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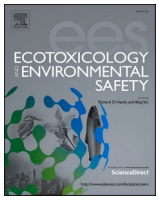

Heterogeneity in biological assemblages and exposure in chemical risk assessment: Exploring capabilities and challenges in methodology with two landscape-scale case studies

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ABSTRACT

Chemical exposure concentrations and the composition of ecological receptors (e.g., species) vary in space and time, resulting in landscape-scale (e.g. catchment) heterogeneity. Current regulatory, prospective chemical risk assessment frameworks do not directly address this heterogeneity because they assume that reasonably worst-case chemical exposure concentrations co-occur (spatially and temporally) with biological species that are the most sensitive to the chemical's toxicity. Whilst current approaches may parameterise fate models with site-specific data and aim to be protective, a more precise understanding of when and where chemical exposure and species sensitivity co-occur enables risk assessments to be better tailored and applied mitigation more efficient. We use two aquatic case studies covering different spatial and temporal resolution to explore how geo-referenced data and spatial tools might be used to account for landscape heterogeneity of chemical exposure and ecological assemblages in prospective risk assessment. Each case study followed a stepwise approach: i) estimate and establish spatial chemical exposure distributions using local environmental information and environmental fate models; ii) derive toxicity thresholds for different taxonomic groups and determine geo-referenced distributions of exposure-toxicity ratios (i.e., potential risk); iii) overlay risk data with the ecological status of biomonitoring sites to determine if relationships exist. We focus on demonstrating whether the integration of relevant data and potential approaches is feasible rather than making comprehensive and refined risk assessments of specific chemicals. The case studies indicate that geo-referenced predicted environmental concentration estimations can be achieved with available data, models and tools but establishing the distribution of species assemblages is reliant on the availability of a few sources of biomonitoring data and tools. Linking large sets of geo-referenced exposure and biomonitoring data is feasible but assessment of risk will often be limited by the availability of ecotoxicity data. The studies highlight the important influence that choices for aggregating data and for the selection of statistical metrics have on assessing and interpreting risk at different spatial scales and patterns of distribution within the landscape. Finally, we discuss approaches and development needs that could help to address environmental heterogeneity in chemical risk assessment.

Abbreviations: BOD, biological oxygen demand; BQE, biological quality element; DF, dilution factor; COD, chemical oxygen demand; EC50, Effective concentration required to achieve 50% effect change from the control; ERA, environmental risk assessment; ETR, exposure:toxicity ratio; GIS, geographic information system; NOEC, no observed effect concentration; OSR, oil seed rape; PE, population estimates; PEC, predicted environmental concentration; PPP, Plant Protection Product; RBMP, river basin management plan; RICT, River Invertebrate Classification Tool; TWA, time weighted average; UBA, Umweltbundesamt; GEA, German Environment Agency; UWWTD, Urban Waste Water Treatment Directive; UWWTP, urban waste water treatement plant; WFD, Water Framework Directive.

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1. Introduction

The natural environment consists of a wide range of land and water patches that can vary in their physical and chemical characteristics and in the occurrence and abundance of organisms inhabiting them. This abiotic and biotic heterogeneity occurs at different spatial and temporal scales. Landscape-scale heterogeneity e.g., separable and quantifiable aspects of landscape features such as the flood plains, forests, agricultural fields and urban areas that occur in a river catchment, is one of the key factors, along with emission scenarios, climate and chemical properties, that determine the extent to which organisms are exposed to chemicals emitted into the environment (Sala et al., 2010). Environmental heterogeneity relevant to chemical risk assessment can comprise several factors including: variation in release of chemicals to receiving habitats leading to variation in exposure; variation in the fate and behaviour of chemicals (and behaviour of organisms) within different receiving habitats also leading to variation in exposure; variation in inherent sensitivity of ecological receptors (e.g. species, life stages) between receiving habitats leading to differing magnitudes of toxic effects; variation in the potential for ecological communities to respond to chemical impacts leading to differing extents of recovery (Armitage et al., 2007, Grill et al., 2015, Oldenkamp et al., 2018, Spurgeon et al., 2020, van Leeuwen and Vermeire, 2007). Furthermore, as the spatial and temporal scales increase and landscape-scale heterogeneity is propagated, there is greater scope for occurrence of different exposures and species assemblages resulting in a broader range of potential risk.

Although consideration of the spatial patterns inherent to multi-use, multi-stressed landscapes has raised important questions about how to assess the risks of chemical stressors in the environment, e.g. Dale et al. (2008), current regulatory prospective chemical environmental risk assessment (ERA) schemes do not directly nor fully address environmental heterogeneity. ERA schemes are largely based on comparisons of chemical exposure estimates, derived from emission data and environmental fate models (and occasionally monitoring data), with generic derivations of protective toxicity thresholds for the types of organism assemblages expected to be exposed. In order to achieve high levels of protection these generic frameworks assume that reasonably worst-case chemical exposure concentrations co-occur, spatially and temporally, with species assemblages that are most sensitive to the chemical's toxicity. Whilst this approach aims to be protective, a more precise understanding of when and where exposure and species co-occur enables risk assessments to be better tailored and mitigation made more efficient.

Use of geo-referenced data enables the influences of environmental heterogeneity on chemical risks to be considered. Indeed, some prospective risk assessment approaches have included spatially explicit estimates of chemical exposure concentrations at appropriate spatial and temporal scales derived from exposure modelling (Kooistra et al., 2005; Faggiano et al., 2010; Linkov et al., 2002; Luo and Zhang, 2010; Nause et al., 2021, Oldenkamp, 2018, Price et al., 2010, Pistocchi, 2008, Wannaz et al., 2018). Geographic Information System (GIS) modelling approaches have been combined with ecotoxicity data to predict spatial distributions of risk (Sala and Vighi, 2008; Dabrowski and Balderacchi, 2013; Liu et al., 2013).

Whilst ecological effects assessments do not generally account for geographic (spatially explicit) patterns of species distributions, several research groups have aimed to correlate site-specific chemical exposure and associated ecotoxicological risk with ecological community composition based on matching biomonitoring data (Hatakeyama and Yokoyama, 1997; Liess and Schulz, 1999; Liess and von der Ohe, 2005; Vaj et al., 2011; Malaj et al., 2014; Lemm et al., 2021; Sumudumali and Jayawardana, 2021). However, many of these studies utilise ecological data from field sampling that represent relatively limited spatial scales or numbers of locations.

The spatial and temporal dynamics of individuals and populations have also been modelled, e.g. using agent or individual-based models of focal or indicator species in terrestrial and aquatic environments (Kooistra et al., 2005; Schmolke et al., 2010; Topping et al., 2015). Many of these models provide highly resolved estimates and when combined with dynamic, landscape-scale exposure models, can address the influence of landscape fragmentation on the impact and recovery of populations exposed to chemicals (Dalkvist et al., 2013; Focks et al., 2014; Topping et al., 2019; Ziółkowska et al., 2021). However, such modelling has mostly been applied to a few focal species and relatively small geographical areas, e.g. local landscapes. Application to prospective risk assessment would ideally apply such approaches over larger regional scales (e.g. pan-European) and consider species assemblages.

Although large-scale spatially referenced information, especially on ecological receptors, has not been generally available for use in prospective ERA, the availability of spatially and temporally referenced landscape scale environmental and ecological data is increasing, in part due to the deployment of remote sensing ground, aviation and satellite technology (Ozesmi and Bauer, 2002; Gergel and Turner, 2017), but also via the provision of data from national, regional and global monitoring and biomonitoring programmes such as the IUCN Red List of Threatened Species (Anon, 2021), the European Environment Agency (EEA) Waterbase – Water Quality, which provides information on concentrations of chemicals (Anon, 2021) and EEA Waterbase – Biology, containing biological quality elements (BQEs) (Anon, 2020) for more than 8200 European sites.

In this study, we investigate the capabilities and challenges of combining three available datasets to account for heterogeneity in the prospective risk assessment of chemicals over a large geographic scale, e.g. regional, national: i) geo-referenced predicted exposure concentrations derived from environmental models, ii) geo-referenced ecological status (quality of the structure (biodiversity) of surface water ecosystems) derived from biomonitoring data, iii) ecotoxicity data for the chemicals considered. We were particularly interested to assess whether high or low risk coincided with high or low ecological status (quality of the biological community) (Anon, 2018). We inform discussion by undertaking two focussed case studies to explore and identify issues and needs for further work, but do not make recommendations for regulatory implementation. We focus on demonstrating whether the integration of relevant data and potential approaches is feasible rather than making comprehensive and refined assessments of specific chemicals.

2. Methods

2.1. Assessment strategy

The key aim was to explore and demonstrate how spatially referenced exposure and ecological receptor data could be integrated for a refined prospective assessment of chemical risk, rather than to explicitly quantify risks. Therefore, the case study ERAs should not be interpreted as consisting of best estimates of exposure or effects, but as examples of how spatially referenced exposure and ecological receptor data could be examined together. The general approach followed was i) estimate and establish spatial exposure distributions using two case studies based on different chemicals, emission pathways and spatial/temporal scale of exposure scenarios; ii) derive toxicity thresholds for various taxonomic groups and determine geo-referenced distributions of exposure-toxicity ratios, i.e. potential risk; iii) overlay risk data with the ecological status of Water Framework Directive, WFD, (Anon, 2018) biomonitoring sites to assess trends between predicted chemical exposure and ecological status (Fig. 1).

