STATISTICAL ECO(-TOXICO)LOGY

IMPROVING THE UTILIZATION OF DATA FOR ECOLOGICAL RISK ASSESSMENT

by

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INTRODUCTION AND OBJECTIVES

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1.2 ECOLOGICAL RISK ASSESSMENT

Ecological risk assessment (ERA) tries to estimate risks to non-human organisms, populations or ecosystems and is used as a tool for decision making under uncertainty. The decision to be made is, whether a (new) pesticide can be approved for usage and a potential release in the environment without a risk to the environment. Ecological risk is defined as a combination of the severity and the probability of occurrence of a potential adverse effect (Suter, 2007). Therefore, ERA is based on two components: Effect- and exposure assessment. A combination of both is needed to characterise ecological risks.

Effect assessment characterizes the strength of effects using laboratory and semi-field experiments. It establishes relationships between the concentration of a compound and the observed ecological effects. In the European Union a tiered approach with increasing complexity and realism. Lower tier assessment is based on highly standardized single species laboratory experiments, whereas higher tier assessment is refined by testing additional species, extended laboratory experiments or model ecosystem experiments. To address the various uncertainties in effect assessment (experimental variation, variation between species, variation in environmental conditions etc) the retrieved toxicity values are multiplied by a assessment factor between 0.01 (lower tier assessment) and 0.5 (higher tier assessment) depending on data quality, which yields to a regulatory acceptable concentration (RAC) (EFSA, 2013).

Exposure Assessment for freshwaters aims to characterise the probability of a adverse effect by deriving a predicted environmental concentration (PEC) in surface waters and sediments (Newman, 2015). It is mainly based on modeling the fate of chemicals in the environment using computer simulations. In the European Union, the FOCUS models are used (FOCUS, 2001; EFSA, 2013). To calculate PECs these model need many compound specific input parameters like the molecular weight, water solubility, partitioning coefficients and dissipation time. Additionally, information on the application regime and crop type is needed. FOCUS models the concentration within edge-of-field streams of 1 meter width and 30 cm depth (Erlacher and Wang, 2011). Such a stream width corresponds to a catchment size of 7 km^2 (See figure **??**) ref to small streams supplement which is considered as small stream (Lorenz et al., 2016). Nevertheless, recent research showed that FOCUS models fail predict measured field concentrations of pesticides (Knäbel et al., 2012; Knäbel et al., 2014).

Risk characterisation is the final step in ERA. It puts together the information gained from effect and exposure assessment. Risk can expressed in several ways, for example simply as the ratio between RAC and PEC, but also as a quantitative description (EFSA, 2013; Suter, 2007).

1.3 ENVIRONMENTAL MONITORING

1.4 STATISTICAL ECOTOXICOLOGY

Ecological effect assessment generates data on ecological effects using experiments. The produced datasets range from small univariate datasets (lower tier assessment) to medium sized multivariate datasets (higher tier assessment). These datasets are analyzed using statistical techniques in order to deliver usable information for assessment.

The relationships between the concentration of a compound and the observed effects are usually analysed using using dose-response models (Ritz, 2010), which can be used to derive an effective concentration for x% effect (EC_x). Nevertheless, such relationships cannot always be established from experimental data. For example, model ecosystem experiments are conducted to characterize effects on whole biological communities. However, because of multivariate responses and potential indirect effects, there is no clear dose-response relationship and no models for this kind of data available. There are also other examples were fitting dose-response models is problematic (Green, 2016). In such theses there is usually a no-observed-effect concentration (NOEC) computed. The NOEC is the highest tested concentration that does not lead to significant deviation from the control response and therefore relies on null hypothesis significance testing (NHST). However, the use of NOEC as toxicity measure in ecological effect assessment has been heavily in the past (Laskowski, 1995; Chapman et al., 1996; Warne and Dam, 2008; Fox et al., 2012; Jager, 2012; Fox and Landis, 2016b). Instead of conducting experiments, toxicity could be also predicted from molecular structures using quantitative structure-activity relationships (QSAR) (Kühne et al., 2013), which are calculated using machine-learning techniques (Murrell et al., 2015; Cortes-Ciriano, 2016). Although, QSARs may save resources they also need huge amounts of input data.

Eco(toxico-)logists produce large amounts of data. For example chemical monitoring produces

Big data can provide new information and opportunities for ERA (Dafforn et al., 2015).

