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A spatiotemporally explicit modeling approach for more realistic exposure and risk assessment of off-field soil organisms

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Abstract

Natural and seminatural habitats of soil living organisms in cultivated landscapes can be subject to unintended exposure by active substances of plant protection products (PPPs) used in adjacent fields. Spray-drift deposition and runoff are considered major exposure routes into such off-field areas. In this work, we develop a model (xOffFieldSoil) and associated scenarios to estimate exposure of off-field soil habitats. The modular model approach consists of components, each addressing a specific aspect of exposure processes, for example, PPP use, drift deposition, runoff generation and filtering, estimation of soil concentrations. The approach is spatiotemporally explicit and operates at scales ranging from local edge-of-field to large landscapes. The outcome can be aggregated and presented to the risk assessor in a way that addresses the dimensions and scales defined in specific protection goals (SPGs). The approach can be used to assess the effect of mitigation options, for example, field margins, in-field buffers, or drift-reducing technology. The presented provisional scenarios start with a schematic edge-of-field situation and extend to real-world landscapes of up to 5 km × 5 km. A case study was conducted for two active substances of different environmental fate characteristics. Results are presented as a collection of percentiles over time and space, as contour plots, and as maps. The results show that exposure patterns of off-field soil organisms are of a complex nature due to spatial and temporal variabilities combined with landscape structure and event-based processes. Our concepts and analysis demonstrate that more realistic exposure data can be meaningfully consolidated to serve in standard-tier risk assessments. The real-world landscape-scale scenarios indicate risk hot-spots that support the identification of efficient risk mitigation. As a next step, the spatiotemporally explicit exposure data can be directly coupled to ecological effect models (e.g., for earthworms or collembola) to conduct risk assessments at biological entity levels as required by SPGs. *Integr Environ Assess Manag* 2023;00:1–15. © 2023 Applied Analysis Solutions LLC and WSC Scientific GmbH and Bayer AG and The Authors. *Integrated Environmental Assessment and Management* published by Wiley Periodicals LLC on behalf of Society of Environmental Toxicology & Chemistry (SETAC)

KEYWORDS: Assessment endpoints; Landscape-scale; Off-field soil risk; Pesticide exposure; Specific protection goals

INTRODUCTION

The authorization process of plant protection products (PPPs) includes comprehensive regulatory risk assessment (RA) for nontarget species, including soil organisms (EC 1107/2009, EU 283/2013, EU 546/2011, European Food Safety Authority [EFSA], 2019; EFSA Panel on Plant Protection Products and their Residues [EFSA PPR Panel], 2017; USEPA, 1992, 1998, 2003). The European Food Safety Authority (EFSA) has released a scientific opinion on "addressing the state of the science on RA of PPPs for in-soil organisms" (EFSA PPR Panel, 2017), in which spray-drift depositions and runoff are identified as the most relevant potential exposure routes of off-field soil organisms, whereby the term "off-field" refers to areas outside the agricultural field boundaries, that is, essentially to (semi-) natural areas present in cultivated landscapes. The EFSA PPR Panel (2017) outlined a first approach to estimate off-field soil exposure, designed closely to the FOCUSsw Step-2 model and scenario approach (FOCUS, 2001), which assumes independent conservative estimates on local spray-drift and runoff entries, and adds them at a single spot. Essentially, this model and scenario definition mean that 100% of individuals in a population occurring "off-field" in a

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cultivated landscape receive such "worst-case" exposures. The approach does not consider real-world variability of exposure conditions in space and time, whereas these two risk dimensions and their scales are essential when assessing effects and risk according to specific protection goals (SPGs, EFSA PPR Panel, 2017; EFSA Scientific Committee, 2016). The conservative character of the approach and the necessity for model and scenario development are indicated in EFSA PPR Panel (2017): "In the absence of appropriate off-field exposure scenarios… Since such models are not yet available for regulatory purposes at the European level, the simplifying assumption is made that the individual exposure routes can be assessed separately. Results of the different entry routes should then be summed, which is a conservative assumption because it neglects the different dynamic behavior of the processes."