We demonstrated the approach using case studies that explored the integration of exposure and ecological receptor data based on the exposure of freshwaters to i) a down-the-drain chemical used in domestic cleaning products (anionic surfactant) and ii) three Plant Protection Products (PPPs) (herbicide, insecticide and fungicide) applied to large area production crops (winter wheat, oil-seed rape and barley). These case studies were selected to examine two chemical classes having

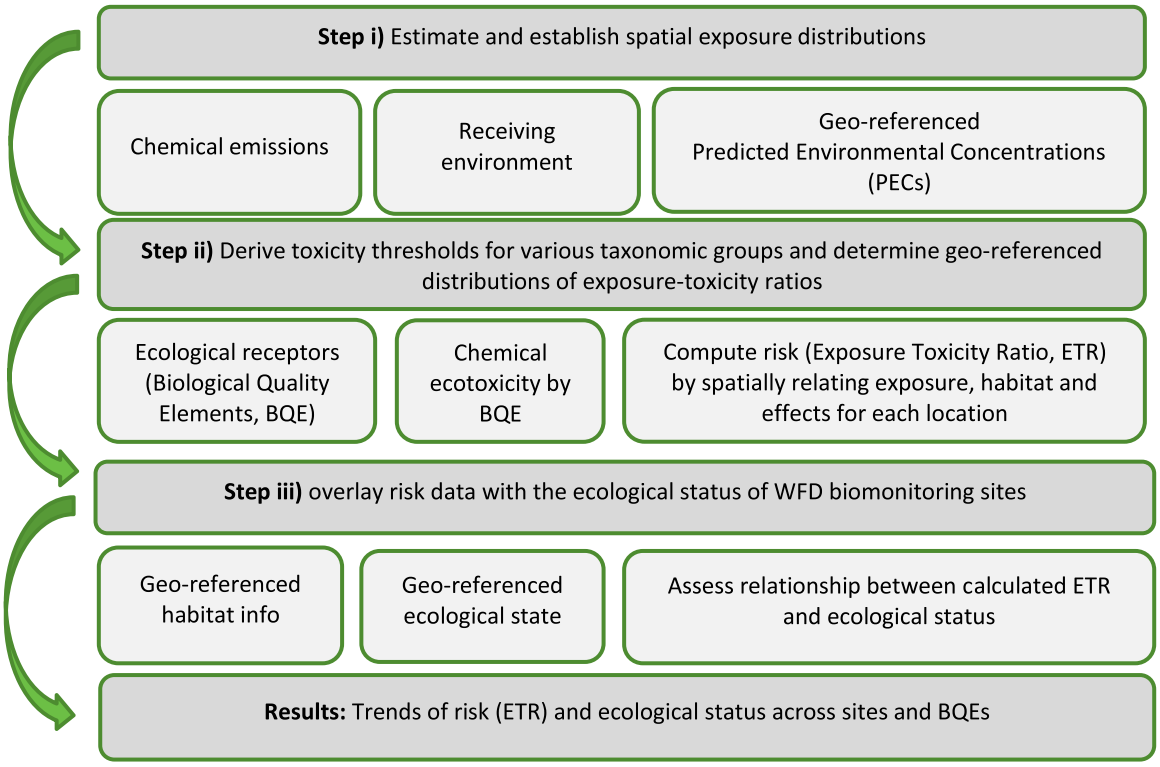

Fig. 1. Overview of assessment strategy steps and associated information utilised to assess trends of risk and ecological status.

different usage and environmental emissions patterns. We also utilised ecological data representing four broad taxonomic groups (WFD biological quality elements, BQE): macroinvertebrates, fish, macrophytes, diatoms. However, the aim of this work was not to determine causal relationships between chemical exposure and ecological effects, as that would have required an eco-epidemiological approach (e.g., Kapo et al., (2008, 2014), Posthuma et al., (2016)). Rather, our main interest was to explore spatially explicit, prospective ERAs.

2.2. Study area

We focused on the German state, Hessen, as a suitable geographic area for demonstrating how to integrate spatial data. Hessen encompasses 21,000 km^2 and contains a population of over 6 million people (300/km^2), mostly located in the southern part of the state which includes the city of Frankfurt (12% of population). There are several large rivers including Main, Lahn, Fulda, Eder and Kinzig. Major land cover includes trees (44%), agriculture (39%) and developed areas (12%), with high yield agriculture located mainly in the lowland area of the south west (Anon, 2021). See Fig. S1 for a map of land covers in Hessen. The study area was chosen primarily due to the availability of high-quality ecological data (WFD biomonitoring data) for aquatic environments in conjunction with detailed hydrologic data to which the ecological sampling data were spatially located. Environmental exposure estimates for PPPs were available for Germany, and it was possible to develop emission and predicted environmental concentrations (PECs) for an anionic surfactant based on available EU-wide data. In principle, a broader, Germany-wide, or even a pan-European, assessment could be made if suitable ecological data were available.

2.3. Ecotoxicology data used for risk estimation

Ecotoxicology data were obtained from public literature sources, including regulatory risk conclusion documents from the European Food Safety Authority (EFSA, 2008; EFSA European Food Safety Authority, 2014a, 2014b). Data were obtianed for organisms broadly representative of the four main WFD BQEs (Table 1).

2.4. Down-the-drain chemicals

2.4.1. Estimation of anionic surfactant exposure concentrations in surface waters

The down-the-drain case study represents an assessment of a widely used substance in home and personal care products with environmental emission into the aquatic habitat via wastewater treatment plant (WWTP) discharges. Surfactant usage occurs in most, if not all, households in Europe, and therefore it was assumed that each WWTP receives a mass of surfactant in influent proportional to the population served, and the concentration of surfactant in this influent is determined by the per capita water use within these households. Locations of contributing WWTPs and receiving stream segments were combined to estimate the spatially explicit mean annual surfactant concentration in receiving waters in Germany. The methodology is summarised in Fig. S2.

We considered aquatic exposure only and there was no assessment of exposure to terrestrial organisms via soil amendment with sewage sludge containing the surfactant. The focus on aquatic exposure was because of limited spatially referenced data on sludge application rates, locations, dates and environmental conditions making estimates of soil exposure highly uncertain within the limitations of this study.

Information describing the geographic location and estimated population served by each WWTP in Germany (n = 3846) was obtained from the EEA Waterbase-UWWTD dataset (Anon, 2017). These data are collected as part of the Urban Waste Water Treatment Directive (UWWTD) addressing the collection, treatment and discharge of urban wastewater. The UWWTD requires discharged wastewater to adhere to specific guidelines for biological and chemical oxygen demand (BOD and COD, respectively) and therefore are assumed to have at least secondary treatment (e.g. activated sludge treatment). Waterbase reported estimated population including commercial and transient populations in addition to residents. Therefore, it is expected that reported population

Table 1
Ecotoxicity data for Surfactant and PPP substances used in the case studies.

	Acute EC50[#] (mg/L)		Chronic NOEC[#] (mg/L)				
Substance	*Daphnia*	Fish	Algae	*Lemna*	*Daphnia*	Fish	*Chir.*
Anionic surfactant[a]	3.5	1.7	2.4	1.2	0.5	0.22	
Acid anilide herbicide[b]	30	4.6	0.0076	0.0071	0.1	1.4	9.8
Pyrethroid insecticide[c]	0.00023	0.000078	0.005 *		0.000002	0.00003	0.00013
Triazole fungicide[d]	2.8	4.4	3.80	0.14	0.01	0.012	2.5

*Endpoint set to water solubility
[#]EC50 (Median effective concentration); NOEC (no observed effect concentration)
[a] Anon (2013)
[b] EFSA European Food Safety Authority (2014a) (2014b)
[c] EFSA (2008)
[d] EFSA European Food Safety Authority (2014a) (2014b)

estimate numbers are equal to or greater than actual population served for the purposes of this study.

An EU-wide average usage of 3 g of surfactant per capita per day (Anon, 2013) was combined with usage of 12 laundry and household care product types containing surfactant for European countries (Euromonitor, 2018) to derive a refined surfactant usage value specifically for Germany of 1463 g yr^{-1} per person (4.0 g day^{-1} per person), i.e., slightly higher than the EU average (Table S1). Following Cavalli et al. (1993) and Hera (2013), we assumed that 99% of surfactant was removed (via biodegradation and sorption to solids) prior to discharge into receiving stream segments. This was a conservative estimate as Freeling et al. (2019), report an average removal of > 99.8% based on a monitoring programme in Germany.

Hydrology information was obtained from the HydroSHEDS dataset (Lehner et al., 2008), including river locations from the HydroRIVERS data layer. These data include medium to large rivers suitable for use with WWTP discharge information (n = 13,877). River flow was accessed from the FLO1K dataset (Barbarossa, 2018), using the 2015 mean annual flow data. The source data are 1-km raster data and therefore multiple 1-km cell values are associated with a single HydroRIVER segment. To estimate a single value for each segment, the median value of all FLO1K cells underneath each HydroRIVER segment was determined and assigned to the segment.

Locations for the Waterbase WWTPs in Germany were geolocated within the GIS using provided coordinates and linked to the closest river (Fig. S3). The HydroRIVERS dataset represents medium and large rivers, but does not include much smaller rivers and streams, therefore if a WWTP was further than 500 m from a HydroRIVERS segment (n = 1263), we assumed the receiving water body was not present in the HydroRIVERS dataset and these WWTPs were excluded from further processing, leaving 2583 WWTPs for analysis. Note that in our analysis the PECs estimated at each WWTP discharge (i.e., the mixing zone) do not account for upstream loadings of chemical. Therefore, while the smaller WWTPs/tributaries may not all be accounted for, their absence would also not affect the PECs for the larger WWTP/rivers. The dilution factors for the rivers included in our Hessen case studies ranged down to 1.6.

A dilution factor (DF) was estimated for each river segment with an associated WWTP discharge location using:

$$DF = (\text{River Flow} + \text{WWTP Flow}) / (\text{WWTP Flow})$$

WWTP flow was based on a constant per capita water use of 46.3 m^3 yr^{-1} (Anon, 2017) and population served by each WWTP (Population Equivalents reported in WaterBase). The minimum DF is 1.0, indicating effluent discharge to a river with no flow (i.e., a dry river).

The 929 HydroRIVERS segments in Hessen have an average length of 5.4 km with a longest stretch of 29 km. In many cases several WWTPs were associated with a single river segment. To associate a WWTP with only the immediate downstream portion of a HydroRIVERS segment, WWTPs (n = 257) were 'snapped' to the closest location on a river segment, and river segments were split at these locations. This resulted in river segments being split at WWTP locations with river PECs specific to the most immediate upstream WWTP (Fig. 2). Each WWTP on the same original river segment discharged to the same river flow. The spatial processing is further described in the SI (Fig. S2, Sections 1.2.1, 1.2.2).

