

STATISTICAL ECO(-TOXICO)LOGY

IMPROVING THE UTILIZATION OF DATA FOR
ECOLOGICAL RISK ASSESSMENT

by

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INTRODUCTION AND OBJECTIVES

1.1 PESTICIDES IN FRESHWATER ECOSYSTEMS

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. 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 experiments. It establishes relationships between the concentration of a compound and the observed ecological effects using dose-response models (Ritz, 2010). Nevertheless, such relationships cannot always be established from experimental data. For example, mesocosm experiments are conducted to characterize effects on 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 where fitting dose-response models is problematic (Green, 2016). In such cases there is 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 this 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, 2016). Instead of conducting experiments, toxicity can be also predicted from molecular structures using quantitative structure-activity relationships (QSAR) (Kühne et al., 2013; Pradeep et al., 2016).

Exposure Assessment for freshwaters aims to characterise the probability of an 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). To calculate PECs these models 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 small streams of 1 meter width and 30 cm depth (Erlacher and Wang, 2011). Such a stream width corresponds to a catchment size of 7 km² [ref to small streams supplement](#). Nevertheless, recent research showed that FOCUS models fail predict measured field concentrations of pesticides (Knäbel et al., 2012; Knäbel et al., 2014).

1.3 STATISTICAL ECOTOXICOLOGY

1.4 ENVIRONMENTAL MONITORING

1.5 OBJECTIVES AND OUTLINE OF THE THESIS

This thesis pursues three objectives:

- i to scrutinize new methods in statistical ecotoxicology,
- ii explore available monitoring data and
- iii provide tools to deal with data in ERA

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 (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?

ERA focuses with its predictions on small streams. Chapter 2 focuses on realised environmental concentrations. Specific goals were:

- Compile all available monitoring data on pesticides in Germany, with a focus on small streams.
- Derive thresholds for agricultural use and catchment size.
- Assess the current pollution in german streams.

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 names
- link them to other datasets
- search properties and identifiers

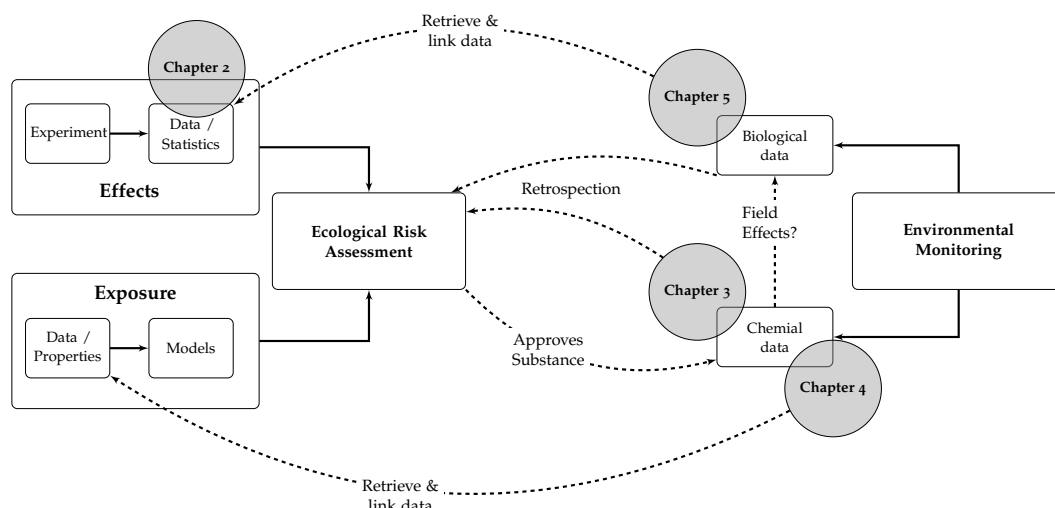


Figure 1.1: Conceptual overview on data in ecological risk assessment and environmental monitoring, as well as parts addressed by this thesis.

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LARGE SCALE RISKS FROM PESTICIDES IN SMALL STREAMS

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2.1 ABSTRACT

2.2 REFERENCES

DISCUSSION

3.1 STATISTICAL ECOTOXICOLOGY

3.2 LEVERAGING MONITORING DATA FOR ECOLOGICAL RISK ASSESSMENT

3.3 CHALLENGES TO UTILIZE 'BIG DATA' IN ERA

3.4 CONCLUSIONS AND OUTLOOK

3.5 REFERENCES