With this background, the aims for the present work are (i) to develop a model approach to appropriately combine off-field soil exposure due to runoff and drift, (ii) to develop scenarios based on real-world conditions, and (iii) to conduct a case study to gain insights into off-field soil exposure and risk, including mitigation options. The developments are guided by the EFSA Scientific Opinion (EFSA PPR Panel, 2017) and by preceding opinions discussing SPGs (EFSA Scientific Committee, 2016). Results are intended to feed the discussion in the scientific community on the design of off-field soil exposure, effect, and risk characterization approaches in a tiered RA scheme and to support the development of assessment endpoints (AEs, e.g., spatiotemporal percentiles of off-field exposure and effects addressing SPGs). This includes the identification of effective risk-mitigating options.

METHODS

Regulatory RA framework

The developments and the case study of our work are embedded into the regulatory framework and its scientific basis of pesticide risk to nontarget organisms. Specific protection goals and RA schemes distinguish between habitats of soil organisms occurring within the cultivated field (in-field) from those occurring outside (off-field) (Figure 1). The xOffFieldSoil approach is applicable to any scenario delineating in-field and off-field. Any land cover patch type can be included in the risk analysis, even when actually located within the property of the farmer. In our scenario development, we define off-field as land cover patches occurring outside farmers' property.

The advent of the framework of SPGs (EFSA PPR Panel, 2010, 2017; EFSA Scientific Committee, 2016) moved RA for nontarget species from single-point worst-case exposure estimates and simple risk quotients (RQs) to ecologically meaningful RAs, including the implementation of more realistic scenarios. Specific protection goals define biological entities and their attributes and require quantifying effect magnitudes in the spatial and temporal dimensions. Corresponding explicit AEs will have to be provided in future RAs, quantifying effect magnitudes in space and time for a defined biological entity (e.g., individuum, population, functional group) and attributes (e.g., behavior, survival and/or growth, abundance and/or biomass). Although the presented xOffFieldSoil approach currently has a focus on exposure assessment (Model design section below), its underlying concepts are built to address the full SPG framework (Bub et al., 2020; Schad, 2013; Schad & Schulz, 2011).

Model design

xOffFieldSoil is a Monte Carlo (MC) approach that is spatiotemporally explicit. Scales are explicitly considered in the representation of spatial and temporal variabilities (implemented as probability density functions [PDFs]) and their propagation to model outcome. This is essential to simulate exposure and effect patterns that can realistically occur in the modeled system. Any variable phenomenon of the modeled system can be represented by a suitable spatiotemporally and scale-explicit PDF; for example, if day-to-day variable wind directions are to be represented across a region, a corresponding PDF can be defined. During simulations, wind directions will be the same for all drift processes in the region on a given day, yet will vary from day to