Surfactant PECs were calculated for each river segment with an associated WWTP discharge location (i.e., the mixing zone for WWTP effluent) using:

$$Conc_{influent} = \text{per capita surfactant usage / per capita water usage.}$$

$$Conc_{effluent} = Conc_{influent} * (1 - Removal_{surfactant}) \quad PEC = Conc_{effluent} / DF$$

WWTP locations, connected populations and associated rivers are presented in Fig. 3A. The level of spatial data available enabled integration of emissions from individual WWTPs with receiving water body flow rates and site-specific exposure estimates. Complete mixing of surfactant in receiving water was assumed and dilution factors (and therefore exposure concentrations) were calculated as a representative annual value based on mean, annual average, river flows.

2.4.2. Calculation of surfactant ETR values

Surfactant PECs were converted to exposure:toxicity ratios (ETRs) using available ecotoxicity data for the four main WFD BQEs: macroinvertebrates, fish, macrophytes, diatoms (Table 1). Whilst the species selected to represent the BQEs do not provide a detailed distribution of the sensitivity of the species present at each site, they are generally considered to be sensitive to chemical toxicity within their broad taxonomic groups. A more refined approach utilizing the ecotoxicological sensitivity of each of the species found at each biomonitoring location would have provided a distribution of risk values that better reflected the range in responses of biological species likely to be exposed. However, such an approach, which also applied to the PPP case study, was not achievable because of the availability of relatively few species-specific ecotoxicity data.

Both acute (fish and *Daphnia*) and chronic (fish, *Daphnia, Lemna*, algae) ETRs were calculated using annual mean PEC estimates. Therefore, for the purposes of our analysis, no account of temporal variation is made for the surfactant case study.

2.5. Plant protection products

2.5.1. Estimation of PPP predicted environmental concentrations in surface waters

The PPP case study incorporates several refinements from the down-the-drain case study. In this case study, multiple substances with different modes of action are included, the spatial scale is more highly resolved, and the temporal dimension is included. The methodology is summarised in Fig. S4.

For this study, three widely cultivated crops were selected to use as the target application of the PPPs: winter wheat (*Triticum aestivum*),

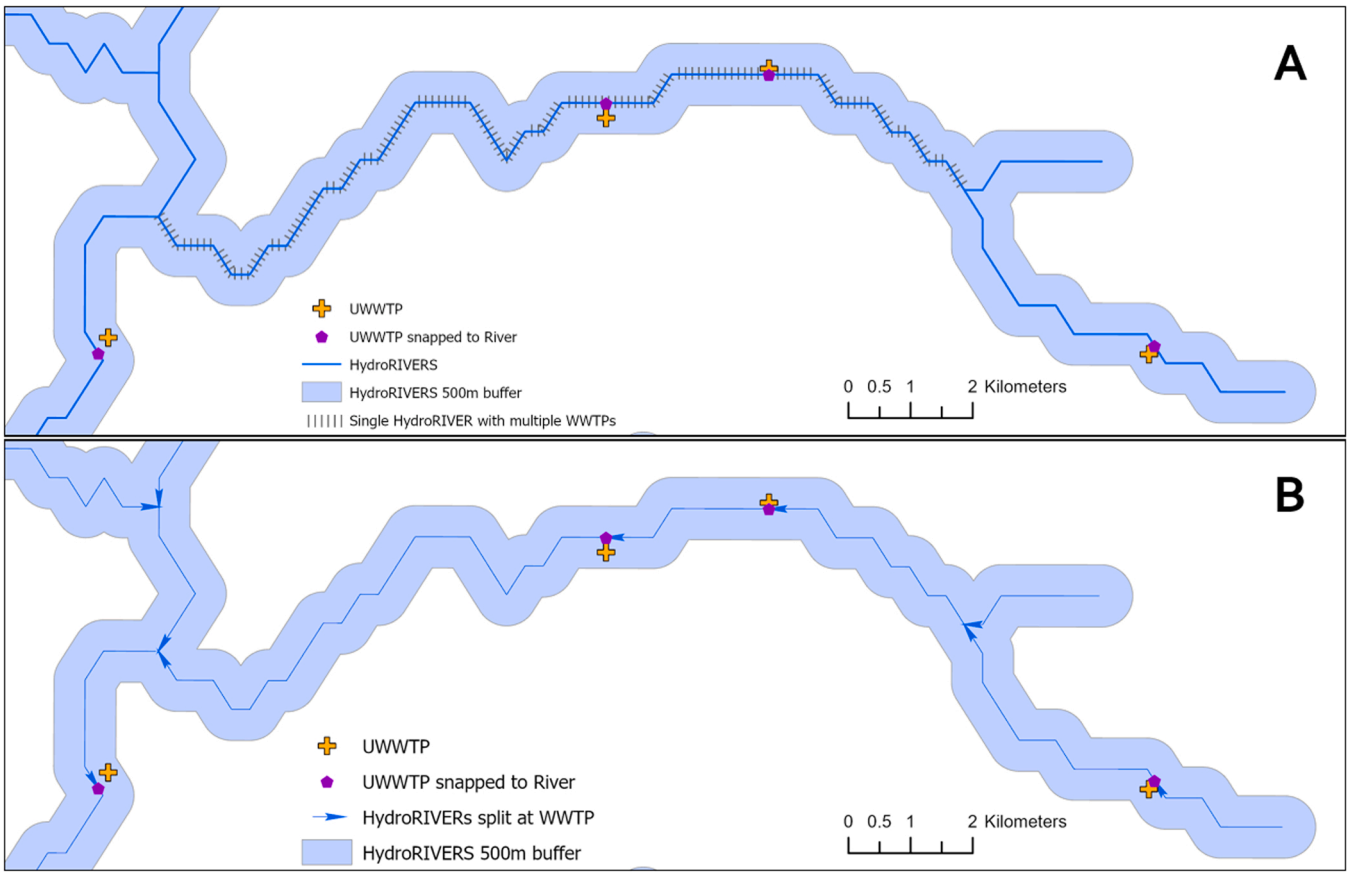

Fig. 2. Example of 500 m distance to rivers and multiple WWTPs associated with a single river segment (grey hatched segment) (A) and resulting split river segments for each WWTP (B) [UWWTP = urban waste water treatment plant].

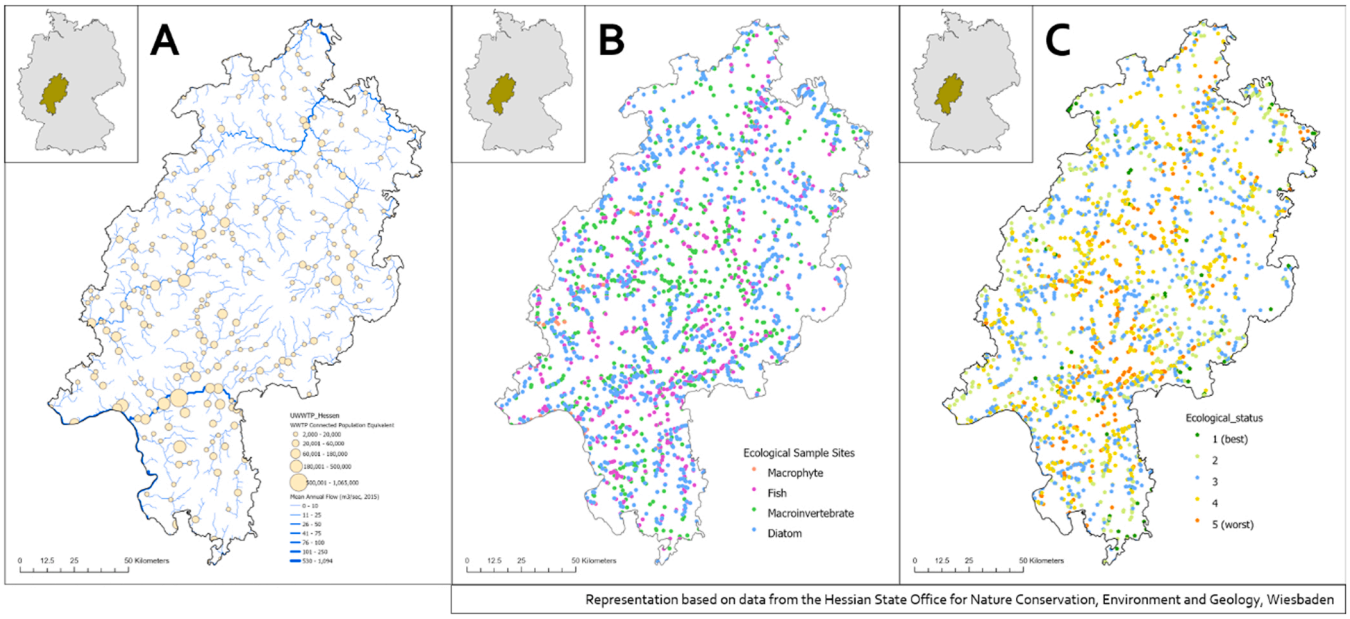

Fig. 3. A) Spatial distribution of WWTPs showing connected population (equivalents) and HydroSHEDS river network with FLO1K mean annual flow (2015), B) Location of 3970 biomonitoring sites in Hessen showing BQE (fish, macroinvertebrates, diatoms, and macrophytes) and C) diversity of ecological status values (note that a single location may represent more than one BQE and/or ecological status) [UWWTP = urban waste water treatment plant; WWTP = waste water treatment plant].

winter barley (*Hordeum vulgare*) and winter oilseed rape (*Brassica napus*) (Fig. S5 shows the spatial distribution of these crops within Hessen). A PPP was selected for each category of fungicide, insecticide and herbicide that was representative of widely used active ingredients in their class: a triazole fungicide, a pyrethroid insecticide, and an acid anilide herbicide. Within our study area, 134,183 applications (73461 winter wheat, 14144 winter barley, 46578 winter oilseed rape) were simulated on 81,822 fields over a 1-year period. Of the fields, 42% received a single PPP, 52% had two PPPs, and 6% received all three PPPs. Further details on applications are available in Tables S2 and S3 in the SI.

