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XDrift—An R package to simulate spatially explicit pesticide spray-drift exposure of non-target-species habitats at landscape scales

Sascha Bub [a,*], Thorsten Schad [b], Zhenglei Gao [b]

[a] *Institute for Environmental Sciences, University of Koblenz–Landau, D-76829 Landau, Germany*
[b] *Bayer AG, Alfred-Nobel-Str. 50, 40789 Monheim, Germany*

A R T I C L E I N F O

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A B S T R A C T

Authorization of pesticides in the European Union is based on a risk assessment that aims at prevention of unacceptable ecological effects. This ecological risk assessment increasingly requires data and tools to base informed decisions on a more realistic modeling of processes at different scales. *XDrift* is the R implementation of such a data-driven model dealing with spray-drift exposure resulting from pesticide spray-applications. It employs the same data on spray-drift depositions as used in the regulatory risk assessment but conserves observed variability. Applied in a multi-scale modeling environment, *XDrift* projects measured drift deposition patterns into landscape scenarios. Both, users and researchers benefit from the publication of the R package and its source code.

Code metadata

Current code version	*1.0.0*
Permanent link to code/repository used of this code version	https://github.com/ElsevierSoftwareX/SOFTX_2020_73
Legal Code License	*CC0* https://creativecommons.org/publicdomain/zero/1.0/legalcode
Code versioning system used	*git*
Software code languages, tools, and services used	*R*
Compilation requirements, operating environments & dependencies	*Linux, OS X, Microsoft Windows. Runs within the R software environment.*
If available Link to developer documentation/manual	
Support email for questions	thorsten.schad@bayer.com

Software metadata

Current software version	*1.0.0*
Permanent link to executables of this version	
Legal Software License	*CC0* https://creativecommons.org/publicdomain/zero/1.0/legalcode
Computing platforms/Operating Systems	*Linux, OS X, Microsoft Windows*
Installation requirements & dependencies	*R 3.4.3 or above from* https://cran.r-project.org
If available, link to user manual - if formally published include a reference to the publication in the reference list	
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1. Introduction

The introduction of Specific Protection Goals into the ecological risk assessment of pesticides [e.g., 1–4] has shifted the focus of risk characterization towards ecosystem services and the units providing these services. The changed focus demands development of risk assessment scenarios as well as re-evaluation and development of tools applicable in these scenarios. To identify the driving factors of risk at specific scales, spatiotemporally explicit exposure models operating at landscape scales have to be combined with ecological effect models characterizing risk at population level. With *XDrift*, we present here a conceptual

* Corresponding author.
E-mail addresses: bub@uni-landau.de (S. Bub), thorsten.schad@bayer.com (T. Schad), zhenglei.gao@bayer.com (Z. Gao).

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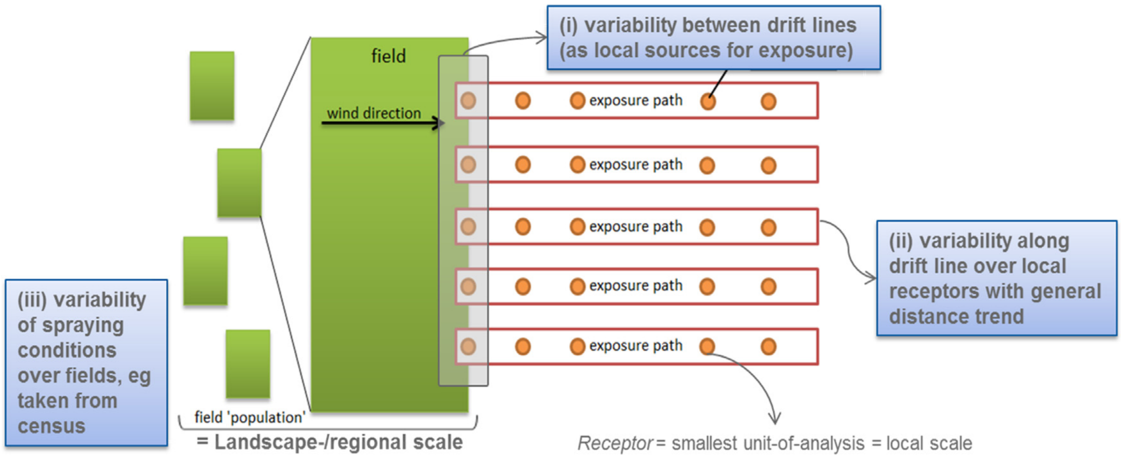

Fig. 1. Variability affecting spray-drift exposure at different scales.

and implemented model that deals with the requirements of the landscape scale for the specific exposure route of spray-drift.