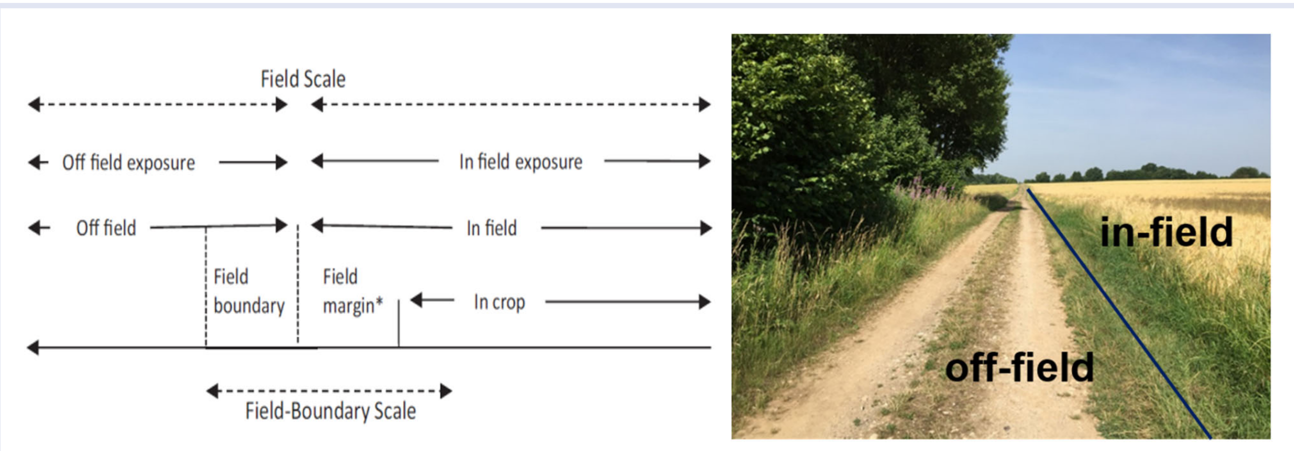

FIGURE 1 Schematic definition (left, EFSA, 2017) and real-world illustration (right) of off-field and in-field areas in cultivated landscapes

day over the simulation period. If the variability of wind direction is observed at different scales, for example, for individual application events on fields with 10 min frequency, PDFs can be defined accordingly. Other variabilities in landscape-scale exposure and effect modeling typically deal with farmers' decisions, for example, crop cultivation or PPP application. During simulation, all variabilities in the system are "resolved" and result in a spatiotemporal pattern of exposure and effects for a defined smallest-unit-of-analysis (e.g., exposure: [1 m^2, day], effects: [individuum, day]). From these spatiotemporally explicit data, meaningful statistical aggregates are derived, again taking explicit scales into account (e.g., a local smallest-unit-of-analysis segment belonging to an edge-of-field vegetation margin, which, together with other margins, is part of a region). In this way, AEs can be built that directly address the entities, dimensions, and scales defined in SPGs for off-field soil organisms, for example, in the spatial dimension for an ensemble of edge-of-field habitats and in the temporal dimension for the spring season from all spring seasons in the full simulation period.

Endpoints can focus on exposure values (as in the case study herein), soil function, or populations of soil organisms, if corresponding population effect models are integrated into xOffFieldSoil. Such model adaptations are possible as xOffFieldSoil is built on a generic modular landscape modeling framework (Figure 2; Schad, 2013). The aims of this framework are (i) to provide concepts and a toolbox to build landscape models capable of propagating variability to model outcome while complying with fundamental principles of MC modeling (e.g., outcome pattern to represent a possible status of the modeled system); (ii) to enable the integration of existing models as components (also to facilitate model validation); (iii) to assure consistent data and information states within the model; and (iv) to transparently build AEs that directly link to the attributes, risk dimensions, and scales defined in SPGs (e.g., EFSA PPR Panel, 2017; EFSA Scientific Committee, 2016). The full xOffFieldSoil model scheme, including additional components, as well as geodata and utilized technology, is illustrated in Supporting Information: Figure S1.

From a user's perspective, xOffFieldSoil can be employed using any simulation model with any scenario (limited by computing resources). The xOffFieldSoil version used in the present case study has been published on GitHub (https://github.com/xlandscape/xOffFieldSoilRisk). Given its conceptual foundation, xOffFieldSoil can be adapted and extended for subprocesses and functionality in a modularized way. The components of the current implementation are summarized in the following sections.

Plant protection product use

Simulated PPP use on fields is done by the xOffFieldSoil component xPProtection ("Plant Protection"; Figure 2). In the present study, a simplified version of xPProtection simulates the spatiotemporal variability of applications of a single PPP to a single crop type. The spatial variability of PPP uses in the landscape is given by the land use data set. Plant protection product applications are defined by PPP use rates (either product use [mL PPP/ha] or as the contained active substance [a.s.] [g a.s./ha]) together with application time windows. During simulations, the PPP is applied during variable dates according to a PDF. For our case study, a uniform distribution was applied (i.e., each day within the defined application window was equally likely to become the application date of the PPP on an individual field).

