD models, the correlation of the EC50 and slope parameters to morphological and physiological species traits is limited compared to TKTD parameters (Rubach et al., 2012).

4.2.3 Species demography and dispersal

Following the concept of Van Straalen (1994), population sustainability describes the potential for a population to recover from any toxic effect by demographic dynamics and by recolonisation. In our simulations, recovery of abundances in the high spray-drift and high sensitivity scenario (Figure 5, bottom) was only observed at the edges of the most affected regions. This recovery process is due to re-colonising individuals that slowly spread into the affected area by dispersal. Recovery by local regrowth was not possible in this case because in the most affected regions total wipe-out of the populations occurred. Under very high exposure concentrations, total wipe-out events have been found in semi-field experiments for λ -cyhalothrin and *Chaoborus* sp. and *Caenis horaria* (Arts et al, 2004), so in general the simulation results are not unrealistic. Unfortunately, information about abundances of *A. aquaticus* is not given in that study. However, *C. horaria* and *A. aquaticus* have a similar order of magnitude of the EC50 for λ -cyhalothrin (Schroer et al, 2004), so we suspect that the intensity of effects on the water lice was comparable to that on the mayfly.

In contrast, for the scenario with high spray-drift and low sensitivity a certain level of survivors remained even in the most affected areas and ensured a faster recovery by local regrowth. Apparently, already low levels of survivors between 1 and 10% of respective control simulations led to drastic decreases in recovery times (Figure 7).

5 These findings confirm the observation of Galic and co-workers that population recovery is mainly driven by reproductive periods (Galic et al., 2012). Also their finding that local survivors play an important role for autogenic recovery of populations of *A.aquaticus* was clearly confirmed by the differences in recovery times between the high and low sensitivity high spray-drift scenarios. All these results have been, however, obtained from simulations under the given parameterisation of
10 the dispersal submodule, while it is not clear how the dispersal rates used relate to in-situ movement of the Asellids.

In general, local regrowth as the major recovery mechanism leads to the fast increase of population abundances, but it happens only during the reproduction periods. Dispersal behaviour on the other hand drives the recovery dynamics more continuously also between the reproduction periods, but
15 the re-colonisation occurs at a lower rate. As a consequence of the combination of these two recovery mechanisms, recovery times can depend critically and very non-linearly on the intensity of pesticide effects. These findings underline the importance of taking into account sensitivities and other species traits with the appropriate accuracy. Concerning our own modelling approach, density-dependence of demographic processes of the MASTEP model are only weakly corroborated by
20 empirical data, and the dispersal part is supported by only one experimental study. Hence we have to state critically that the absolute values in our results for population recovery need to be interpreted with care. Experimental research on density dependence and dispersal parameters is urgently needed to increase the level of trust of prospective effect and recovery simulations (Augusiak et al., subm., this issue).

25 **4.3 Did effects remain local in the water network or did they spread out over a larger spatial scale?**

When performing the simulations, one of our main hypotheses was that downstream transport and pollution of remote parts of the water network leads to distinct effects in remote areas. However, from the results it appeared that remote effects of λ -cyhalothrin were lower than expected. There were strong remote effects in the high spray drift and high sensitivity scenario, but they were restricted to sections of the water course network adjacent to the input sections. For example, abundances in the first part of section 32, downstream of section 23, were reduced to values below 25% of the control, but the spatial extent of this effect remained below 500 m (Figure 5, bottom). Additional remote effects of pesticide loads were prevented by the fast dissipation of the substance. Pollution of unpolluted sections in the water course network was observed, e.g. in section 36 that received pesticide input from section 125, but the magnitude of effects remained limited also because of the fast dissipation of the pesticide from the water phase.

4.4 Landscape ecotoxicology and the options for ecological risk assessment

Embedding the population model into a realistic landscape shape in terms of a concrete water course network offers the possibility to assess not only a single application under idealised conditions, but to simulate the consequence of a label-conforming usage of a given compound within an agricultural landscape on a series of crop fields. In this sense, our approach is one further step towards extrapolating from laboratory results to real-world landscapes. It follows the request for research as formulated by Artigas et al. (2012), who called for the development of a coherent modelling framework to establish links between exposure to toxicants and effects at all scales and complexity levels. The generality of our framework 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; simulations are then automatically performed for a freely definable network of water courses. In our case studies, the chemical exposure patterns were calculated for λ -cyhalothrin and population dynamics were simulated for the water louse *A. aquaticus* in a typical Dutch drainage ditch network, but it is easily possible to perform a next set of

simulations for another pesticide and another aquatic species in a different landscape, as long as the concentration profiles are provided externally and the population model is implemented in NetLogo.