Spray-drift exposure is affected by many environmental and agricultural conditions at different scales. Relative location of agricultural fields and habitats, timing of applications on different fields, local wind and spraying conditions as well as other factors all result in a phenomenon that is highly variable in space and time (Fig. 1). Especially at the local field-edge scale (1 to 10 m around fields), that is supposed to be crucial to the risk of non-target terrestrial and aquatic species, the understanding of spatiotemporal patterns of drift exposure is decisive for risk characterization. Worst-case point estimates, that are used in lower-tier assessments to indicate risk (e.g., 'Abdrifteckwerte', [5]), do hardly allow to quantify risk at real-world landscape scales, a prerequisite for adequate and effective risk management decisions. This is especially true if the lower-tier drift exposure estimation is coupled with ecological effect models [e.g., 6–8].

XDrift uses the same observations as the official data (Rautmann et al. [5]; for methodology, see Supplementary Material) but preserves its variability. Applied along field edges in Monte Carlo simulations, it is thus a data-driven model that allows for quantitative assessments at scales relevant for Specific Protection Goals.

XDrift has been applied in risk assessments using *Xplicit* and has shown to produce reasonable outcomes [6,9]. Through the publication of *XDrift* as an open-source R package, we intend to broaden its field of application to other modeling environments and research questions. We assume that both regulatory and scientific risk assessments may benefit from its application. It can also be a valuable input for the development of management and decision models that require scale-explicit spray-drift exposure data.

XDrift can be installed and used like most R packages. It can be compiled from the source code provided at GitHub and published here. The package consists of R code, object documentation and three vignettes. The first vignette ("X3 Spray-Drift Package for R") gives an overview of the package's functions and their usage. The second vignette ("Using the X3 package in a small real-world landscape") explains the steps required to apply the package's functions to real-world data. The third vignette ("Using the X3 package in a Geo-Workflow") outlines measures that enable the package to run in large-scale settings.

In an earlier work, Wang and Rautmann [10] evaluated spray-drift variability to derive probability density functions (PDFs) for each individual drift trial using an approach similar to that of *XDrift*. The analysis was focused on orchards and used gamma distributions to fit the single trial deposition data. Application of these single trial PDFs was found to be limited due to the small sample size of measured spray-drift depositions in the individual trials, which is typically around six data points. Therefore, in *XDrift*, different options of trial pooling were used (see Supplementary Material) and provided as options to the user.

2. R package functions

XDrift is implemented as a standard R package and coded entirely in R. It provides implementations of spray-drift models that operate on the field-edge scale and topological functions that allow downscaling landscape scale data to the field-edge scale (Fig. 2). In its entirety, it can be used to compose spray-drift simulations at various scales.

At its core, the *XDrift* R package exports five functions that are presented here shortly. See the package's vignette "X3 Spray-Drift Package for R" for a more detailed description.

The *mindwdist* function returns the minimum Euclidean distance between points of one set to any point of another set, considering only a specified direction for distance calculation. This function can be used to evaluate the minimum downwind distance between sources of exposure and its sinks. It therefore maps two-dimensional landscape data to a one-dimensional representation along a wind trajectory, a representation that is required by the *XDrift* spray-drift models.

The *bands* function segments a plane into parallel bands of same width. It is an auxiliary spatial function that is used to create areas along a field edge in which the same percentile for the *xspraydrift* model is assumed. This allows depicting variability along a field edge in a defined way.

The *rautmann90* function is an implementation of the Rautmann 90th percentile model. It is based on the 90th percentile regressions of the official drift-deposition values and can be used to simulate exposure according to the underlying worst-case scenario or for comparison with the *xspraydrift* model results.

Based on the same trial data as the Rautmann 90th percentile model, the *xspraydrift* model simulates exposure based on independent PDFs. It is accompanied by the *xspraydriftparameters* function that provides the parameterizations for individual density functions. The parameters returned by this function have been derived by statistical analysis of measured depositions (see Supplementary Material).