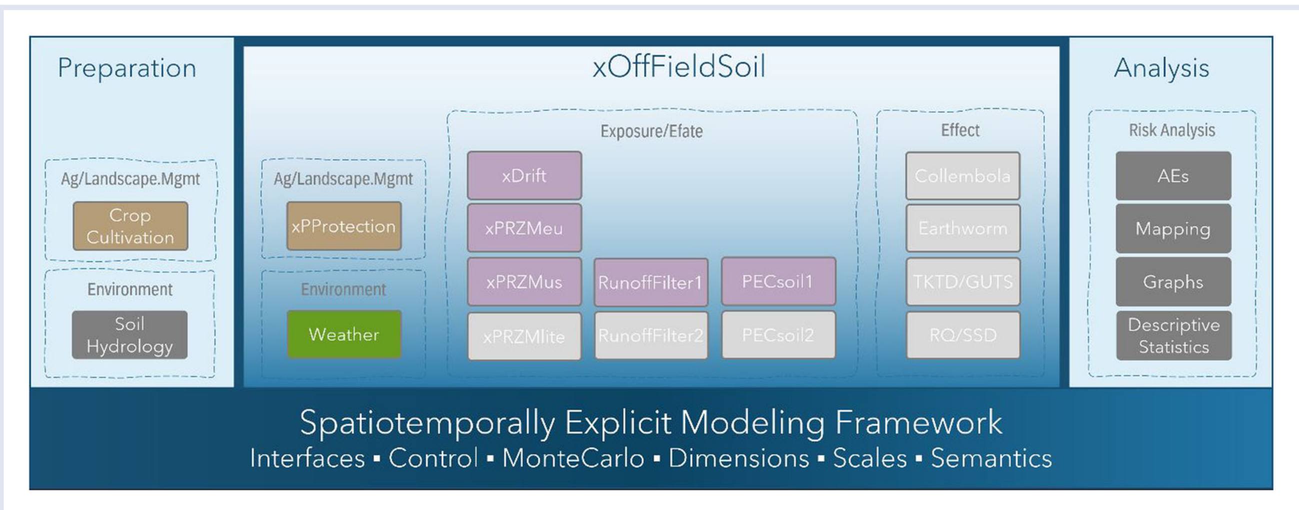

FIGURE 2 xOffFieldSoil model scheme. The model is composed of components (boxes in the central panel, e.g., xDrift; Bub et al., 2020). Components provide major model functionality (e.g., spray-drift or runoff exposure calculation) and are built by wrapping existing models (e.g., PRZM) or by developing new ones (e.g., "RunoffFilter1"). The implementation of xOffFieldSoil is based on a generic modular landscape modeling framework (Schad, 2013). The light gray boxes represent xOffFieldSoil components that were not used in the case study, although they do exist or are under development (full scheme in Supporting Information: Figure S1, https://github.com/xlandscape/xOffFieldSoilRisk). Preparation and analysis panels contain tools, for example, for data preparation and risk analysis of model outcome (Supporting Information: Table S1) and operate closely with the framework, yet are not part of the core xOffFieldSoil model. PRZM, Pesticide Root Zone Model

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Spray-drift deposition

Currently, in Europe, spray-drift exposure is assessed based on empirical data from which local realistic worst-case values are derived (90th percentile for single applications, FOCUS, 2001; Rautmann et al., 2001). However, it is unrealistic to use a 90th percentile spray-drift deposition at 100% of two-dimensional (2D) landscape-scale off-field patches. Therefore, on the basis of Rautmann et al. (2001), a model was developed (xDrift; Bub et al., 2020) that represents the variability of spray-drift depositions along the field edge as observed in the drift trials. Consequently, a range of deposition values are possible with a PPP application event. This may include even higher depositions than the "Rautmann 90th percentile," leading to higher local maximum effects than the standard-tier RA. The mass deposited on an off-field soil segment by a spray-drift event was used to calculate a local off-field predicted environmental concentration in soil (PECsoil). xDrift was integrated as a component into xOffFieldSoil (Figure 2).

