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An R package to calculate potential environmental and human health risks from pesticide applications using the 'Pesticide Load' indicator applied in Denmark

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ABSTRACT

This paper presents and discusses the "PesticideLoadIndicator" package, a new R-package to compute potential environmental and health effects of pesticide applications using the Danish 'Pesticide Load' indicator. The implementation in the R *Statistical Language* makes it easy for researchers, practitioners and institutions to compare potential pesticide risks for a wide range of applications and compute risk indicators at field-, crop-, farm-, regional- or national level. The tool is publicly available. It provides a possibility for the direct integration of pesticide properties needed for indicator computation (ecotoxicity, environmental fate and human health), from the Pesticide Properties Database or other sources and allows users to change default reference values and weights.

1. Introduction

The reduction of environmental and health risks from agricultural pesticide use is at the top of the agenda of food-value chain actors and policymakers worldwide (Möhring et al., 2020). For example, the EU's sustainable use directive (EU Directive 128/2009EC) prescribes the use of Integrated Pest Management and all EU Member States have published National Action Plans for pesticide risk reduction that should be updated regularly. The European Commission has further emphasized these goals in its recent "Farm to Fork" strategy by demanding a 50% pesticide risk reduction by 2030 (Schebesta and Candel, 2020).

However, the extreme heterogeneity of pesticides and their active ingredients complicate the evaluation of pesticide use, the implementation of risk reduction goals but also the development of suitable tools and policies to achieve such risk reductions (Möhring et al., 2019). Thus, tangible and transparent pesticide indicators are needed, which can be aggregated on a field and crop-, farm- or regional level and which account for the heterogeneity of active substances with regard to their potential effects on the environment and human health. However, such indicators have not been developed in most European countries so far (European Court of Auditors, 2020).

As a possible role model, the 'Pesticide Load' indicator, which accounts for potential environmental and health effects of pesticides on a product level, has been developed in Denmark (Kudsk et al., 2018). Other prominent examples for pesticide risk indicators include the EIQ and SYNOPS models (Kovach et al., 1992, Strassemeyer et al., 2017). Further, studies have assessed pesticide risks globally or their development over time (Schulz et al., 2021, Tang et al., 2021). The advantage of the here used Pesticide Load' indicator is that it can jointly account for potential fate, ecotoxicity and human health effects, has comparably low data requirements and is therefore easily scalable. The 'Pesticide Load' indicator is further broadly implemented and tested in practice: i) it is used as an indicator for the spatio-temporal assessment of pesticide risk reduction goals under the Danish National Action Plan and ii) as a basis for the Danish pesticide tax (Kudsk et al 2018). Due to its broad scope in line with current EU policy goals and its scalability, the indicator has a wide range of potential applications in institutions, industry and research (Möhring et al., 2019, Jørgensen et al., 2019, Ehlers et al., 2021). So far, however, no tangible and transparent public tool for indicator computation was available. To make the 'Pesticide Load' indicator easily accessible to a large range of stakeholders, e.g. for research, education and policy evaluation, we here present and discuss a package

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in the R *Statistical Language* (R Core Team, 2020) for indicator computation (Möhring et al., 2021).

The package allows users to compute the Pesticide Load and its sub-indicators for potential Ecotoxicity, Environmental Fate and Human Health effects based on pesticide application data. It further provides a possibility for the direct integration of pesticide properties, needed for the computation, from the Pesticide Properties Database (Lewis et al., 2016). Finally, it is flexible to integrate other data sources and/or adjust default (Danish) reference values and weights for indicator computation.

Following, we briefly describe the indicator, its background and limitations, provide a description of the package and its functions and give an example of its application using integrated test data.

2. Description of the pesticide load indicator

The Pesticide Load and its sub indicators are computed for each pesticide product (eq. 1 & 2). They may then be aggregated at a field and crop-, farm, regional or national level. We further provide the Load Index in the package, given applied standard dosages are provided.

