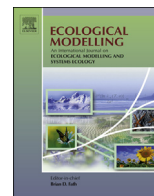




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Two pairs of eyes are better than one: Combining individual-based and matrix models for ecological risk assessment of chemicals

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ABSTRACT

Current chemical risk assessment procedures may result in imprecise estimates of risk due to sometimes arbitrary simplifying assumptions. As a way to incorporate ecological complexity and improve risk estimates, mechanistic effect models have been recommended. However, effect modeling has not yet been extensively used for regulatory purposes, one of the main reasons being uncertainty about which model type to use to answer specific regulatory questions. We took an individual-based model (IBM), which was developed for risk assessment of soil invertebrates and includes avoidance of highly contaminated areas, and contrasted it with a simpler, more standardized model, based on the generic metapopulation matrix model RAMAS. In the latter the individuals within a sub-population are not treated as separate entities anymore and the spatial resolution is lower. We explored consequences of model aggregation in terms of assessing population-level effects for different spatial distributions of a toxic chemical. For homogeneous contamination of the soil, we found good agreement between the two models, whereas for heterogeneous contamination, at different concentrations and percentages of contaminated area, RAMAS results were alternatively similar to IBM results with and without avoidance, and different food levels. This inconsistency is explained on the basis of behavioral responses that are included in the IBM but not in RAMAS. Overall, RAMAS was less sensitive than the IBM in detecting population-level effects of different spatial patterns of exposure. We conclude that choosing the right model type for risk assessment of chemicals depends on whether or not population-level effects of small-scale heterogeneity in exposure need to be detected. We recommend that if in doubt, both model types should be used and compared. Describing both models following the same standard format, the ODD protocol, makes them equally transparent and understandable. The simpler model helps to build up trust for the more complex model and can be used for more homogeneous exposure patterns. The more complex model helps detecting and understanding the limitations of the simpler model and is needed to ensure ecological realism for more complex exposure scenarios.

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1. Introduction

What is the risk that chemicals released into the environment have unacceptable effects on populations and ecosystems? In current regulatory environmental risk assessment (ERA) of chemicals, ecological effects are determined indirectly. Threshold exposure concentrations for detectable effects on individuals measured in

the laboratory are extrapolated to populations in real landscapes by dividing them by so-called assessment, or safety, factors, which are supposed to take into account ecological characteristics of the species, landscape, and ecosystem under consideration. However, whether or not these factors are over- or under-protective remains an open question (Forbes and Calow, 2002).

As a way to incorporate ecological complexity and bridge the gap between laboratory tests and effects on the ecological entities that current risk assessment schemes aim to protect, ecological mechanistic effect models (MEMs) have been recommended as they provide a tool for expressing ecological risks in a way that informs the environmental management process (Forbes et al., 2010) and increases the ecological relevance of risk assessments

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(Forbes et al., 2008; Thorbek et al., 2009). Population modeling has also been included by the European Food Safety Authority (EFSA) in the revised Guidance Document on Risk Assessment for Birds and Mammals (EFSA, 2009) and in a Scientific Opinion on the development of specific protection goals (EFSA Panel on Plant Protection Products and their Residues, 2010) as an appropriate option for higher-tier risk assessment.

Nevertheless, in contrast to exposure modeling (Boesten et al., 1995), effect modeling has not yet been extensively used for regulatory purposes (Schmolke et al., 2010a,b). A main reason for this was identified in a survey among stakeholders from academia, industry, and regulatory authorities involved in ERA (Hunka et al., 2013): the lack of official guidance for developing and using mechanistic effect models. This includes choosing the model types to be used, which is influenced by contradicting expectations (Hunka et al., 2013): models are supposed to be simple and user-friendly enough to be easily understood, parameterized, and used in a standardized way, but at the same time complex enough to be realistic and capable of capturing a wide range of ecological scenarios.

Thus, in addition to developing ecological models for chemical risk assessment, which just have a certain level of complexity, the costs and benefits of this particular level of complexity for ERA procedures need to be demonstrated more often, by contrasting more simple and more complex models. Fully independent comparisons, though, would require that the models were developed by different modelers with no direct or indirect interactions whatsoever, which would be difficult and so far has never been tried. An alternative is starting with a more complex model and then aggregating it into a simplified one. For mechanistic effect models, this was done by Topping et al. (2005), who compared a very complex spatially explicit IBM to a very simple non-spatial matrix model.