Environmental exposure data were obtained from the SYNOPS model (Gutsche and Roßberg, 1997; Gutsche and Strassemeyer, 2007; Strassemeyer et al., 2017), a Germany-wide field-scale model which utilises PPP usage survey data to associate PPP applications to individual fields. PPP applications schemes were generated from the German wide reference farm network 'Netzwerk Vergleichbetriebe Pflanzenschutz' (Dachbrodt-Saaydeh et al., 2021; Freier et al., 2016). Treated fields were randomly selected within soil/climate regions linked to surveyed PPP data (Roßberg et al., 2007) and controlled to match county crop statistics (i.e., if according to the statistics in a certain county, 10% of the agricultural area is maize, only 10% of the field area in the county will be assigned to maize). Timing of PPP applications on crops were taken from the survey data. The weather data came from individual station information from Deutsche Wetterdienst for the 2015/2016 growing season. Each field was paired with the nearest weather station. PPP no-spray buffer zones were implemented within the SYNOPS exposure calculation. PPP exposure modelling was performed at a daily time step using regulatory models to simulate drift, drainage and runoff/erosion. These regulatory models utilize the physical/chemical properties of the PPP (e.g., terrestrial half-life, aquatic-half-life, sorption properties and potential for leaching) coupled with environmental properties (e.g., temperature, rainfall, wind speed, soil properties and field slope) to parameterize empirical equations describing the fate and transport of chemicals via spray drift (Drift Calculator, https://esdac.jrc.ec.europa.eu/projects/drift-calculator), in soil (PRZM_SW model, https://esdac.jrc.ec.europa.eu/projects/przmsw) and water (TOXSWA model, https://esdac.jrc.ec.europa.eu/projects/toxswa) on a daily basis (Anon, 2001). Estimated daily concentrations in field margins, 1- and 7-day time weighted average concentrations in surface water and soil were summarised within the model and stored as the annual 90th percentile of daily PECs associated with the field for that year. While SYNOPS also includes the calculation of risk indices, the model output also represents a suitable realistic prospective scenario for exposure estimation.

2.5.2. Calculation of PPP ETRs in surface waters

A risk index (ETR) for the same broad BQEs as used in the surfactant study was calculated for each field-level PPP using endpoints from Table 1. The sum of risk for all PPPs applied to each field was calculated to account for applications of more than one PPP to a single field in our risk estimation. Acute (daily) risk was calculated for fish and *Daphnia*, while chronic risk (7-day time weighted average (TWA)) was calculated for algae, *Daphnia*, fish, *Lemna* and *Chironomus*.

To match the spatial resolution of the SYNOPS field-level exposure data, as well as containing a direct link to the ecological sampling data, a detailed dataset of streams (Gewässerstruktur aller hessischen Fließgewässerder)[1] was obtained from Hessen State Office for Nature Conservation, Environment and Geology, Wiesbaden. This dataset contained over 77,757 segments (typically 100 m or 500 m in length) and associated attributes within Hessen (Fig. S6). Each agricultural field was spatially linked to the closest surface water segment within 300 m (the maximum distance SYNOPS used for runoff/erosion) within the GIS. If a field was further than 300 m, it was not included in the analysis of surface water risk. A field was associated with only the closest surface water segment, even if multiple segments were within 300 m. For each surface water segment within 300 m of a field (n = 53,624), risk indices for all treated fields were summed for each category (acute & chronic for each BQE) resulting in 18,142 stream segments with ETR values.

To account for hydrologic transport and accumulation, upstream segments on the mainstem comprising a total of 1000 m were identified for each surface water segment (using available attributes within the hydrology data), and the sum of the individual risk indices for all upstream segments was calculated for each BQE. Distances of 500 m and 2500 m were also calculated for evaluation but not presented here. The 1000 m distance was selected after consideration of ten river segments upstream (i.e., 10 ×100 m). The longer 2500 m distance would likely incur greater uncertainty in exposure since degradation and aquatic fate losses are not accounted for. It was judged that it could take approximately 1 h for river water to travel 1000 m at an assumed 0.28 m/s. The 10 upstream segments move downstream as a "sliding window" (1–10, 2–11, 3–12, etc.). Additional information is included in the SI.

The detailed hydrology dataset links individual segments (e.g., 100 m) of a river reach together in order, it does not allow assessment of additional exposure from incoming tributaries/confluences. However, risks in tributaries are assessed as individual river stretches based on their own upstream contribution from treated fields.

2.6. Biomonitoring locations in Hessen

Water Framework Directive ecological data were obtained from Federal State of Hessen, Hessen State Office for Nature Conservation, Environment and Geology, Wiesbaden, Germany (Biologie der Fliessgewässer[2]) containing 3970 unique sampling locations in Hessen which were mapped in the GIS using the provided coordinates. Each biomonitoring location had one or more sample dates between 2004 and 2017 along with the associated observations. Where there were more than one sample per biomonitoring location, we used the most recent sampling event to determine ecological status. Attributes included location, abundance, evaluation of ecological state, as well as other scoring values. Data included observed information on ecological type including fish, macroinvertebrates, diatoms, and macrophytes (i.e., BQEs) (Fig. 3B). Of particular interest was the ranking of ecological status for each site (Fig. 3C). A rough visual assessment suggested no clear spatial aggregation of ecological status in Hessen.

We excluded highly modified water bodies because they are classified in terms of their potential for reaching one of the ecological classes whereas their current observed status may be lower. Non-highly modified streams are given actual ecological status classification. This excluded approximately 100 sites which are clustered in a heavily agricultural region.

In order to relate our calculated exposure/risk values with the measured ecological sampling information, i.e., taxonomic presence and abundance data, each biomonitoring location was associated with the nearest hydrology segment using GIS functionality. For the down-the-drain case study, biomonitoring sites within 250 m of the river segments downstream of a WWTP were linked (see SI for details) so that surfactant PEC and ecotoxicity values could be combined to calculate site-specific ETR values for the relevant BQEs (Fig. 4A). This process resulted in 800 biomonitoring sites linked to rivers with surfactant PECs. For the PPP case study, a more detailed river network was used to complement the refined spatial nature of the agricultural fields. Over 25,000 agricultural fields within 300 m had the potential to influence surface water. Biomonitoring sites within 300 m of the detailed stream network were spatially selected (n = 3815) and associated with the closest stream segment (Fig. 4B).

[1] https://www.hlnug.de/themen/wasser/fliessgewaesser/fliessgewaesser-struktur

[2] Biologie der Fließgewässer at https://www.hlnug.de/themen/wasser/fliessgewaesser/fliessgewaesser-biologie

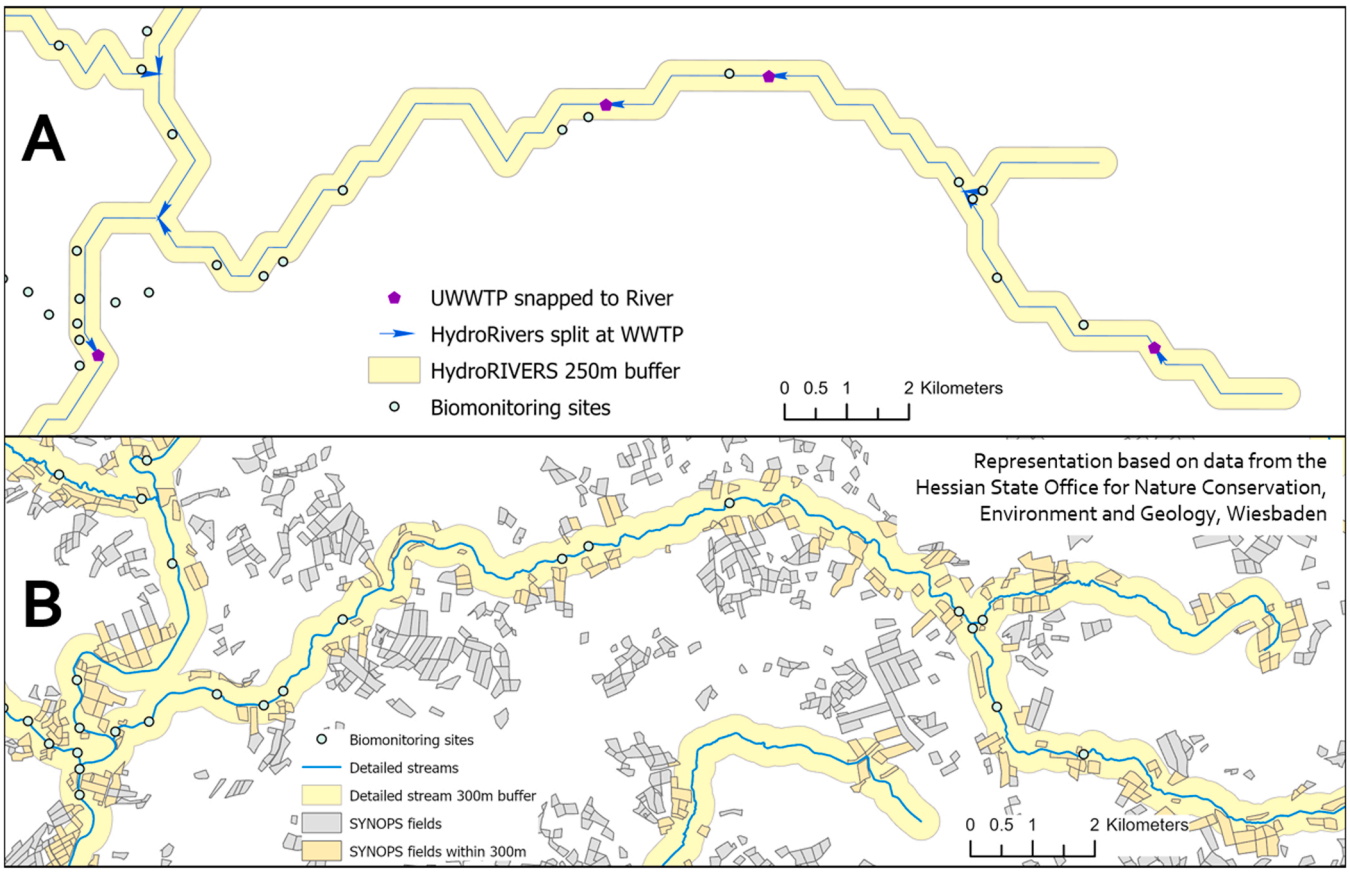

Fig. 4. Example of biomonitoring sites linked to river segments for WWTPs in surfactant case study (A) and SYNOPS fields in the PPP case study (B) [UWWTP = urban waste water treatment plant].