(1) Pesticide Load [Load units per kg/l product] = Ecotoxicity Load + Environmental Fate Load + Human Health Load
(2) Load Index [Load per standard dosage] = Pesticide Load * Applied standard dosages of product (standard dosage of product defined in national pesticide databases)

The *Ecotoxicity Load* is calculated, based on 11 LC/LD/EC50 (median lethal dose/concentration) and NOEC (No Observed Effect Concentration) parameters. Eight of these parameters relate to acute ecotoxicity/short-term effects of active substances on birds, mammals, fish, daphnia, algae, aquatic plants, earthworms, bees, while three relate to chronic ecotoxicity/long-term effects on fish, daphnia and earthworms, respectively. Values for chronic ecotoxicity are adjusted for degradation rate of the active ingredient in case half-life values in soil and water are available.

The *Environmental Fate Load* is based on three parameters: the half-life in soil (DT_{50}), the bioaccumulation factor (or the log P_{ow} value if no BCF value is reported) and the SCI-GROW index that reflects the mobility and risk of leaching to the groundwater of the active ingredient and the major metabolites listed in the Pesticide Properties Database.

Whereas the calculation of the Ecotoxicity and Environmental Fate Loads are based on properties of the active ingredients in the product and are then aggregated on a product level, the *Human Health Load* is directly calculated based on the risk phrases and symbols on the product label and the formulation of the products. It should be noticed that the Human Health sub-indicator primarily addresses the potential exposure of operators (and to a lesser extent by-standers), but not consumers, who are mainly exposed via pesticide residues in food and drinking water. All ecotoxicology and environmental fate values are normalized by reference values (the active ingredient with the maximum or minimum value depending on the parameter in question) and weighted according to the (Danish) weighting scheme described in Kudsk et al. (2018). The weighting scheme was introduced to ensure that Ecotoxicology, Environmental Fate and Human Health each contributed with approx. 1/3 at a national level in the reference year 2007. Furthermore, it guaranteed that all Ecotoxicology and Environmental Fate parameters contributed to the overall values. For example, in 2007 aquatic ecotoxicity related parameters, bees, bird, as well as mammals and earthworms (=soil organisms) contributed 41, 21, 18 and 21% to the Ecotoxicology load aggregated at national level. However, the package explicitly allows users to also change reference values and weights to adapt the indicator to other countries and circumstances and easily access respective changes in Load values. This allows testing hypothetical scenarios of changes in reference values and weighting, e.g. for the implementation in other countries with different preferences. However, note that such changes shift weights between the three main categories (Human Health, Fate, Ecotoxicity) and relative importance of pesticide properties (e.g. ecotoxicity for bees vs. aquatic organisms). For a detailed description of the Pesticide Load and the Load Index on different aggregation levels see Kudsk et al. (2018) and Möhring et al. (2019).

It should be stressed that the "PesticideLoadIndicator" tool made available here is not identical to the Danish Pesticide Load used by the Danish authorities and the calculated pesticide loads may therefore be different. This is because pesticide products and their formulation may differ and change over time and country and pesticide properties data from the Pesticide Properties Database may have been amended and completed. The here computed indicators should further not be confused with the so called "Pesticide Load Indicator (PBI)", which indicates Load on a national level divided by a reference area (conventionally grown and sprayed crops in 2010) and is sometimes used in Denmark.

3. Data availability, requirements, and preparation

Computation of the Pesticide Load and the Environmental Fate, Ecotoxicity and Human Health Load with the package requires pesticide application data and human health properties (risk statements) on a product level, as well as information on active ingredients of the applied pesticides, their concentration and fate, as well as ecotoxicity properties, as indicated above. Data on standard dosages and human health properties (risk statements) of products is publicly accessible in national pesticide registers. Substance properties data used for the computation of the 'Pesticide Load' indicator is publicly accessible, e.g. through EU dossiers on the authorization of pesticide products. A central collection of this information is, for example, provided by the Pesticide Properties database (PPDB, Lewis et al., 2016). The here presented tool allows users to integrate a database version of the PPDB (licensed) and automatically draw required information for indicator computation[1] or provide information from other information sources themselves.

Due to the heterogeneity (in quality) of pesticide use data and the low accessibility of national databases on registered pesticides, the computation of the 'Pesticide Load' indicator often requires substantial work to collect and prepare data. Further tools for data scraping and manipulation, complementing the here presented tool for indicator computation should be developed to render pesticide risk indicators more accessible.

