Frederik DE LAENDER

Predicting effects of chemicals on freshwater ecosystems: model development, validation and application

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Concurrently with the increasing human population and its associated activity, the number of chemical substances found in water bodies has augmented substantially during the last century. Because these different chemicals have a wide range of biological modes of action, it is not unlikely that their presence in water bodies results in adverse effects on aqueous ecosystems. Within the field of ecotoxicology, ecological effect assessment of chemicals aims at assessing and predicting these effects. It has become a routine practice to perform such assessments solely relying on single-species toxicity test results. Results from this type of tests reflect the **direct effect** of a chemical on one isolated species in a laboratory setting. These test results are mostly expressed as concentrations resulting in x% effect (EC_x) on a given test population. Current approaches to extrapolate single-species toxicity test results to ecosystem-level effects are based on a set of largely untested assumptions which **ignore ecological interactions** between different populations. One such an approach is to use a statistical distribution of single-species toxicity test results of different species for a given chemical, termed species sensitivity distribution (SSD).

It has been shown that ecological effects are determined by (1) **ecological interactions** and (2) **direct effects**. Hence, predictions of ecological effects by current extrapolation methods (e.g. the use of SSDs) will most likely be inaccurate. Therefore, ecological effect assessments relying on such inaccurate predictions result in accurate assessments of chemical risk to aquatic ecosystems.

The use of **dynamic ecosystem models** has been proposed as an alternative to current approaches. These models may consist of (1) a food web model; (2) toxic effect sub-models; and (3) a model for nutrient and detritus cycling. The advantage of these models in comparison to current approaches is that they **can account for ecological interactions** between populations by incorporating feeding and competition relationships. Unfortunately, no information exists on which type of toxic effect sub-model results in the most accurate predictions of an ecosystem model. Also, quantitative validations of effects predicted by such ecosystem models are scarce. As a result, it is unknown if and how ecosystem models can contribute to ecological effects assessments.

Because current approaches for ecological effect assessments rely on the relationship between single-species toxicity test results and effects on ecosystems, this dissertation starts with a review of studies which were designed to examine this relationship (**chapter II**). These studies can be divided in (1) experimental ecosystem studies and (2) studies using ecosystem models. For both study types, changes in abundances or biomasses of populations were most frequently studied.

Experimental ecosystem studies with insecticides report EC_xs for invertebrate species (with biomass or abundance as endpoint) which differ less than a factor two of single-species EC_xs for the same species based on the same endpoint. Results from the few modelling studies found indicate that EC_xs within an ecosystem can be lower than corresponding single-species EC_xs. The overestimated effects produced by the reviewed ecosystem models and the focus on toxicants for which prey are more sensitive than predators can explain the difference between results from experimental ecosystem studies and results from modelling studies.

In **chapter III and IV** the development and application of a new ecosystem model is described. A dynamic ecosystem model is constructed in such a way that it can be customized to represent different lentic (i.e. non-running) aquatic ecosystems. Also the toxic effect sub-models can be customized. The ecosystem model aims at accurately predicting ecological effects, rather than pursuing the exact replication of observed population dynamics. Ecological effects of copper, which were observed in a previously conducted ecosystem study, were predicted accurately by the developed ecosystem model (**chapter IV**). In contrast, extrapolation based on single-species toxicity test results alone did not accurately predict ecosystem effect levels.

While a default toxic effect sub-model was chosen in chapter IV, an effort was made in **chapter V** to determine which toxic effect sub-model is most suited for the developed ecosystem modelling approach. To this end, four ecosystem models were constructed, each with a different toxic effect sub-model. The capacity of each of these models to predict biomass changes and no observed effect concentrations (NOECs) established in an experimental microcosm was evaluated. The ecosystem model with a toxic effect sub-model incorporating effects on zooplankton mortality using a logistic concentration-effect function was superior to the other three models since it made accurate NOEC predictions for most populations. Additional incorporation of sub-lethal effects on zooplankton did not result in better predictions. Ecosystem models using linear concentration-effect functions predict biomass decreases already occurring at concentrations which are 4 times lower than the observed NOECs.

In **chapter VI** the ecosystem model which gave the best predictions in chapter V was further validated using literature data. Predicted NOECs were compared with population and ecosystem - NOECs observed in 11 experimental ecosystems. For each of those studies, the model was customized to account for the specific ecological interactions within the studied system. Population-NOEC predictions were accurate, or at least protective (i.e. smaller than the observed one), for 60 and 86% of all considered populations, respectively. For all 11 studies, a protective ecosystem-NOEC could be derived, i.e. accurate and conservative predictions in 8 and 3 cases, respectively. It was concluded that the inclusion of the relevant populations and taking the median of model outputs can increase the accuracy of model predictions.