Runoff

With the aim of staying close to the current regulatory exposure assessment approaches in Europe, the well-established runoff model Pesticide Root Zone Model (PRZM, FOCUS, 2001) was used for the runoff calculation component (xPRZMeu, Figure 2). This allows verification of local exposure patterns resulting from xOffFieldSoil using standard FOCUSsw PRZM results. Parameterization of the runoff component uses the same data structure as standard FOCUSsw PRZM regarding PPP application, efate of the substance, and soil and weather data input, yet taken from local environmental conditions. The runoff process consists of three subprocesses using a grid-based approach (Supporting Information: Section S1.4.2): (i) soil surface hydrology, (ii) runoff (erosion) generation on fields, and (iii) runoff filtering in off-field habitats. The local calculation of the soil surface hydrology uses local water flow direction determined using a digital elevation model (EEA, 2019). For each daily time step, PRZM calculates local water volume, eroded sediment, and chemical mass transfer to the downstream grid cell.

Mitigation

A range of options exist to mitigate exposure to off-field habitats from spray-drift and runoff entry (e.g., Alix et al., 2013; FOCUS, 2007a, 2007b). The most prominent ones were implemented in the present version of xOffFieldSoil. The in-crop-buffer represents a no-spray, yet cropped, strip of a certain distance from the field boundary (e.g., 5 m). An in-field margin is a noncropped strip of a certain distance from the field boundary, often cultivated as a flowering strip. Both cause a spraying distance to off-field soil areas of the untreated strip width, that is, a spray-drift reduction, whereas we conservatively assume that runoff filtering only occurs in the in-field-margin. Drift-reducing spraying technology reduces spray-drift by a certain fraction (e.g., 90%), typically implemented using drift-reducing nozzles.

Runoff filtering

Exposure of off-field soil organisms due to runoff is a result of filtering and deposition of run-on, that is, of water together with its dissolved and particle-bound substances, for example, by off-field soil vegetation (EFSA PPR Panel, 2017). FOCUS (2007a, 2007b) provides minimum, maximum, and mean filter efficacy values for pesticide filtering (Supporting Information: Figure S2). From these data, exponential deposition curves were calculated to determine the relative soil loading as a function of filter length (Supporting Information: Section S1.2). In the case study, mean filter efficacy was chosen; however, the appropriate curve for regulatory RA use is to be discussed. The mass deposited on an off-field soil segment by a runoff and/or erosion event was used to calculate a local off-field PECsoil. A more sophisticated component using VFSMOD (Muñoz-Carpena et al., 1999) is under development.

PECsoil

A simple xOffFieldSoil component (PECsoil1; Figure 2) was implemented to calculate exposure of soil-dwelling organisms (PECsoil) from the combined spray-drift and runoff deposited mass, assuming a soil depth of 5 cm and a dry bulk density of 1.5 kg/L. At each time step, deposition mass is added to already present residues taking first-order degradation into account based on the input DT50 (days). Publication of a more sophisticated PECsoil component using the EPA model PRZM-5 (Young & Fry, 2014) is in preparation (GitHub https://github.com/xlandscape/xOffFieldSoilRisk).

Effects

Specific protection goals for off-field soil organisms are defined for biological entities and attributes (EFSA PPR Panel, 2017). Correspondingly, AEs have to directly address effects at these protection endpoints (e.g., modeling effects on individual and population levels, experimental endpoints). To this end, effect models are under development (see the Outlook section), whereas current standard-tier RA is based on a straightforward RQ. The RQ is a comparison of the regulatory acceptable concentration (RAC; Supporting Information: Section S2.3) of an a.s. with the modeled exposure (PEC), (RQ = PEC/RAC). Risk quotients are calculated and compared to a threshold. Typically, acceptable risk is indicated for RQ < 1.

The present version of xOffFieldSoil comes with a simple component (xRQ/species sensitivity distribution [SSD]; Figure 2) that calculates RQs from spatiotemporally explicit exposure values using ecotoxicological test data. Analysis of resulting spatiotemporally explicit RQ distributions produce visualizations and AEs as exposure outcomes. Using SSDs, the fraction of species affected in space and time can be estimated. However, with the aim of providing AEs that directly relate to the biological entities of SPGs for soil organisms, effect model components should be integrated in future versions of xOffFieldSoil, directly linking exposure and effect models (see the Outlook section).