4. Package structure and functions

The package is publicly accessible to (R) users through the CRAN network. It provides several functions to compute the Load Index, the Pesticide Load, the Fate Load, the Ecotoxicity Load and the Human Health Load for application-level pesticide use data:Table 1

5. Reproducible example

Following, we provide a reproducible R code on how to compute the pesticide indicators and discuss the outcome. We compute the indicators for four pesticide applications in Switzerland (example data provided in the package):

```
# Install and load the PesticideLoadIndicator package
install.packages("PesticideLoadIndicator")
library(PesticideLoadIndicator)
# Load the dataframe containing the pesticide use data.
```

[1] Further, note that the package is regularly updated to account for potential changes in the PPDB so that workload for users with an updated version (i.e. licensed users) is significantly reduced. CRAN further provides the possibility to use previous version of the package, which might be more compatible if older versions of the PPDB are used.

Table 1
Functions of the 'PesticideLoadIndicator' package.

Function	Description
compute_pesticide_load_indicator (…)	Computes indicators based on user supplied tables of pesticide applications and information on their active ingredients, including ecotoxicity, human health and fate properties.
match.ppdb (…)	Expands basic pesticide use data with information on pesticide properties (ecotoxicity, fate and human health), needed to compute the Pesticide Load, based on CAS numbers. Requires access to the Pesticide Properties Database.
compute_risk_score(…)	Compute human health risk sum scores on a product level based on a list of H-Phrases.
check_substance_column_names (…)	Check names of supplied tables with active substance information.
check_products_column_names (…)	Check names of supplied tables with pesticide application information.

products_user <- products.load()

 # Load the (user-supplied) dataframe with detailed information on used pesticides.

substances_user <- substances.load()

 # Example for optional changes of reference values and weights: here earthworms (not executed)

 # substances_user$Reference.Value.Earthworms.Chronic <- 0.3

 # substances_user$Load.Factor.Earthworms.Chronic <- 3

 # Compute the Pesticide Load and its sub-indicators using the supplied data.

indicators_user <- compute_pesticide_load_indicator(substances = substances_user,

products = products_user)

This provides us with the following indicator values for the Pesticide Load, Health Load, Ecotoxicity Load, Fate Load, Standard Treatment Index and Load Index for the four pesticide applications (note that the optional adjustments to reference values and weights for earthworms were not executed):

Product applied	Crop	Amount applied (kg/ha)	Health Load	Ecotoxicity Load	Fate Load	Pesticide Load	Standard Treatment Index	Load Index
Agora®	Sugar beets	0.4	0.750	0.31	0.18	1.24	0.50	0.62
Alanto®	apple	0.53	0.125	0.57	0.03	0.72	1.67	1.20
Aniten®	wheat	0.25	0.100	0.06	0.14	0.30	0.09	0.03
Artist®	potato	2.0	0.650	0.27	0.15	1.07	0.80	0.85

Please see the package description for a reproducible example of how to compute the indicators only based on simple pesticide use data, i.e. using the Pesticide Properties Database to expand data with needed information on pesticide properties.

6. Discussion & conclusion

We here describe and discuss the "PesticideLoadIndicator" package. It allows practitioners, researchers and administrations to straightforward compute potential environmental and health risks of pesticides, based on the Danish 'Pesticide Load' indicator. The 'Pesticide Load' indicator has a high relevance for current debates on pesticide risk reduction (e.g. in the European Union), as it jointly accounts for potential ecotoxicity, fate and human health effects of pesticides and is easily scalable across products and aggregation levels.

The package thus contributes to i) make the indicator available to a wide range of interested stakeholders, ii) standardize its computation and make it transparent, and iii) easily assess effects of changes in default (Danish) reference values and weights.

Additional tools to collect and prepare data on pesticide use and properties would complement the here presented tool for indicator computation. Further, a transfer of the developed tool into a more accessible and interactive format in the future (e.g. an R Shiny application) would make it more attainable to a broader audience, such as certain groups of practitioners.

CRediT authorship contribution statement

Niklas Möhring: Conceptualization, Software, Validation, Investigation, Visualization, Supervision, Project administration, Writing – original draft, Writing – review & editing. **Per Kudsk:** Conceptualization, Resources, Writing – original draft, Writing – review & editing. **Lise Nistrup Jørgensen:** Resources, Writing – original draft, Writing – review & editing. **Jens Erik Ørum:** Resources, Writing – original draft, Writing – review & editing. **Robert Finger:** Conceptualization, Supervision, Project administration, Writing – original draft, 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.

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