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Do predictions from Species Sensitivity Distributions match with field data?

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ABSTRACT

Species Sensitivity Distribution (SSD) is a statistical model that can be used to predict effects of contaminants on biological communities, but only few comparisons of this model with field studies have been conducted so far. In the present study we used measured pesticides concentrations from streams in Germany, France, and Finland, and we used SSD to calculate msPAF (multiple substance potentially affected fraction) values based on maximum toxic stress at localities. We compared these SSD-based predictions with the actual effects on stream invertebrates quantified by the $SPEAR_{pesticides}$ bioindicator. The results show that the msPAFs correlated well with the bioindicator, however, the generally accepted SSD threshold msPAF of 0.05 (5% of species are predicted to be affected) severely underestimated the observed effects (msPAF values causing significant effects are 2–1000-times lower). These results demonstrate that validation with field data is required to define the appropriate thresholds for SSD predictions.

1. Introduction

Freshwater ecosystems are contaminated with various toxic compounds that may strongly affect populations, community composition, biodiversity, and ecosystem functions (for meta-analyses and reviews see: Beketov et al., 2013; Millennium Ecosystem Assessment, 2005; Schäfer et al., 2012; Schwarzenbach et al., 2006). However, reliable prediction of the ecological risks and impacts associated with contaminants remains a considerable challenge.

One method used for the risk assessment of toxic compounds is the Species Sensitivity Distribution; SSD (Posthuma et al., 2002; Van Straalen and Denneman, 1989) This method uses available toxicity values for different species with respect to a particular chemical to derive a joint sensitivity distribution, from which the fraction of species affected by a certain toxicant concentration can be determined (i.e. a quantile of that distribution). It was originally developed for the risk assessment of single substances through the setting of thresholds: either a hazardous concentration affecting x % of species (HCx, i.e. x-th percentile) or the fraction of species potentially affected by a certain concentration (PAF; Traas et al., 2002). For example, in Europe, a concentration of a single substance potentially affecting 5% of species (i.e. HC5) is deemed protective for the whole community when applying the appropriate assessment factor 1–5 (EC, 2011) or 3–9 (EFSA, 2013) (depending on the types of substances and taxa used for SSD).

Given that toxic compounds frequently occur as mixtures, concentration addition (CA) and response addition (RA) models have been incorporated into the SSD framework (De Zwart and Posthuma, 2005; Traas et al., 2002) to allow for prediction of the potentially affected fraction of species by mixtures (multiple substance potentially affected fraction – msPAF) and consequently for the risk assessment of chemical mixtures (Carafa et al., 2011; Comte et al., 2010; Faggiano et al., 2010; Fedorenkova et al., 2013; Schuler and Rand, 2008).

Environmental quality standards based on SSDs are regarded as less uncertain in comparison to those based on one or just several standard species (EC, 2011). However, an SSD is a statistical model based on several assumptions that may not be met under realistic conditions (Forbes and Calow, 2002). Problems connected with assumptions such as (i) *the equal importance of all species*, (ii) *the equal sensitivity of laboratory and field organisms* or (iii) *the choice of ecologically relevant endpoints to derive the SSD model* can be at least partially solved by various approaches (Duboudin et al., 2004;

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Hayashi and Kashiwagi, 2010; Kefford et al., 2005; Maltby et al., 2005; Van den Brink et al., 2006). Nevertheless, the assumptions of (iv) *no interactions between species* or (v) *structure as the target of concern* remain problematic (Van den Brink et al., 2008), as species interactions may alter sensitivities (Knillmann et al., 2012) and recovery time (Foit et al., 2012). Another limitation is the availability of data used in SSD. Since chronic data (NOEC) are scarce and unreliable for many substances (Crane and Newman, 2000; Jager, 2012), usually acute EC50 data are used, which do not capture chronic and delayed toxic effects.

In addition, the taxonomic groups that are included in a SSD should be carefully selected, as different group selection leads to different PAF values (De Zwart and Posthuma, 2005; Jesenska et al., 2013; Van den Brink et al., 2006). According to a European Union Guideline (EC, 2011) and several studies (Maltby et al., 2005; Van den Brink et al., 2006), only the most sensitive taxonomic group should be used when deriving a SSD for substances with a specific mode of action (e.g. pesticides) and when clear gaps exist between the sensitivities of different taxonomic groups. The HC5 or PAF values are then related to effects on the most sensitive group of organisms. However, various studies still derive one SSD for all taxonomic groups pooled together, even for substances with a specific toxic mode of action like herbicides (Faggiano et al., 2010).

To our knowledge, only a few studies have compared SSD predictions to the effects in real-world ecosystems (i.e. not micro- and mesocosms). Posthuma and De Zwart (2006) found no statistically significant correlation between msPAF values of mixtures (metals, ammonia, household chemicals) and fish species richness or abundance in rivers in Ohio, USA. This was attributed to the influence of additional stressors. A significant correlation and good agreement (in terms of values) were observed only between msPAF and the estimated *"fraction of species likely lost due to toxicant mixture"*. A similar study with mixtures of 45 different contaminants investigated correlations between msPAF and the abundance of 103 individual macroinvertebrate taxa, and found significant correlations of msPAF only with the abundances of 11% of the studied species (Posthuma and De Zwart, 2012). Only a fraction of species with strong abundance changes (>50% decline) showed a closer association with the affected fraction predicted by msPAF. To summarize, the latter two studies found no overall correlation between the abundances of all monitored species and msPAF, presumably because of other stressors influencing the populations and the non-specificity of abundance as an endpoint. A good concordance between predicted and observed effects was detected only after several modelling and data analysis steps. In a study by Carafa et al. (2011), a significant correlation between msPAF for mixtures of 60 different substances and two biotic indices for macroinvertebrates and diatoms is reported. In addition, a range of semi-field studies exhibited a good match with SSD derived thresholds for particular substances (Hose and Van den Brink, 2004; Kefford et al., 2006; Maltby et al., 2005, 2009; Mebane, 2010; Schmitt-Jansen and Altenburger, 2005). However, these comparisons focused mainly on the HC5 instead of the whole SSD and did not account for mixture toxicity.