3. Application of XDrift

We illustrate here the application of the *XDrift* R package in a multi-scale context conceptually. For a working example,

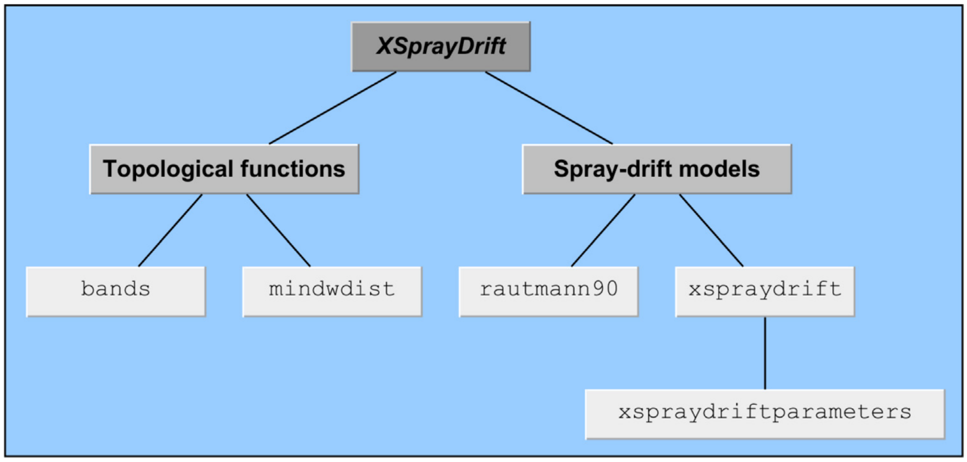

Fig. 2. Functions provided by the *XDrift* R package.