2.7. Comparison of ETR values with ecological data

Our interest was in the methodology for generating prospective risk assessments rather than establishing retrospective trends in chemical exposure and ecological status over time. Once ETR values were spatially linked to the river/stream dataset we compared them to the ecological status (Anon, 2018) of approximately 4000 WFD biomonitoring sites in Hessen (based on data for fish, diatoms, macrophytes and macroinvertebrates). Values for ecological status range from 1 (best ecological status) to 5 (worst ecological status).

For a single BQE at a location, more than one sampling event/date may be reported. Comparing some biomonitoring data to ETRs from different individual years can introduce uncertainty due to temporal variation in species occurrence and abundance. Nevertheless, as a demonstration of our assessment approach we assumed the exposure data would be representative of typical use patterns and used the most recent ecological status class where a temporal range occurred.

For a single location, more than one BQE could be reported, each of which has a BQE-specific ecological status. We develop an analysis which addressed three "levels" of ecological resolution for our assessment.

Level 1 –The "Best" ecological status of all BQEs sampled at a site (i.e., lowest ecological status value) was compared to the ETR of highest (maximum) risk across all BQEs (chronic & acute separately). The comparison includes all BQE types in a single analysis. Comparing the highest ecological status with the highest risk provides a conservative approach to identifying risks to relatively unimpacted sites, i.e., with ecological status class 1 or 2.

Level 2 – Ecological status at a site was compared to the ETR of highest (maximum) risk across all BQEs (chronic & acute separately). The comparison includes separate analyses for each BQE type and represents a more refined approach than Level 1 whilst keeping a conservative (worst case) metric for risk.

Level 3 – Ecological status at a site was compared to the most taxonomically relevant ETR (chronic & acute separately). The comparison includes separate analyses for each BQE type. Comparing ecological status and risk derived from the same BQE represents the highest level of resolution and the most scientifically relevant of the three approaches.

3. Results

3.1. Down-the-drain chemicals

3.1.1. Predicted environmental concentrations (PECs)

Surfactant PECs were estimated at each WWTP location in Germany located within 500 m to the river network, resulting in 2583 location-specific concentrations in this 'mixing zone' using mean annual river flow. WWTP population served (uwwLoadEnteringWWTP) ranged from 532 to 1.75 million population equivalents, with a median value of 10,803. Per capita water use was constant at 127 L d^{-1}. River flows (2015 annual average) ranged from 0.01 to 1590 m^3 sec^{-1} with a median value of 1.03 m^3 sec^{-1}. Dilution factors ranged from 1.1 to more than 300,000, with a median value of 72.4. Estimated mean annual surfactant concentrations ranged from 9.5×10^{-7} to 2.9×10^{-1} mg L^{-1}, with a median value of 4.4×10^{-3} mg L^{-1}.

For Hessen, WWTP population served ranged from 2000 to 1.06 million population equivalents, with a median value of 9760. River flows (2015 annual average) ranged from 0.04 to 1093 m^3 sec^{-1} with a median value of 0.79 m^3 sec^{-1}. Dilution factors range from 1.6 to more than 151,000, with a median value of 56.0. Estimated mean annual surfactant concentrations ranged from 2.1×10^{-6} to 2.0×10^{-1} mg L^{-1}, with a median value of 5.6×10^{-3} mg L^{-1}. See corresponding

figures in SI for charts and maps of these results (S8-S11).

3.1.1.1. PEC comparison to published data. During the course of our analysis, data were published reporting surfactant concentrations at 33 WWTPs across Germany (Freeling et al., 2019). We worked with the German Environment Agency (Umweltbundesamt, UBA) to compare their measured results to those predicted using our methodology. To maintain confidentiality, specific information about WWTPs could not be divulged by UBA, and therefore UBA performed the comparison analysis based on the full dataset of 2583 surfactant PECs that we provided.

In order to identify the 33 WWTP with measurements in the UBA data with the 2583 predictions, the WWTP name and capacity was used. Twenty two of the 33 sites were clearly identified and three other sites were excluded due to release into large lakes. The remaining 8 UBA sites were not readily identified in our data, however PECs were estimated using our estimate of the constant effluent concentration (3.16×10^{-1} mg L^{-1}) and measured removal and flow values from Freeling et al. (2019). The highest concentration measured directly in the 33 wastewater effluent samples was 4.74×10^{-2} mg L^{-1}.

Overall, our river concentrations consistently overpredicted the UBA concentrations based on a regression slope of 0.85 and R-square of 0.94. Concentrations were generally overpredicted by slightly more than an order of magnitude and are therefore conservative.[3] The overprediction is likely related to the net balance between lower WWTP removal rates that we used (99% compared to >99.8% UBA, almost an order of magnitude difference in mass remaining in the effluent) counterbalanced by using annual mean river flow conditions compared to low flow conditions in the UBA results.

3.1.2. Surface water ETR (risk)

A total of 717 of the 3970 biomonitoring sites were associated with the 257 river segments having a WWTP within 500 m, and a BQE-specific ETR was calculated based on the ecotoxicity data from Table 1. The resulting risk values were examined in relation to the ecological status of each BQE at that biomonitoring site (Fig. 5). Additional chronic risk maps for the remaining BQEs, as well as acute risk maps are available in the SI. The risk maps did not indicate any obvious spatial trends or hot spots within Hessen.

3.1.3. Comparison of ETRs and ecological status

Data were grouped by BQE and sorted by ecological status for examination of risk distributions and visualisation (Fig. 6). Three levels of association were performed for both acute and chronic ETRs. We present only chronic Level 3 comparisons here, while the remaining results, including risk maps, are available in the SI (Figs. S8-S22). Chronic ETRs should be most relevant to the assessment of the down the drain chemical since it has a continuous exposure profile.

Chronic risks to fish and macroinvertebrates were generally higher than to macrophytes and algae due to greater sensitivity to surfactants (Table 1). However, there were no trends in surfactant acute or chronic ETR values and ecological status indicating that ecological status was not primarily influenced by exposure to surfactant present in emissions from WWTP (Fig. 6). With minor differences, Level 1 and 2 analyses indicate similar ETR values whereas Level 3 analyses tend to indicate lower ETR values than comparable Level 1 and 2 values. Nevertheless, all Levels indicate similar trends across the range of ecological status classes. These results can also be used to assess what proportion of sites with high ecological status are at risk. In this case, the proportion of BQE-specific ecological class sites at risk (ETR >1) is zero for all taxa and all ecological classes. This outcome is consistent with existing surfactant risk assessments (Hera, 2013, Van de Plassche et al., 1997).

[3] Results of the comparison study are available from the corresponding author.

3.2. Plant protection products

3.2.1. Predicted environmental concentrations (PECs)

For the PPP case study, surface water PECs were generated at the field-level for the herbicide, insecticide and fungicide applied to that crop (i.e., winter wheat, winter barley or winter oil seed rape (OSR)) (Figs. S23 to S25). Prior to combining into a single field-level risk value, the PPP-specific PECs can be reported based on the crop to which it was applied. Figs. S23 through S25 in the SI show the distribution of aquatic PECs in relation to the chronic and acute ecotoxicological endpoints for insecticide, herbicide and fungicide.

The modelled PPP PECs could not be compared to measured data because SYNOPS output does not reflect an actual point in time (from which measurements could be made and compared). SYNOPS PECS are based on applying historic PPP usage data to the population of all agricultural fields selected in a stratified random approach (described in Nause et al., 2021 for sugarbeets). However, the underlying pesticide fate models used within SYNOPS (Strassemeyer et al., 2017) are also used by EFSA for risk assessment purposes (Anon, 2001).

3.2.2. Surface water ETR (risk)

PPP ETRs were estimated for each stream segment within 300 m of an agricultural field that had one of the three PPPs applied to winter wheat, barley and OSR (n = 25,523 fields). A total of 3731 biological sampling sites were located 1000 m downstream of at least one treated field. A BQE-specific ETR was calculated based on the ecotoxicology data from Table 1 and mapped in Fig. 7A. The resulting risk values were examined in relation to the ecological status of each BQE at that biomonitoring site (Fig. 7B). Additional chronic risk maps for the remaining BQEs, as well as acute risk maps are available in the SI (Figs. S26-S33). The risk maps did not indicate any obvious spatial trends or hot spots within Hessen.

3.2.3. Comparison of ETRs and ecological status for BQEs

Data were grouped by BQE and sorted by ecological status for examination of risk distributions and visualisation of possible trends (Fig. 8). Three levels of association were performed for both acute and chronic ETRs. Unlike the down-the-drain assessment, acute and chronic ETRs are relevant for PPP assessment because exposure can be short, i.e., < few days. We present only chronic Level 3 comparisons here, while the remaining results figures are available in the SI (Figs. S8-S22).

Risks to macroinvertebrates and fish were generally higher than to macrophytes and algae indicating that, in this case with just three different types of active ingredient, there was relatively greater influence from the insecticide than from the fungicide and herbicide. Although exposure to the insecticide was lower than that to the fungicide and herbicide, the inherent toxicity of the insecticide is relatively high and drives risk. However, there were no trends in PPP acute or chronic maximum ETR values and ecological status indicating that ecological status was not primarilly influenced by exposure to the three PPP chemicals. As with the surfactant case study, Level 1 and 2 analyses indicated similar ETR values whereas level 3 analyses tended to indicate lower ETR values than comparable Level 1 and 2 values (Figs. S28 to S33). Nevertheless, all Levels indicated similar trends across the range of ecological status classes. There was also no suggestion of any geographic distribution of high or low risk. The results can also be used to indicate the proportion of BQE-specific ecological class sites at risk (ETR >1). In this case, 6.5% of all sites have chronic ETR> 1% and 6.4% Class 1 & 2 sites have chronic ETR > 1; no site has acute ETR > 1. The proportion of sites at chronic risk is low and Class 1 & 2 sites are no more or no less at risk than Class 3 & 4 & 5 sites, i.e., there is no correlation of sites at high or low ecological status with ETR values > 1.