We see our approach as a development within the field of landscape ecotoxicology, because we provide a modelling framework where chemical exposure patterns, toxicity, and ecological population models are integrated within a realistic landscape setting. In this sense, the framework provides a platform to account for movement patterns of a species, toxicity and lifecycle characteristics, expressed at the landscape level according to the request of Van den Brink (2008). This possibility of an ecotoxicological assessment of endpoints appropriate to the spatial and temporal scales across which pesticides are dispersed is currently missing in the environmental risk assessment framework of pesticide registration. Examples like Topping et al. (2013), Topping and Lagisz (2012), Galic et al. (2012) and the framework introduced in this manuscript show the potential of spatially-explicit individual-based models to elucidate questions about pesticide effects in realistic landscape settings. These modelling approaches provide, for example, the potential to estimate risks to or in remote areas, and also to consider large-scale heterogeneity of exposure patterns. The representation of the recolonisation potential in a spatially realistic landscape naturally emerges from the landscape structure and need not be imposed artificially. In general, the landscape approach adds a proper spatial dimension to risk assessment, that introduces more realism in exposure and recovery of the aquatic species.

In this way, spatially explicit integrated simulation models can help to tackle some of the challenges for ERA on a landscape level, for example that the effect and recovery patterns on a landscape scale emerge from quite a number of processes on different spatial scales. While pesticide transport occurs at the larger spatial scale, local dispersal by walking of the Asellids remains a strictly local phenomenon as long as drift is not considered, but population demography leads to changes at larger spatial scales. The modelling approach that we followed in this paper integrates all these scales by mechanistically linking the respective processes. This approach can be challenged as

introducing a high level of complexity into ERA, as being parameter- and data-hungry and also as being demanding in terms of computation times. However, mechanistic modelling of the combined exposure and effect dynamics are conceptually simple and straightforward and facilitate exploration of risks of pesticide applications in at least semi-realistic landscape settings.

5 The present study contributed new possibilities for the simulation of pesticide effects on aquatic macroinvertebrates on a landscape scale. The results from the case study with λ -cyhalothrin do not change the risk estimates for this substance, but it shows a blueprint for an assessment for new registrations. Risk assessors can use integrated simulation frameworks like the one proposed in this study for the aquatic environment or ALMaSS for the terrestrial domain to add information about
10 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
15 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 in the end pesticides are not used in isolation and with single applications.

This study cannot provide endpoints that are immediately operational for environmental risk
20 assessment in its current shape. A candidate for such an endpoint would be the ratio of affected area, that integrates over chemical fate and effects. Hopefully, this study initiates discussions about what new indicators could look like and how they could be integrated into the current ERA framework.

25 **5. Conclusions**

This study shows a proof of concept of the chosen modelling approach to assess the risks of pesticide exposure to aquatic organisms in a spatially-realistic landscape context. The observed differences in effect and recovery patterns that range between no observable effects for the low spray-drift and low sensitivity scenario (Fig. 6) and severe reduction of abundances for the high spray-drift and high sensitivity scenario (Fig. 5) illustrate the sensitivity of our modelling approach, but also shows the necessity of precise calculations of pesticide inputs and model parameterisation.

Further on, this study demonstrates the possibilities of model approaches for risk assessors. Modelling can deliver more and more realistic simulations of pesticide fate and effects, and risk assessors can test scenarios or simulate assumptions that have effects on the scale of agricultural landscapes. Coupled fate-and effect modelling delivers the potential to explore situations that differ from current risk assessment, hence to extrapolate to different exposure situations, or to different climate situations. Further options could involve exploring the effects of mitigation measures on the risk estimates on the landscape scale and hence going a step towards risk management, or to support field monitoring studies with spatially realistic landscape-scale simulations.

Our results underline the importance of taking into account ecological processes that determine population recoveries after pesticide stress on an appropriate spatial resolution and with the appropriate accuracy. To increase the level of trust in effect and recovery simulations, experimental research on density dependence and dispersal parameters of *A. aquaticus* is urgently needed.

Chemical fate simulations did not include a sediment compartment. For the chemical fate of λ -cyhalothrin and other strong sorbing pesticides, the addition of a sediment compartment to the CASCADE-TOXSWA model would increase the realism of the concentration patterns and is therefore recommended. A sediment compartment would act as a buffer that releases low-level concentrations of chemicals over longer times, so it is important for chronic effect assessments, and certainly has to be introduced for studies that involve uptake of chemicals from the sediment.

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Supplementary data

A comprehensive model documentation in the ODD format and more information about model formulation, development and testing in the TRACE format is attached.