Experiments

An xOffFieldSoil experiment is defined by a set of MC simulations using the same model parameterization. xOffFieldSoil runs the simulations using parallel computing according to the number of CPU cores specified by the user. Analysis is performed at the level of the individual MC simulation (e.g., a 90th percentile over space of the local median exposure values over time, PEC[x90{t50}]) as well as on the experiment level (e.g., expectancy values < PEC[x90{t50}] > represented by the arithmetic mean) over the set of MC simulations. Typically, the "control" defines an experiment without PPP use. In the absence of effect models (e.g., population models), that is, for exposure AEs, this is just the zero-exposure situation.

Local realistic worst-case exposure

As proposed by EFSA PPR Panel (2017), the FOCUS surface water STEP 2 approach (FOCUS, 2001) was used to estimate local realistic worst-case spray-drift and runoff loadings for comparison with xOffFieldSoil outcome. This approach is built on independent conservative assumptions regarding local spray-drift and runoff and combines them at a single point in time (the application date) at a single local spot (see Supporting Information).

Scenarios

Present regulatory RA of PPPs depends on scenarios (e.g., EFSA PPR Panel, 2017; FOCUS, 2001, 2007a, 2007b) that cover land use and coverage distribution, environmental conditions, and agricultural practices including PPP use, with an outlook to more explicitly including species' habitat conditions, species occurrence, and ecosystem services. In the absence of established scenarios for the RA of off-field soil organisms, (i) first, research on off-field habitat types occurring in the agricultural landscape was conducted, from which (ii) example schematic and landscape scenarios were developed. These scenarios are available with the xOffFieldSoil model (Supporting Information: Section S1.4).

Schematic scenarios

With a focus on lower-tier RAs, schematic scenarios were developed addressing the edge-of-field scale. In our case study, a schematic scenario (Schematic-1) was used that includes a 100 m × 100 m field ("in-field," optionally surrounded by an off-crop margin, Figure 3A) and an off-field area to the east (Figure 3A). In the analysis of the xOffFieldSoil outcome, the off-field soil area can be parameterized as a small strip