4. Discussion

GIS-based ERA can better relate to landscape scale targeted

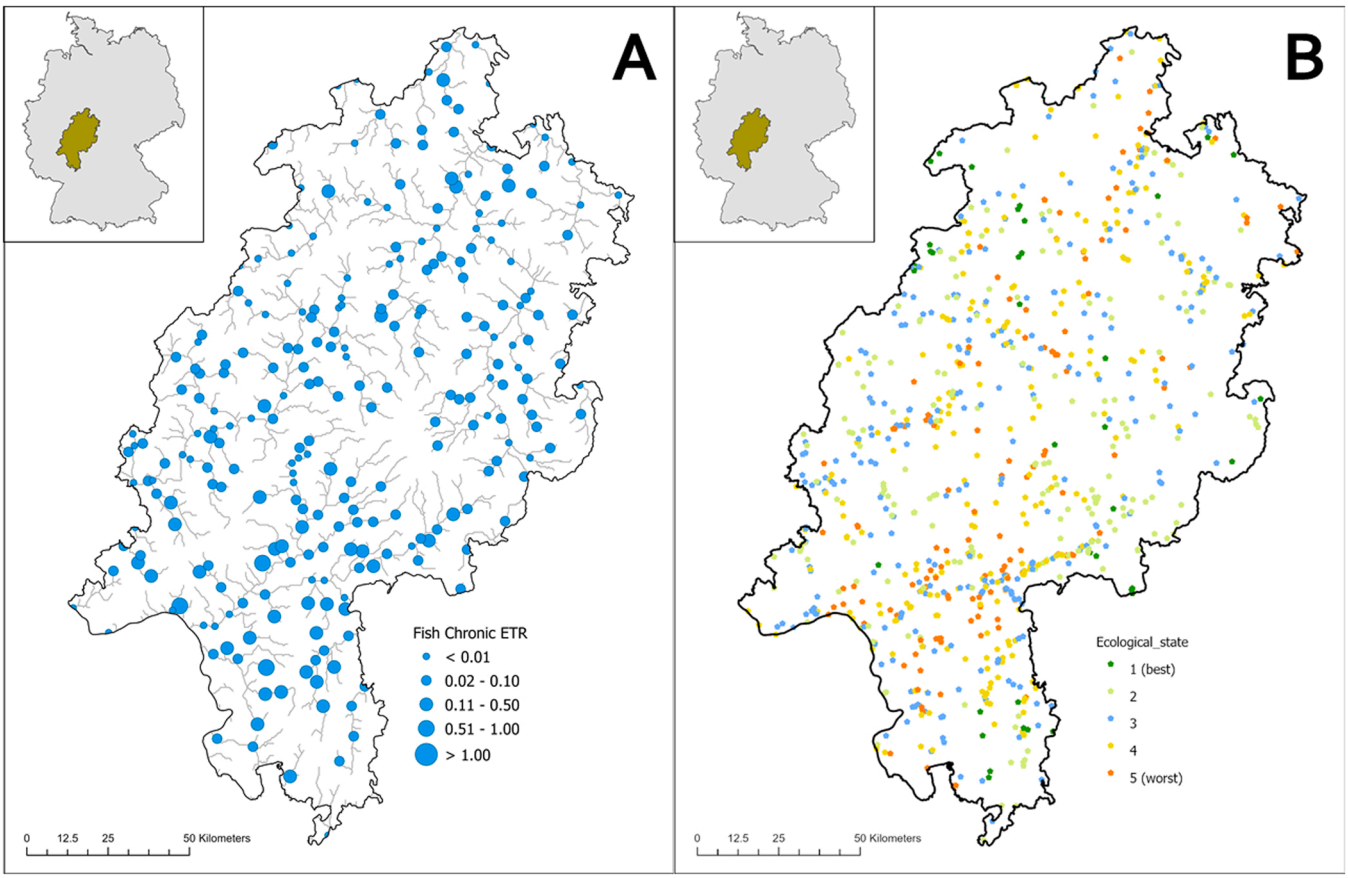

Fig. 5. Spatial distribution of surfactant chronic risk values for fish (A) and fish ecological status of biomonitoring locations (B) [ETR = exposure:toxicity ratio].

environmental management objectives than can current chemical ERA frameworks (e.g. EU REACH regulation, Pesticide Regulation No 1107/2009) that use generic scenarios and assumptions of species presence, because it provides assessments tailored to local landscape/watershed abiotic characteristics and accounts for ecological heterogeneity. The two case studies developed here demonstrate the feasibility of i) deriving large scale (i.e. 21,000 km^2) spatially explicit exposure concentrations for disparate chemicals and emission scenarios, i.e. PPP chemicals and chemicals disposed down the drain, ii) converting location-specific PECs to a range of risk indices representative of several broad taxonomic groups and iii) comparing these indices over a large geographic area e.g. > 250 locations for the surfactant study and > 3700 locations for the PPP study, to matched site-specific ecological status to determine any geo-spatial trends or location-specific "hot spots". The approach presented was intentionally made to be applicable across the EU i.e., national or pan-European, and at high levels of spatial resolution.

The aim of this work focused on demonstrating the potential approaches and challenges in integrating relevant geo-spatial data rather than making comprehensive and refined assessments of specific chemicals. However, the approach exemplified in our prospective case studies could be used to identify discontinuous levels of risk across broad geographical areas, whether the distribution of high or low risk coincides with high or low ecological status or to focus on the impact of chemicals on specific lotic systems. Whilst our case studies did not consider any additional ecotoxicological risks from other chemicals co-occurring with the chemicals selected, the assessment approach could be extended to multiple chemicals using assessment schemes developed for assessing mixture toxicity.

Identifying a trend where poor ecological status tends to coincide with high exposure or risk does not necessarilly indicate causality because of other (unknown) influencing factors including prior exposure to the same or other chemicals. Whilst our case studies did not find such relationships, they could indicate a need for further assessment and consideration of local mitigation where necessary. It follows that GIS-based risk assessment would be particularly relevant for chemicals with emission profiles that lead to variable spatial exposure in the environment, e.g. PPPs. Such assessments could be useful input to the implementation of Water Framework Directive (WFD) river basin management plans (RBMPs) as well as providing higher tier refinements for prospective risk assessments.

4.1. *Landscape-scale exposure estimation*

Our approach to deriving surfactant exposure concentrations was generally consistent with other assessments of chemicals used in consumer products (Price et al., 2010; Keller et al., 2014; Wannaz et al., 2018). In order to make a large-scale, spatially explicit but relatively simplistic assessment of surfactant exposure, we used non-varying values for national average surfactant use, potable water usage and removal of surfactant in all WWTPs. This resulted in effluent surfactant concentrations being the same for all WWTPs. We assumed complete mixing of effluent discharges and no upstream contributions of surfactant mass. It was considered that the upstream contribution of surfactant mass would not be significant given the short aquatic half-life of the surfactant being modelled, i.e. 3 h (Anon, 2013). We also did not account for temporal variation in dilution, likely to be the dominant factor influencing exposure to surfactant over an annual cycle. Temporally-referenced flow data are available and can be purchased (e.g. Low flows 2000 (Young et al., 2003)) or are freely available but require extensive processing for this use (FLO1K (Barbarossa et al., 2018)). Temporal variation in exposure of the surfactant was not

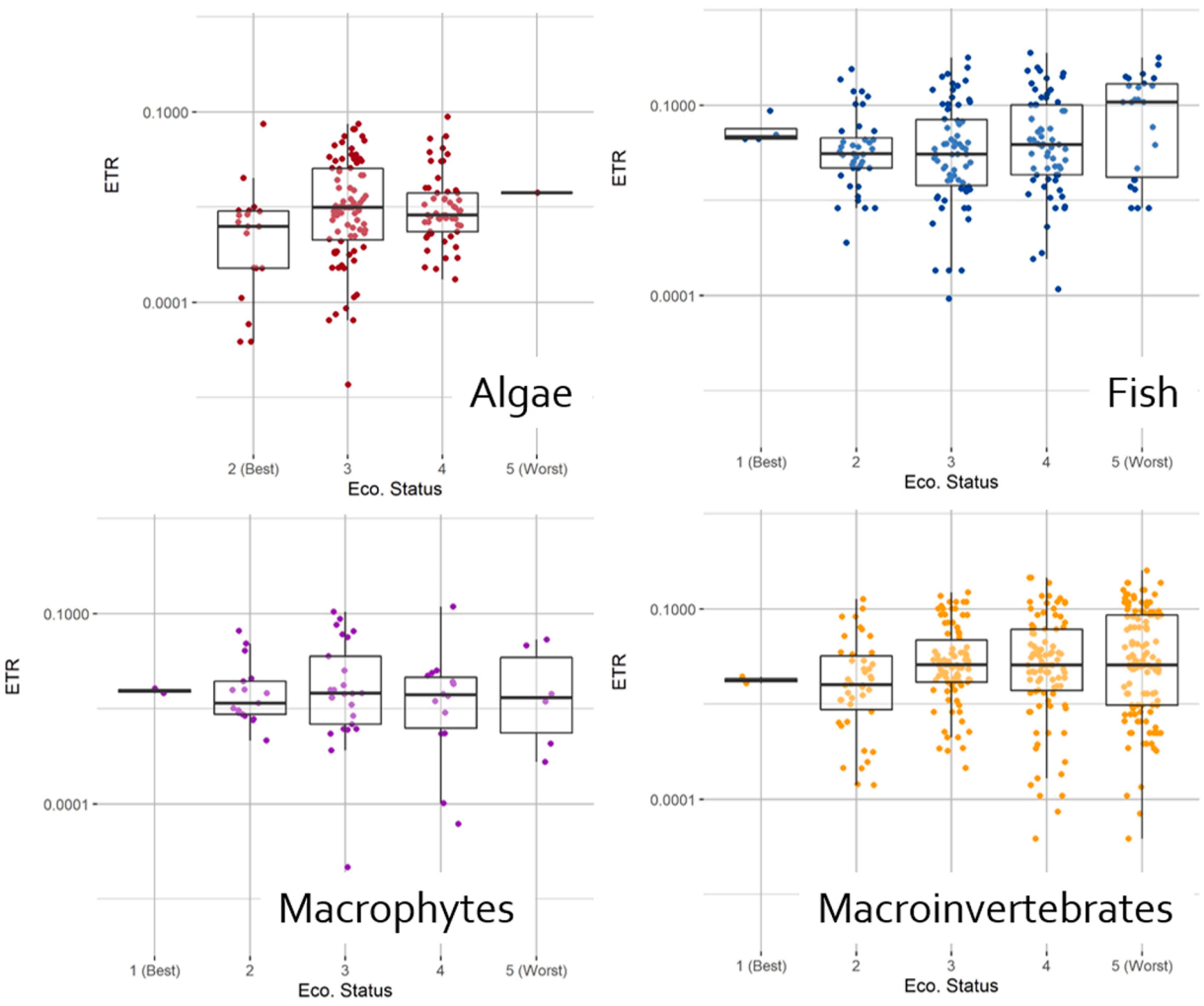

Fig. 6. Boxplots of surfactant chronic ETR v ecological status (Eco.status) derived from the same taxonomic group (Level 3). Boxes represent the lower (25th) and upper (75th) quartiles, and line represents the median value. [ETR = exposure:toxicity ratio].

considered to add perspective to our main focus on spatial influences. Utilising annual average river flow data will be both over and under conservative depending on variation in annual flow profiles. Despite these simplifications, the range of dilution factors exceeded a factor of 10^5, hence the range of exposure concentrations also extended over several orders of magnitude. Diamond et al. (2018) discuss an approach for deriving representative, site-specific concentrations of chemicals in waste water discharges.