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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),
Reproduction	Repro_date_1 (Age at reproduction 1 st period)	120	day	Galic et al. (2012)
	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), Tolba and Holdich (1981) therein
	Repro_len_1 (Length of 1 st reproduction period)	1 to 28 (uniform)	day	Galic et al. (2012), Chambers (1977) therein
	Repro_len_2 (Length of 2 nd reproduction period)	1 to 45 (uniform)	day	Galic et al. (2012), Chambers (1977) therein
Growth	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
	K (Size growth rate constant)	0.02	1/day	Galic et al. (2012)
	Mat_age (Age at maturity)	45	day	Galic et al. (2012), Williams (1962) therein
Movement	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

Table 2: Affected areas and recovery times.

Scenario		Extent of affected area (%) ^a			
Spray drift	Sensitivity	Sec. 19	Sec. 23	Sec. 58	remote ^b
5 %	24 ng/L	100	100	100	22.8
	48 ng/L	100	100	98.0	12.7
1 %	24 ng/L	100	100	12.4	2.5
	48 ng/L	23.8	27.7	14.6	2.6
		Recovery times (days) ^a			
		Sec. 19	Sec. 23	Sec. 58	remote ^b
5 %	24 ng/L	930	841	791	67
	48 ng/L	429	456	211	12
1 %	24 ng/L	14	20	-	-
	48 ng/L	-	-	-	-

^a: see Material and Methods for exact definition.

^b: remote areas: all segments of the downstream transect exclusive those sections that were subject to direct spray drift input, i.e. section 19, 23 and 58 (ref. to Fig. 1).

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Table 3: Flow velocities in some selected sections of the case study area (see Fig. 2).

Application date	Flow velocity (m/d)			
	Section 19	Section 20	Section 23	Section 58
1-5-1994	73.0	221.6	606.5	752.0
8-5-1994	8.6	118.0	11.7	407.5
15-5-1994	7.9	104.5	10.2	124.7
22-5-1994	77.4	191.8	653.9	1066.0
29-5-1994	10.6	138.0	14.4	80.1
5-6-1994	74.8	225.3	623.9	729.8
12-6-1994	68.8	212.0	567.4	583.2
19-6-1994	70.6	221.7	579.7	745.8
26-6-1994	7.6	104.7	9.6	383.6
3-7-1994	4.8	67.3	6.6	45.5
10-7-1994	53.8	116.5	477.9	122.3
17-7-1994	5.2	66.2	7.1	151.6
24-7-1994	3.2	42.3	4.4	95.0
31-7-1994	1.7	22.8	2.4	39.7
7-8-1994	0.6	8.0	0.8	5.3

5 Figure captions

Figure 1: Flow chart of the upscaling framework. *: local capacities (individuals) are calculated per segment based on the specific area of each segment.

Fig. 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 for the local model. rand(1) are uniformly distributed random numbers between 0 and 1.

Figure 4: Space-time plot of the simulated water concentrations (mg/L) of λ -cyhalothrin for the 5%-drift scenario. Values are shown along the transect from section 19 to 111 (see Figure 1). The vertical grid lines between days 122 and 220 indicate the days of pesticide application. The horizontal grid lines indicate the beginning of downstream sections along the transect, starting with section 19 in the bottom. The colours indicate pesticide water concentrations as given in the legend, the maximum value is about 4.55×10^{-5} mg/L.

Figure 5: Space-time plot of the relative abundances of *Asellus aquaticus* as simulated for the 5 % - spray drift scenario using an EC50 value of 48 ng/L (**top panel**) and 24 ng/L (**bottom panel**). Relative abundances are shown along the transect from section 19 to 111 (see Figure 1). The black vertical grid lines between April 94 and August 94 indicate the days of pesticide application. The white, 5 dashed vertical grid lines indicate the times of population peaks , that is end of April and mid-July every year. The horizontal grid lines indicate the beginning of the downstream section along the transect, starting with section 19 in the bottom. The colours indicate the relative abundances as given in the legend on the right hand side.

Figure 6: Space-time plot of the relative abundances of *Asellus aquaticus* as simulated for the 1 % - 10 spray drift scenario using an EC50 value of 48 ng/L (**top panel**) and 24 ng/L (**bottom panel**). Relative abundances are shown along the transect from section 19 to 111 (see Figure 1). The black vertical grid lines between April 94 and August 94 indicate the days of pesticide application. The white, dashed vertical grid lines indicate the times of population peaks , that is end of April and mid-July every year. The horizontal grid lines indicate the beginning of the downstream section along the 15 transect, starting with section 19 in the bottom. The colours indicate the relative abundances as given in the legend on the right hand side.

Figure 7: Log10-transformed relative abundances of *Asellus aquaticus* along the downstream transect 19 to 111 on day 228, i.e. two days after the last pesticide application for the 5%-drift scenario. The blue line shows results from the low toxicity simulations (EC50 = 48 ng/L), and the red 20 line shows results from high toxicity simulations (EC50 = 24 ng/L).