Effect assessment relies heavily on statistical methods. Statistical ecotoxicology combines statistics with the specific needs and constraints of ecotoxicology. It aims to provide solutions to statistical challenges in ecotoxicology (Fox and Landis, 2016a), guidance on experimental designs (Johnson et al., 2015) and tools to integrate big data (Van den Brink et al., 2016) to improve accuracy of ERA.

1.5 OBJECTIVES AND OUTLINE OF THE THESIS

The overall goal of this thesis was to contribute to the emerging field of statistical ecotoxicology and ERA. The main objectives were (i) to scrutinize new methods in statistical ecotoxicology, (ii) explore available monitoring data and (iii) provide tools to deal with big data. Figure 1.1 provides an overview on the research performed and its relation to ERA as outlined in the previous sections.

The thesis starts with a comparison of statistical methods to analyse ecotoxicological experiments in effect assessment (Chapter **??**). Specific questions addressed were:

- Are newer statistical methods more powerful than currently used methods?

- How much statistical power do current experimental designs in ecotoxicology exhibit?

Exposure assessment makes predictions on concentrations in small streams. Chapter 2 focuses on large-scale realised environmental concentrations and the drivers thereof. Specific goals were:

- Compile all available monitoring data on pesticides in Germany, with a focus on small streams.
- Explore the relationship between agricultural land use and streams sizze and measured pesticide concentrations.
- Study annual dynamics of pesticide exposure, as well as influence of precipitation on measured pesticide concentrations.
- Assess the current pollution in German streams and identify responsible pesticides.

The compilation of monitoring data from different data sources, lead to a big inhomogeneous amount of data that first needs to be harmonized. Chapters **??** (chemical data) and **??** (biological data) describe software solutions to simplify and accelerate the workflow of:

- validating and harmonizing chemical and taxonomic data
- linking to other datasets
- searching properties and identifiers

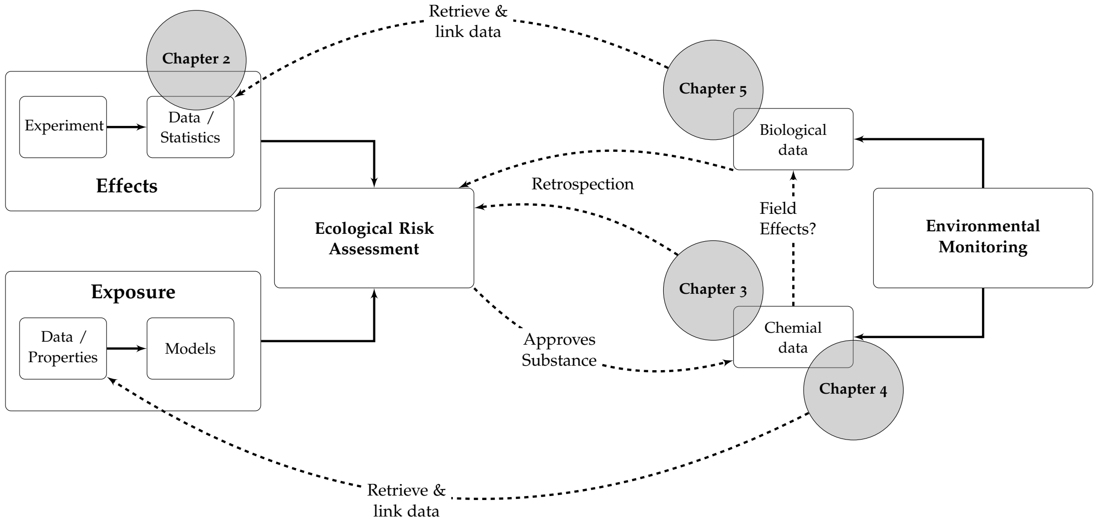

Figure 1.1: Conceptual overview on data in ecological risk assessment and environmental monitoring, as well as parts addressed by this thesis.

1.6 REFERENCES

Chapman, P., P. Chapman, and R. Caldwell (1996). "A warning: NOECs are inappropriate for regulatory use". *Environmental Toxicology and Chemistry* 15 (2), 77–79.

Cortes-Ciriano, I. (2016). "Bioalerts: a python library for the derivation of structural alerts from bioactivity and toxicity data sets". *Journal of Cheminformatics* 8 (1).

Dafforn, K. A., E. L. Johnston, A. Ferguson, C. Humphrey, W. Monk, S. J. Nichols, S. L. Simpson, M. G. Tulbure, and D. J. Baird (2015). "Big data opportunities and challenges for assessing multiple stressors across scales in aquatic ecosystems." *Marine and Freshwater Research*.