Overall, there is still a need for the validation of SSD predictions regarding the effects of toxicant mixtures on biological communities in the field. Therefore, the aim of the present study was to directly validate SSD-based predictions (msPAF) with respect to effects on stream invertebrates quantified by the SPEAR bioindicator approach (Liess and Von Der Ohe, 2005). We used the $SPEAR_{pesticides}$ index, which has been shown to be stressor specific as reviewed in Liess et al. (2008) and Schäfer et al. (2012). In contrast to indices reflecting general ecological degradation such as the BMWP (Armitage et al., 1983) and the EPT index (Wallace et al., 1996), the $SPEAR_{pesticides}$ index is based on biological traits. These traits are assumed to be responsive to pesticide effects in the field: the physiological sensitivity of species and the spatio-temporal co-occurrence of organisms and toxicants, and traits fostering post-contamination recovery, i.e. generation time and migration ability (Beketov et al., 2009; Liess and Von Der Ohe, 2005). Although various other indices and methods could be used to validate the SSD-based predictions with field data (e.g. see Rubach et al., 2010; Beketov et al., 2013), we applied the $SPEAR_{pesticides}$, as this index had been successfully employed in the field studies, from which we obtained the data.

A recent analysis by Schäfer et al. (2013) found a clear correlation between the msPAFs for pesticides (based on invertebrates) and $SPEAR_{pesticides}$. In the present study, we tested whether an effect threshold PAF of 5%, which is generally accepted in Europe for setting threshold concentrations for individual substances (i.e. HC5), is protective for the freshwater ecosystems (i.e. msPAF = 5% as an effect threshold). We used previously measured pesticide concentrations from streams in three European regions (Germany, France, and Finland) and calculated both acute and chronic msPAF based on toxicity data for different taxonomic groups.

2. Materials and methods

2.1. Pesticide concentrations and biomonitoring data

The study included event-driven monitoring of 25 pesticides (12 herbicides, 6 insecticides and 7 fungicides; see Table S1) and stream macroinvertebrate abundance data from 45 sites in Lower Saxony (Germany, years 1998–2000) (Liess and Von Der Ohe, 2005), Brittany (France, 2005), and Southern Finland (2005) (Schäfer et al., 2007). Macroinvertebrate samples were collected twice during the main period of pesticide application (Finland – July and August, France – April and May, Germany – May and June). Sites were selected to exclude the influence of waste-water treatment plants, industrial facilities, and mining drainage upstream. Thus, chemical pollution other than from agricultural sources was unlikely. For more details see Liess and Von Der Ohe (2005) and Schäfer et al. (2007).

2.2. SPEAR index calculation

The abundance-based $SPEAR_{pesticides}$ values were calculated according to Beketov et al. (2009) on the basis of the SPEAR approach from Liess and Von Der Ohe (2005):

$$SPEAR_{pesticides} = \frac{\sum_{i=1}^{n} \log(x_i + 1)y}{\sum_{i=1}^{n} \log(x_i + 1)} 100; \quad (1)$$

where n is the number of taxa, x_i is the abundance of the taxon i, and y is 1 if the taxon is classified 'at risk', or 0 if not. A taxon is regarded as 'at risk' only if it has: (i) a $S_{organic}$ value > -0.36, (ii) a generation time ≥ 0.5 year, (iii) aquatic stages which are unable to avoid exposure during periods of intensive pesticide usage, and (iv) a low migration ability (see Beketov et al., 2009 and Liess and Von Der Ohe, 2005 for details).

Additionally, the $SPEAR(number)_{pesticides}$, was calculated (Schäfer et al., 2007; see also Liess and Von Der Ohe, 2005), which gives the fraction of species at risk:

$$SPEAR(number)_{pesticides} = \frac{\sum_{i=1}^{n} y}{n} 100. \quad (2)$$

Multiple SPEAR values derived per site were averaged to reduce estimation bias.

2.3. SSD derivation

Ecotoxicity data for SSD derivation were collected from the US EPA ECOTOX database (http://cfpub.epa.gov/ecotox; last access in February 2014) and IUCLID Chemical Data Sheets (available at http://esis.jrc.ec.europa.eu/; last access in February 2014) and complemented with published data (Supplementary Table S1). Only acute EC50 values for the endpoints of growth, biomass, mortality, and immobilization from tests with the active pesticide ingredient (minimal purity 90%) and exposure duration of 1–7 days were used (see Jesenska et al., 2013 for the rationale). In the case of outliers (i.e. EC50 values outside the 3-σ interval of the SSD distribution), the original articles were studied to assess the reliability of the data value. In the case of multiple EC50 values per one species and a compound, the geometric mean was used. We did not base our analysis on chronic NOEC data because of the scarcity of data and major uncertainties related to NOEC derivation (Crane and Newman, 2000; Laskowski, 1995).

In SSD calculation, a log-normal distribution was assumed and the mean and standard deviation (SD) for different taxonomic groups were calculated (see Table S2) if a minimum of five EC50 values were available. This is in concordance