We used the SYNOPS tool (Strassemeyer et al., 2017) to estimate PPP chemical exposures. A number of spatio-temporal models exist to estimate daily aquatic exposures at the landscape level (Schad and Schulz, 2011). Due to the complexities of landscape scale PPP exposure modelling, it can be time intensive to develop PPP estimates across a large spatial expanse (i.e., all of Germany). Because SYNOPS incorporates in-use regulatory PPP exposure models coupled with real-world PPP usage information applied at the field scale (Nause et al., 2021), and was available as a resource for this study, it was deemed suitable to demonstrate the principles of spatio-temporal exposure estimation of PPPs across a large landscape. If data sets for agrochemical application and timing are available, the SYNOPS framework can be adapted to other countries and provides estimates of exposure and risk to terrestrial, surface water and ground water systems (Dominic et al., 2017).

Use of SYNOPS included fewer generalised assumptions in predicted environmental concentration (PEC) estimation than in the surfactant case study. Consequently, PPP PECs were likely to reflect the influence of more of the relevant variables and so have potential to be more representative of the range of expected environmental concentrations.

4.2. *Landscale-scale estimation of exposure toxicity ratios (ETRs) and risk distributions*

Whilst ETRs incorporate variation in chemical exposure and sensitivity to chemical toxicity, the influence of toxicity will usually be limited to a coarse scale by the relatively small range of ecotoxicity data available. ETRs were generated for the same range of biological quality elements (BQEs: fish, macroinvertebrates, macrophytes, diatoms) at all assessment locations since these BQEs were routinely represented in the biomonitoring data. A more resolved range of ecotoxicological sensitivity, i.e., representing the variability of species found at each biomonitoring location would have provided a distribution of risk values that better reflected the heterogeneity of biological species likely to be exposed. The development of approaches to enhance the derivation of species sensitivity to chemicals is a key development needed to maximise the value from geo-referenced risk assessment (see 4.3), as it is for conventional prospective risk assessment. The ETR calculation for the three PPP chemicals involved aggregating ETRs for all contributing chemicals (i.e., concentration addition) at the same location (including 1000 m upstream). This represents a conservative approach, i.e., a reasonable worst case, since chemicals with different modes of action

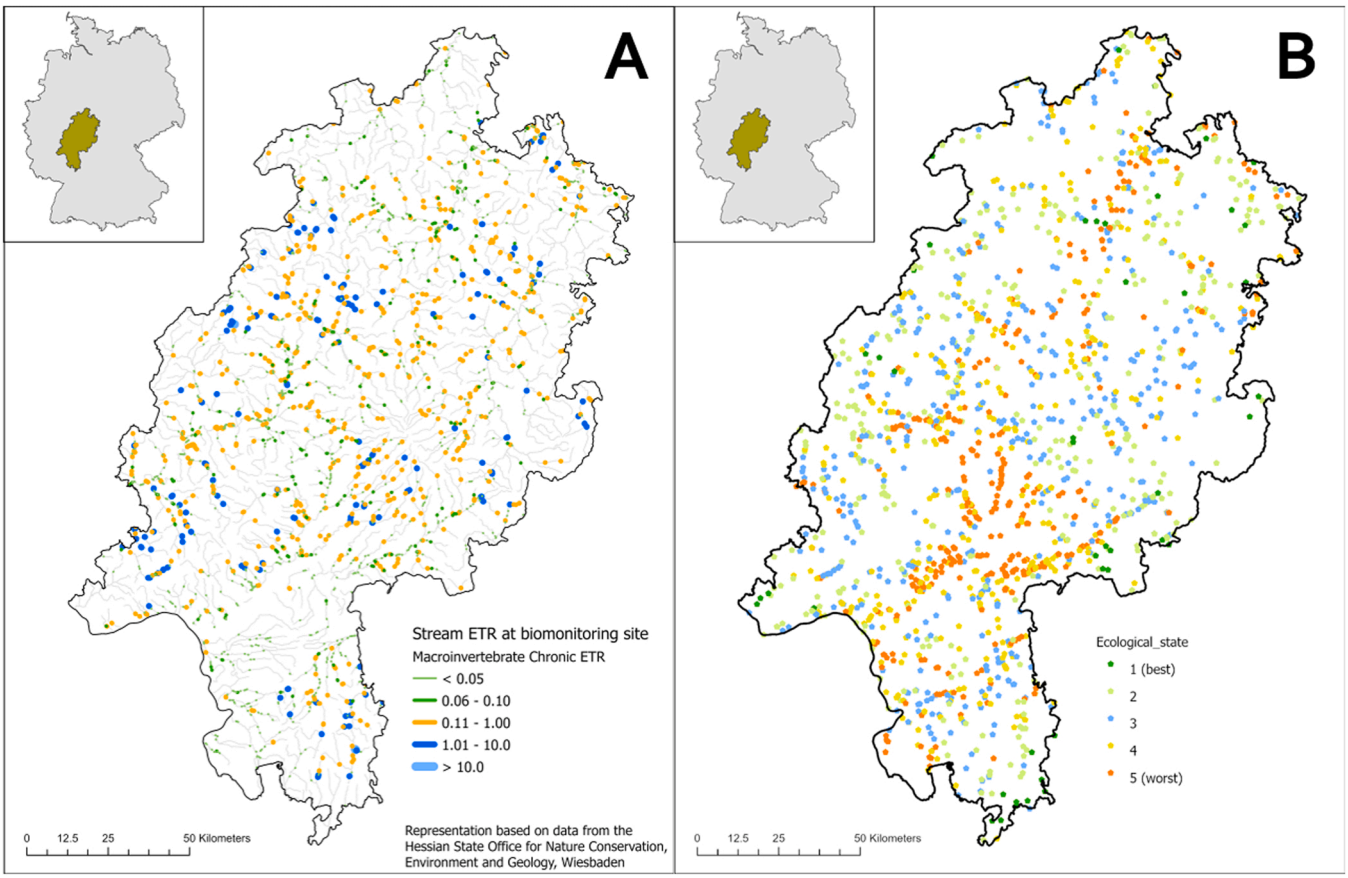

Fig. 7. Spatial distribution of PPP chronic risk values for macroinvertebrates (A) and ecological status of spatially associated biomonitoring locations (B) [ETR = exposure:toxicity ratio].

most likely do not act additively (SHER, 2012).

There are many approaches for using distributions of spatially referenced exposure concentrations and ecological receptor occurrence/abundance in deriving risk estimates. Clear expression of the assessment objectives enables appropriate procedures to be selected. To illustrate this point and recognising the limited availability of ecotoxicity data needed to determine risk, we considered three simple correlative uses of the biomonitoring data with the ETR distributions. A conservative or screening approach is represented by our level 1 assessment which compared the "Best" ecological status BQE per site to ETR of highest (maximum) risk across all BQEs (chronic & acute separately). Whilst this approach makes broad use of the ecological data, interpretation of the ETR values is difficult for chemicals with wide differences in species sensitivity. For example, ecological status may not always be driven by taxa that are relatively sensitive to a chemical. An intermediate approach is represented by Level 2 where each BQE and ecological status per site are compared to ETR of highest (maximum) risk across all BQEs (chronic & acute separately). The most credible approach, Level 3, compares each BQE and ecological status per site to the most relevant ETR (chronic and acute separately).

One approach to reducing the complexity of assessment options is to compare chemical exposures or ETRs with only those sites classed with a high ecological status, i.e., sites considered relatively unimpacted by anthropogenic stressors, including habitat degradation. Liess and von der Ohe (2005) report a similar approach using multiple stream sites likely to be relatively unimpacted by pollutants or hydrodynamic stress in which to assess any relationship between PPP chemical concentrations and community composition. In our case studies higher ETR values did not occur less often at sites with high ecological status than at sites with lower ecological status. This might suggest a low level of concern if the biomonitoring data are taken as spatially and temporally representative. Apart from the specific chemicals selected, we did not investigate other factors that could have influenced ecological status.

In our case studies, 90th percentile annual PECs were used to remove temporal variation thereby enabling a focus on spatial heterogeneity. Assessment of both spatial and temporal influences on risk could be made by comparing field-level acute or chronic exposure with ecotoxicity data or biomonitoring data at multiple time points (Holmes et al., 2018). Consideration of temporal variation in risk could include the timing of occurrence of sensitive life stages, e.g. by focusing the assessment at times and locations where chemical exposure coincides with occurrence of early life stages. However, given that most chronic ecotoxicity tests include sensitive life stages, and that use of 90th percentile PECs is reasonably conservative, excluding temporal variation may not represent an under-estimation of risk.