EFSA (2013). "Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters". *EFSA Journal* 11 (7), 3290.

Erlacher, E. and M. Wang (2011). "Regulation (EC) No. 1107/2009 and upcoming challenges for exposure assessment of plant protection products – Harmonisation or national modelling approaches?" *Environmental Pollution* 159 (12), 3357–3363.

FOCUS (2001). *FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC.* Report of the FOCUS Working Group on Surface Water Scenarios EC Document Reference SANCO/4802/2001-rev.2.

Fox, D. R., E. Billoir, S. Charles, M. L. Delignette-Muller, and C. Lopes (2012). "What to do with NOECS/NOELS—prohibition or innovation?" *Integrated Environmental Assessment and Management* 8 (4), 764–766.

Fox, D. R. and W. G. Landis (2016a). "Comment on ET&C perspectives, November 2015-A holistic view". *Environmental Toxicology and Chemistry* 35 (6), 1337–1339.

Fox, D. R. and W. G. Landis (2016b). "Don't be fooled-A no-observed-effect concentration is no substitute for a poor concentration-response experiment: NOEC and a poor concentration-response experiment". *Environmental Toxicology and Chemistry* 35 (9), 2141–2148.

Green, J. W. (2016). "Issues with using only regression models for ecotoxicity studies". *Integrated Environmental Assessment and Management* 12 (1), 198–199.

Jager, T. (2012). "Bad habits die hard: The NOEC's persistence reflects poorly on ecotoxicology". *Environmental Toxicology and Chemistry* 31 (2), 228–229.

Johnson, P. C. D., S. J. E. Barry, H. M. Ferguson, and P. Müller (2015). "Power analysis for generalized linear mixed models in ecology and evolution". *Methods in Ecology and Evolution* 6 (2), 133–142.

Knäbel, A., K. Meyer, J. Rapp, and R. Schulz (2014). "Fungicide Field Concentrations Exceed FOCUS Surface Water Predictions: Urgent Need of Model Improvement". *Environmental Science & Technology* 48 (1), 455–463.

Knäbel, A., S. Stehle, R. B. Schäfer, and R. Schulz (2012). "Regulatory FOCUS Surface Water Models Fail to Predict Insecticide Concentrations in the Field". *Environmental Science & Technology* 46 (15), 8397–8404.

Kühne, R., R.-U. Ebert, P. C. von der Ohe, N. Ulrich, W. Brack, and G. Schüürmann (2013). "Read-Across Prediction of the Acute Toxicity of Organic Compounds toward the Water Flea Daphnia magna". *Molecular Informatics* 32 (1), 108–120.

Laskowski, R. (1995). “Some good reasons to ban the use of NOEC, LOEC and related concepts in ecotoxicology”. *Oikos* 73 (1), 140–144.

Lorenz, S., J. J. Rasmussen, A. Süß, T. Kalettka, B. Golla, P. Horney, M. Stähler, B. Hommel, and R. B. Schäfer (2016). “Specifics and challenges of assessing exposure and effects of pesticides in small water bodies”. *Hydrobiologia*, 1–12.

Murrell, D. S., I. Cortes-Ciriano, G. J. P. van Westen, I. P. Stott, A. Bender, T. E. Malliavin, and R. C. Glen (2015). “Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules”. *Journal of Cheminformatics* 7 (1).

Newman, M. C. (2015). *Fundamentals of ecotoxicology: the science of pollution*. Boca Raton: CRC Press, Taylor & Francis Group.

Ritz, C. (2010). “Toward a unified approach to dose-response modeling in ecotoxicology”. *Environmental Toxicology and Chemistry* 29 (1), 220–229.

Suter, G. W., ed. (2007). *Ecological risk assessment*. Boca Raton: CRC Press/Taylor & Francis.

Van den Brink, P. J., C. B. Choung, W. Landis, M. Mayer-Pinto, V. Pettigrove, P. Scanes, R. Smith, and J. Stauber (2016). “New approaches to the ecological risk assessment of multiple stressors”. *Marine and Freshwater Research* 67 (4), 429.

Warne, M. S. J. and R. van Dam (2008). “NOEC and LOEC data should no longer be generated or used”. *Australasian Journal of Ecotoxicology* 14, 1–5.

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LARGE SCALE RISKS FROM PESTICIDES IN SMALL STREAMS

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2.1 ABSTRACT

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DISCUSSION

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