Here we take a recent spatially explicit individual-based population model, which was developed for risk assessment of soil invertebrates (Meli et al., 2013), and contrast it with a simpler, more standardized model, which is based on the generic metapopulation matrix model RAMAS Metapop 5.0 (Akçakaya and Root, 2005). RAMAS falls into the family of “canned” programs (Reed et al., 2002), which corresponds to the widely held belief among the stakeholders involved in ERA of chemicals that using standardized software is the best way to establish MEMs for regulatory risk assessment.

In our example models, we focus on soil invertebrates, which are key drivers of important ecosystem services such as nutrient cycling and soil formation (Lavelle et al., 2006). For these species, an important ecological factor that is largely ignored in current regulatory risk assessments is spatial heterogeneity in exposure. It is well known that in soils both natural properties, such as moisture and organic matter concentrations, and chemical contamination are heterogeneously distributed (Lavelle and Spain, 2001; Becker et al., 2006), which has important consequences for the distribution and functioning of populations of soil organisms (Hoy and Hall, 1998). Thus, the real risk posed by the use of chemicals in agricultural practices or industrial activities is likely not to be adequately captured by current risk assessment procedures.

The two models we are contrasting are mostly based on the same input data and, similarly to Topping et al. (2005), the IBM is used to determine some of the parameters of the metapopulation model, as it was not possible to find appropriate values in the scientific literature. Therefore in this study we are not trying to compare independent predictions of two models, but to explore the consequences of model aggregation. Aggregating a complex individual-based model into a metapopulation matrix model, where all the individuals within a grid cell are not treated as separate entities anymore and the spatial resolution is lower, will allow us to understand whether it really is necessary to look at single individuals for a species with a relatively simple life-cycle in

order to assess toxic effects at the population level. Furthermore, we will explore which benefits the parallel development of more simple and more complex models can have within a regulatory perspective, for instance in terms of trust and model acceptance.

2. Methods

The species used in the simulations is *Folsomia candida* Willem 1902, which belongs to the order *Collembola*, suborder *Entomobryomorpha*, family *Isotomidae*. This species is used as a standard test organism for toxicity tests: a 28-day reproduction test (International Organization for Standardization, 1999; Organisation for Economic Co-operation and Development, 2009) is included in the refinement options for ecological risk assessment of plant protection products to soil organisms in the EU (EC, 2009). A more detailed description of *F. candida* is given in Meli et al. (2013).

Copper sulfate (CuSO_4) was used as a model contaminant: it is proven to cause toxic effects to *F. candida* survival and reproduction (LC50 equal to 1810 mg kg^{-1} , EC50 for reproduction equal to 751 mg kg^{-1} ; Greenslade and Vaughan, 2003) and to elicit behavioral responses like avoidance (Boiteau et al., 2011). Moreover it is the most widely distributed pollutant among all metals, and therefore it is relevant from the practical point of view of ecological risk assessment.

2.1. Individual-based model

The purpose of the model is to investigate how populations of *F. candida* are affected by spatial distribution of toxic contamination in soil, with a special focus on interactions with food availability and local population density (Meli et al., 2013). The model comprises the entities eggs, juvenile and adult female springtails, and grid cells. Springtails are mobile and are characterized by the state variables age (days), position (continuous coordinates), direction for movement, energetic status (days-to-death), cumulative distance (in cm) walked in each hourly time-step, and time (h) spent on contaminated grid cells. Grid cells are characterized by their food level and concentration of toxicant (mg kg^{-1} soil). The model world is a two-dimensional grid of 100×100 square grid cells, whereas each grid cell represents 1 cm^2 of soil. The model proceeds on two time scales: hourly time steps are used for the foraging procedure, while the following processes are repeated at daily time steps: updating the seasonal re-growth of food, aging and growth, reproduction, hatching, density dependence on fecundity and survival, and mortality.

Values of almost all parameters are drawn from uniform or normal probability distributions, in order to reflect heterogeneity among individuals. Stochasticity is also used for initializing springtails' starting positions, as well as causing individual behaviors (movement, reproduction, hatching, mortality) to occur with specified frequencies. Simulations start with 1000 individuals located on the upper left corner of the model arena, in order to simulate a recolonization scenario. The initial population is divided in a stage distribution that randomly varies around the mean values of all the stable stage distributions used for the metapopulation model. Food resources are also randomly assigned at the beginning of a model run to grid cells which are initialized to be food sources, with different maximal food levels. Four different scenarios for the extent and spatial distribution of contaminated areas are used (see Section 2.3). A key feature of the model is that it represents avoidance behavior: individuals can, depending on the toxicant's concentration, sense and avoid contaminated areas. The stage distributions used to initialize the model and the TRACE documentation of the model (Schmolke et al., 2010a), which includes a full description

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