In **chapter VII** the validity of a theoretical assumption underlying species sensitivity distributions (SSDs), used for deriving “safe concentrations” based on single-species toxicity test results, was examined in a simple freshwater lentic pelagic ecosystem. The tested assumption was that ecological interactions do not alter a sensitivity distribution. For each of 1000 hypothetical toxicants, a lognormal SSD was fitted to chronic single-species toxicity test results, i.e. without taking into account ecological interactions and therefore termed ‘conventional SSD’ (cSSD). Next, corresponding sensitivity distributions, which do take ecological interactions into account, were constructed (eco-SSDs) using the ecosystem modelling-approach described and validated in the previous chapters. For 254 of the 1000 hypothetical toxicants, mean and/or variance of the cSSD were significantly higher than mean and/or variance of the eco-SSD, as such rejecting the general validity of the tested assumption. A classification tree approach further indicated that especially for toxicants exerting direct effects on phytoplankton (e.g. herbicides), the cSSD may have a higher mean than the eco-SSD. Conversely, means of eco-SSD and cSSD are likely to be equal for toxicants targeting zooplankton and fish.

A second theoretical assumption underlying SSDs was tested in **chapter VIII**. Here, the tested assumption was that ecosystem structure (i.e. species composition) is as or more sensitive than ecosystem function. This test was performed using the same ecosystem as that used in chapter VII. NOECs were calculated for ecosystem structure and function for each of the 1000 hypothetical toxicants. For 979 of these toxicants, the ecosystem structure-NOEC was lower than or equal to the ecosystem function-NOEC, indicating that the tested assumption is valid. For 239 of these 979 toxicants, both NOECs were equal. For half of the 1000 toxicants, structure of lower trophic levels (i.e. phytoplankton) appears to be more sensitive than structure of higher trophic levels (i.e. fish). As such, ecosystem structure-NOECs are primarily determined by the sensitivity of the structure of lower trophic levels. In contrast, ecosystem functions associated with higher trophic levels (e.g., total ingestion by fish) are more sensitive than functions associated with lower trophic levels (e.g., total photosynthesis by phytoplankton) for 749 toxicants. Top-down regulation of ecosystem structure and cascading effects from lower trophic level functions to higher trophic level ecosystem functions are discussed as possible explanations for these two contrasting findings.

When applying SSDs in ecological effect assessments, it is generally accepted that a concentration corresponding to a percentile y of this SSD is a hazardous concentration for y% of the species within an ecosystem (HC_y). To elucidate the ecological significance of this concept, the ecosystem model developed and validated in the previous chapters was used in a practical ecosystem study (**chapter IX).** The ecological effects of different HC_ys of copper on ecosystem structure (biomass) and function (photosynthesis of phytoplankton, $PS_{all\ phytoplankton}$; and ingestion by zooplankton, $I_{all\ zooplankton}$) were estimated with the developed ecosystem model. Zooplankton biomass and the associated ecosystem function rate ($I_{all\ zooplankton}$) remained unaffected when the system was exposed to concentrations $\leq HC_{30}$ of an SSD based on EC_{20}s derived from single-species tests. Phytoplankton biomass and $PS_{all\ phytoplankton}$ increased at concentrations > HC_5 or HC_{30} of an SSD based on EC_{20}s or EC_{10}s, respectively. Thus, exposing the ecosystem studied to other percentiles than the commonly chosen HC_5 does not necessarily result in ecological effects on 5% of the species.

A summary of the conclusions drawn in the different chapters is provided in **chapter X**. In general, it is concluded that the type of ecosystem models constructed in this dissertation can serve as an ecology-based method to accurately **predict ecological effects**, provided that the relevant populations are included in the model and a logistic toxic effect sub-model is used to integrate direct effects on mortality of animals. The use of ecosystem models in ecological effect assessments benefits from the limited data needs of such models. The amount of standard single-species toxicity test results needed to use such an approach is comparable to the amount of data needed to apply conventional extrapolation approaches. Moreover, the models developed here can also **support** current extrapolation approaches. The validity of the assumptions underlying these extrapolation approaches is related to the toxicant type. For toxicants directly targeting zooplankton and fish, these assumptions are likely to be valid, while the opposite holds for toxicants directly targeting phytoplankton. These findings, together with results from experimental ecosystem studies aid in understanding the significance of current extrapolations approaches. As such, they can assist risk assessors in applying approaches that more accurately predict no effect concentrations for chemicals.