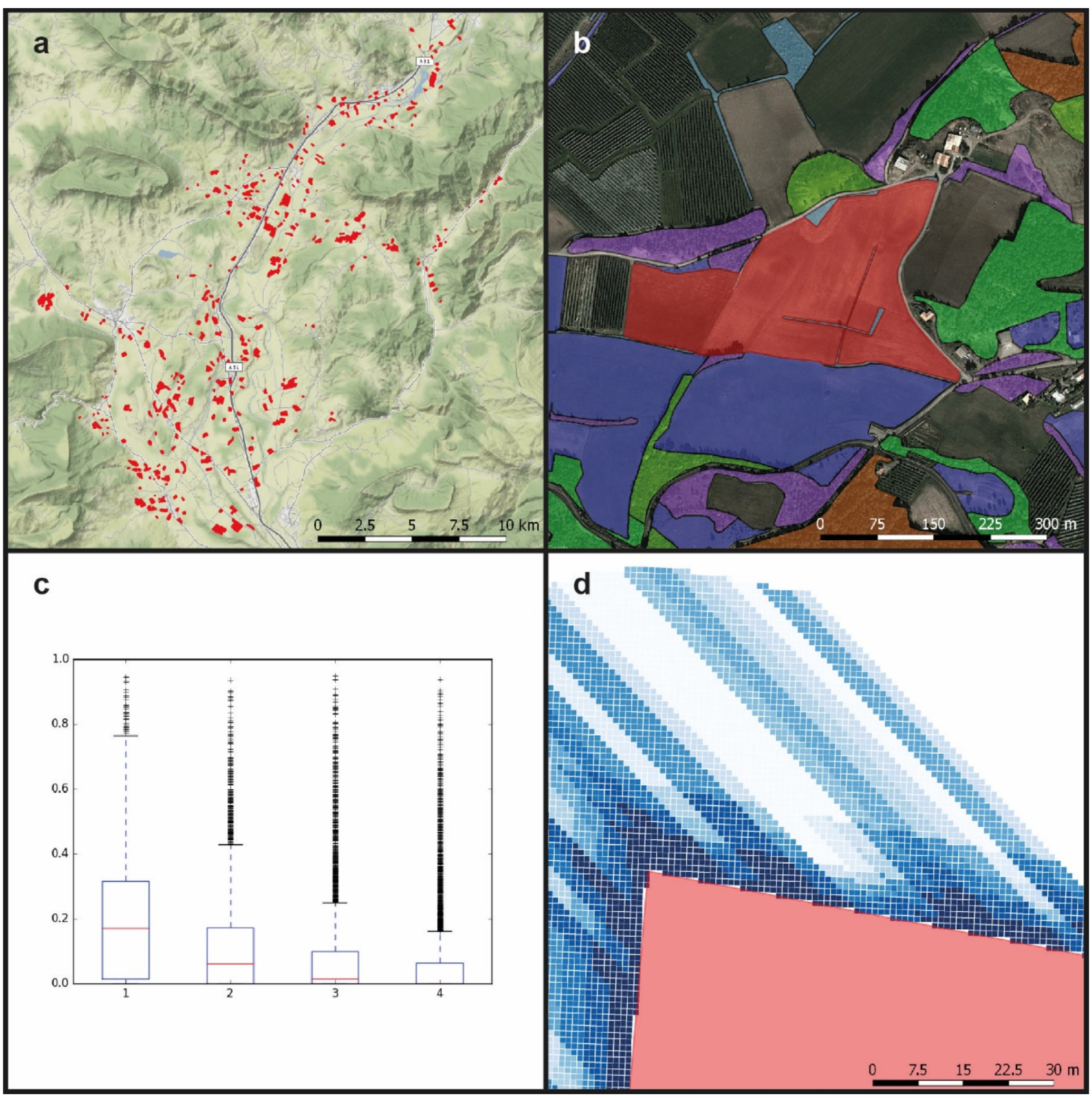

Fig. 3. Important scales of spray-drift exposure. **a** Landscape or regional scale. Applied fields on the current simulation day (modeled) in red. **b** Field scale. An applied field (red) and habitats in its vicinity (other colors) as derived from real-world data. **c** Patch scale. Assessment of areal fractions at which individual habitats are affected for different distance classes (1 to 4) as derived from *XDrift*. **d** Field-edge scale. Exposure pattern simulated by *XDrift*.

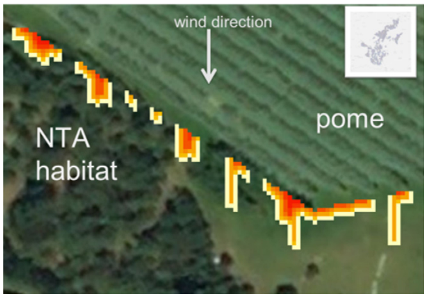

Fig. 4. Local spots violating toxicity–exposure ratio threshold from a single Monte Carlo run. The spots have a mean area of 12 m^2 and a mean distance to non-violated areas of 2 m.

Table 1
Results of a case study about herbicide effects in a plant community using *XDrift* [7].

Scenario	Endpoint	Effect extent [%]	Effect frequency (# of years out of 30)
Overspray	Biomass	26.1	30
	Richness	38.6	30
Wind towards habitat	Biomass	14.4	27
	Richness	18.6	1
Variable wind	Biomass	12.8	17
	Richness	0	0

including code, please refer to the vignette "Using the X3 package in a small real-world landscape".

A key scale in ecotoxicological risk assessment is the landscape scale (Fig. 3a). Landscapes vary in their spatial and temporal distribution of agricultural use. Which crop is planted at which field is decided from year to year or for multiple years and may change within the course of a year. Farming actions like plowing, seeding, harvesting or, in particular, pesticide application occur in hourly to daily changing spatial patterns within certain periods of the year. Within a simulation, these actions have to be determined either using empirical data or by applying a model.

Individual farming actions take place at the field scale (Fig. 3b) and the spatial composition and structure of this scale is crucial for ecological effects of farming actions. In the case of spray-applications, the vicinity of plant and animal habitats to the applied field may potentially impose risks while high vegetation may also filter drift loads. The field scale is commonly derived from geodata but may also be modeled, e.g., by applying a vegetation growth model to static geodata.

In a landscape scale risk assessment, risk characterization typically focuses on specific parts of the landscape. Depending on the protection goal, the risk assessment scale may be, for instance, the habitat (patch) scale. In this case, parts of the landscape may comprise the entirety of habitats in a landscape, habitats of a specific type or habitats within a given distance to fields etc. (Fig. 3c). Defining the assessment scale before running the model can often increase performance as it allows reducing the model to elements that are actually relevant for the assessment.

After identification of application events at the landscape scale and deriving local conditions from the field scale, *XDrift* can be used to simulate exposure patterns at the field-edge scale (Fig. 3d). The simulated exposure can be used as input for environmental fate or effect models, or can be directly mapped to the assessment scale. If combined with models for farm management, weather, environmental fate, exposure models for other exposure paths etc., detailed long-term simulations considering spray-drift exposition are possible using *XDrift*.