4.3. *Further developments*

Direct comparisons of predicted environmental concentrations with specific taxa are feasible if the full biomonitoring data are available (Vaj et al., 2011; Liess and von der Ohe, 2005), but will likely be limited by the lack of knowledge of ecotoxicological sensitivity of most of the species present. Since relatively few species are included in standard ecotoxicity tests, e.g. OECD, ASTM, ISO, there will be many data gaps for exposed species and functions (Maltby et al., 2017). Assessment of adverse effects then requires approaches to account for use of surrogate ecotoxicity data as well as the other uncertainties in extrapolating from (mainly) single species laboratory tests to assemblages of species in the field (Spurgeon et al., 2020; Van den Berg et al., 2021). Such approaches are set out in existing regulatory frameworks which aim to be protective

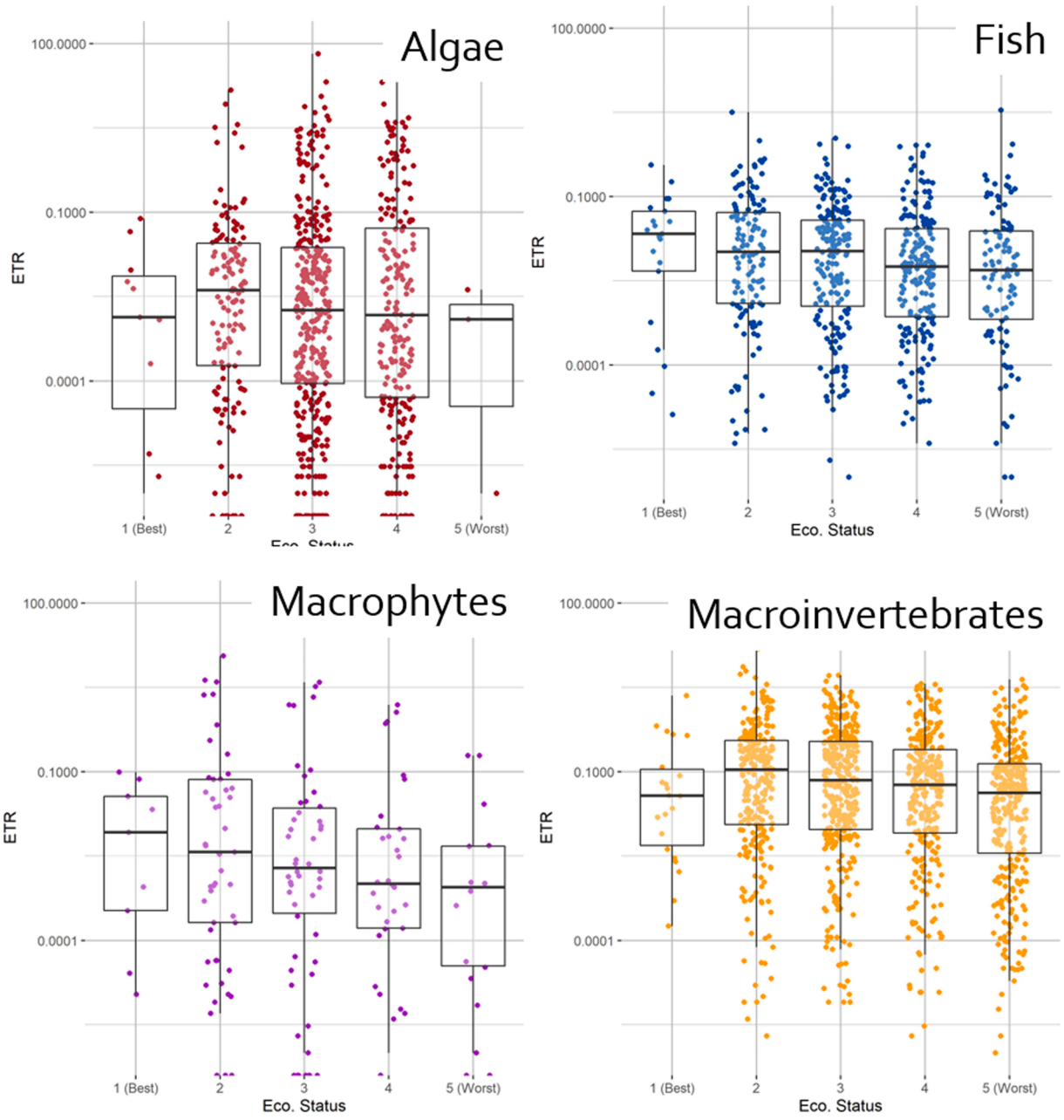

Fig. 8. Plant Protection Product (PPP) chronic Exposure Toxicity Ratio (ETR) v ecological status derived from the same taxonomic group (Level 3).

of broad ranges of taxa. Continuation of approaches to address this issue, e.g. the use of species sensitivity driven by traits (Van den Berg et al., 2019), is key to achieving risk assessments of high ecological resolution.

A mid-way approach between the current generic models used in ERA and a site-specific approach could be to develop representative scenarios (Rico et al., 2015, Goussen et al., 2016, Franco et al., 2017). Ecological scenarios can be viewed as representative food webs or major taxonomic groups within food webs. Developing environmental and ecological scenarios could provide the basis for achieving a simplified and pragmatic approach to the number of assessments required for an individual chemical. Scenarios could be aligned to local specific protection goals, e.g. as set out in terms of WFD biological quality elements, BQEs RBMPs, or to other management goals, e.g. in terms of ecosystem services.

4.4. Challenges

Two main challenges were identified during this research that related to data availability and temporal variation in exposure.

4.4.1. Data availability

A search for available and accessible geo-referenced ecological data sources indicated scarce data suitable for risk assessments on a pan-European scale. The most useful data set was the WFD biomonitoring data as required for assessment of ecological status. Whilst these data are collected by national agencies they aim to provide comparable Europe wide assessment at the required spatial scale and resolution. However, ease of access varies even within Member States with some internal regions providing data freely whilst others require a financial payment. There are concerns over comparability when using indices specific to member states for ecological quality assessment. Nevertheless, there have been intercalibration exercises to ensure the comparability of

ecological quality class limits between EU Member States (Birk et al., 2013; Poikane et al., 2014).

Broader application of WFD ecological monitoring data is limited by their hydrological scope and ecological relevance. The UK River Invertebrate Classification Tool, RICT, is only applicable to freshwaters whereas the German Perlodes assessment (Pottgiesser and Sommerhäuser, 2004) includes some transitional waters (backwater and brackish water influenced Baltic Sea tributaries). There are other tools for transitional and coastal ecosystems based on similar approaches to the use of WFD BQEs in freshwater assessment (Ponti et al., 2009; Borja et al., 2009, Hernández et al., 2010, Vinagre et al., 2016, Souza and Vianna, 2020). Linking these integrative biological indices with reference hydromorphological typologies provides potential incorporation into GIS-based tools. We did not identify large scale geo-referenced ecological data sets for other environmental compartments.

Whichever approach is used, the comparisons lead to a spatial distribution of aggregated risk for the PPP case study or individual chemical risk for the consumer product study. These distributions then require interpretation in order to determine acceptable chemical uses and risk management measures. Since ecological communities are influenced by local landscape and climate characteristics and stressors, simple correlative links between chemical exposure or ETR and ecological status require cautious interpretation. Determining the importance of a specific environmental factor using field data is challenging because other environmental factors may obfuscate possible effects.

Temporal variation in exposure: for streams, flow may dissipate the acute 1-day PEC rapidly such that the 90th percentile of daily values at a given site is lower than the respective chronic 7-day TWA PEC for the same site. Concern for missing short-term exposure spikes has been discussed elsewhere (Lorenz, 2017). Furthermore, accounting for temporal variation generates a huge amount of additional data to assess and present even though the biomonitoring data were obtained on relatively few time points during the annual cycle. Since biomonitoring data obtained at high temporal resolution are not generally available, it would be necessary to extrapolate occurrence/abundance data which would introduce a high level of uncertainty.

4.5. Future needs

Whatever approach is applied to landscape-scale assessment, it seems critical to develop guidance on assessing and interpreting the outcomes of complex data integration necessary to determine the level of risk that is acceptable and to inform decision making. Guidance on the use and integration of exposure, ecotoxicity data and ecological quality, e.g. occurrence/abundance, is key to this as is the interpretation of this mapping. For instance, if an assessment should lead to 90th percentile protection on a spatial or temporal scale, does that mean risks up to the 10th percentile are acceptable irrespective of how they are distributed, or should a spatially clumped concentration of risk be assessed differently? Identifying certain landscape characteristics or times of the year that lead to particularly high risk might also inform better management or mitigation decisions. If such high-risk situations are identified and managed with mitigation, does that then mean that in/at other areas/times of the year higher chemical use rates could be acceptable? Furthermore, should highly diverse and/or sensitive ecosystems have higher protection than species poor and insensitive assemblages? If there is no indication of spatial clustering of risk, is a landscape scale assessment necessary for deciding on any management or mitigation measures?

Our studies do not provide answers to these questions, but these are aspects that regulatory agencies and risk managers need to discuss if landscape scale risk assessments are to be used. In addition to further research to develop data and methods, we recommend stakeholder workshops to gain consensus on scoping and interpreting landscape scale assessments, leading to greater overall acceptance of the approaches.

5. Conclusions

Framing (problem formulation) of landscape-scale risk assessment is a critical step that requires a clear statement of the questions to be addressed and must consider data handling, e.g., aggregation, required resolution, methods for integrating data layers. Whilst we focused on demonstrating whether the integration of relevant data and potential approaches is feasible rather than making comprehensive and refined risk assessments of specific chemicals, we demonstrated that prospective derivation of spatially referenced exposure concentrations was technically feasible but that assessment of risk is less well resolved because of the limited range of ecotoxicity data. Furthermore, there is a limited breadth of ecological data sets that are comprehensive and consistent and that span large geographic areas. The challenges of adopting geo-referenced ERA over continental scales might be addressed by further development and application of spatially explicit ecological effects models. Further development towards increasing efficiency, simplifying and normalising assessment and interpretation methods would also be required. This includes the development of guidance on how to assess spatial and temporal distributions of risk for decision making.

CRediT authorship contribution statement

Stuart Marshall: Conceptualization, Methodology, Writing – original draft, Writing – review & editing. **Chris Holmes**: Conceptualization, Data curation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing. **Lorraine Maltby**: Conceptualization, Methodology, Writing – review & editing. **Paul Sweeney:** Conceptualization, Methodology, Writing – review & editing. **Pernille Thorbek**: Conceptualization, Methodology, Writing – review & editing. **Jens Otte**: Conceptualization, Data curation, Methodology, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data will be made available on request.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.ecoenv.2022.114143.

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