4. Impact

XDrift is implemented in the context of the current scientific developments regarding risk assessment of pesticides, especially considering Specific Protection Goals. Its application as a module of spatiotemporally explicit simulations allows studying the effects of spray-drift exposure to local populations at different scales. Due to its focus on spray-drift exposure, it can be applied to a wide range of ecological risk assessment problems, e.g., the assessment of non-target terrestrial plants, non-target arthropods, aquatic organisms, bees and voles, and may also be applied in monitoring at the catchment scale.

Although the *XDrift* R package has not been published until now, it has already been used for several case studies. In one of the studies of a pome cultivating region, the spray-drift induced risk of spray-application to non-target arthropods has been assessed for the local, habitat and regional scale by integrating an *XDrift* call into a Python geo-process. At the regional scale, 2.5% of the habitat area in up to 20 m vicinity of the 2800 ha pome fields, violated the regulatory threshold assuming worst-case conditions. Analysis at the local scale allowed to statistically derive the size of affected patches and their distance to unaffected habitats (Fig. 4).

Another case study used *XDrift* results to simulate the exposure of 3 m x 3 m plant communities in 1 m, 5 m and 10 m distance of a cereal field in which herbicide was applied for 30 consecutive years. The plant communities, represented by the IBC model [7], were assessed regarding biomass and plant family richness for one scenario with variable wind direction, one where the patches were located downwind every year and an overspray scenario (Table 1). The results exemplify how the consideration of variability, as a measure to model processes in a landscape more realistically, alters the quantification of risk considerably.

With its publication, *XDrift* becomes freely available to the scientific community. Researchers or commercial environmental consultants can include *XDrift* in their own environmental models that require variable and more realistic spray-drift exposure. Applied by these groups, *XDrift* may help to answer many current risk assessment and risk management questions.

5. Conclusion

XDrift is an R package for simulating spray-drift exposure of pesticides. Used in multi-scale modeling environments, it can help addressing the requirements of current and future risk assessment and management. In this regard, it also gives an example of modular implementations for spatiotemporally explicit models in landscape modeling context. Exemplary applications show the value of this approach. The publication of *XDrift*'s source code is intended as a contribution to the discourse of the scientific community.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: The research has been funded by Bayer AG, Alfred-Nobel-Str. 50, 40789 Monheim, Germany.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2020.100610.

References

[1] EFSA. EFSA guidance document on the risk assessment of plant protection products on bees (Apis mellifera, Bombus spp. and solitary bees). EFSA J 2013;11(7):3295, 268 pp. http://dx.doi.org/10.2903/j.efsa.2013.3295.

[2] EFSA. Draft opinion on the temporal and spatial ecological recovery of non-target organisms for environmental risk assessments. 2015.

[3] EFSA. DRAFT guidance to define protection goals for environmental risk assessment in relation to biodiversity and ecosystem services. 2015.

[4] EFSA. Guidance to develop specific protection goals options for environmental risk assessment at EFSA, in relation to biodiversity and ecosystem services. EFSA J 2016;14(6). http://dx.doi.org/10.2903/j.efsa.2016.4499.

[5] Rautmann D, Streloke M, Winkler R. New basic drift values in the authorisation procedure for plant protection products. In: IMitt. Biol. Bundesanst. Land-Forstwirtsch. Berlin-Dahlem; 2001, Heft 81.

[6] Schad T. Xplicit – a modelling framework for ecological risk characterisation at landscape-scales in regulatory risk assessment and risk management of plant protection products. DIssertation, Universität Koblenz–Landau; 2013.

[7] Reeg J, Schad T, Preuss TG, Solga A, Körner A, Mihan C, Jeltsch F. Modelling direct and indirect effects of herbicides on non-targetgrassland communities. Ecol Model 2017;348(2017):44–55.

[8] Ashauer R, Boxall A, Brown C. New ecotoxicological model to simulate survival of aquatic invertebrates after exposure to fluctuating and sequential pulses of pesticides. Environ Sci Technol 2007;41(4):1480–6.

[9] Schad T, Schulz R. Xplicit, a novel approach in probabilistic spatiotemporally explicit exposure and risk assessment for plant protection products. Integr. Environ. Assess. Manag. 2011;7:612–23.

[10] Wang M, Rautmann D. A simple probabilistic estimation of spray driftfactors determining spray drift and development of a model. SETAC Press. Environ Toxicol Chem 2008;27:2617–26.