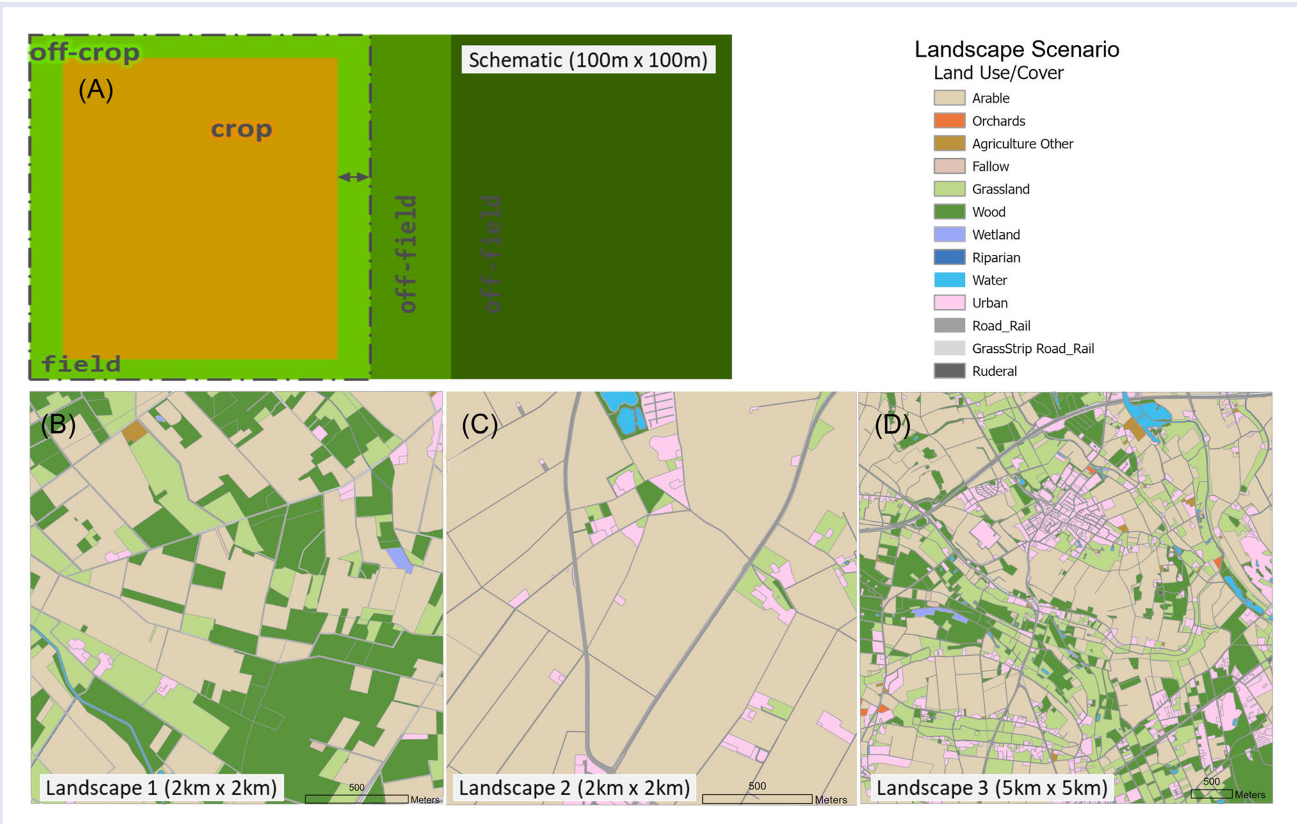

FIGURE 3 Schematic edge-of-field (A) and landscape (B–D) scenarios. The brown "field" patch (A) represents farmers' property and can be entirely cultivated or can optionally include a noncropped "in-field off-crop" margin (light green). The 100 m × 100 m schematic scenario (A, Schematic-1) has an "off-field" patch in the eastern direction. Its light and dark green colors indicate optional different sizes representing different real-world off-field habitat types. The landscape scenarios (B–D) are of 2 km × 2 km extent (B/"Landscape-1," C/"Landscape-2") or 5 km × 5 km (D/"Landscape-3") and reflect real-world agricultural landscape conditions, and are hence composed of different land use and off-field soil habitat types (Supporting Information: Figures S7–S9)

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(e.g., representing a field margin, wood margin, or hedge) or a larger off-field soil patch (e.g., representing grasslands). Experiments can be parameterized with risk mitigation options, including a noncropped margin within the field boundary ("in-field off-crop") and an in-crop no-spray buffer. Given their simplicity, edge-of-field schematic scenarios are important to understand and verify the complex spatiotemporally explicit system behavior. For the assessment of SPGs that operate above the level of an individual edge-of-field population of off-field soil organisms, as a first step, an ensemble of edge-of-field scenarios can be used, including schematic scenarios of different compositions. To adequately provide AEs addressing population, community, or even biodiversity attributes, the use of landscape-scale scenarios is recommended.

Landscape scenarios

Landscape scenarios represent excerpts in time and space of real-world agricultural landscapes. Thus, landscape scenarios per se come with a purpose-driven level of reality, and hence cover a portion of the natural variability of land use and/or cover composition, landscape structure, environmental and agricultural conditions, and their dynamics. The effectivity and efficiency of risk mitigation options can be assessed more realistically for individual PPP use (e.g., in-crop buffer) or for generic risk management (e.g., runoff filter strips, landscape design) (e.g., Alix et al., 2013; FOCUS, 2007a, 2007b). The development of landscape scenarios can be separated into (i) scenario site selection and (ii) actual scenario construction. As examples for our case study, three landscape scenarios were developed located in North Rhein Westfalia (Germany; Figure 3B–D and Supporting Information: Figures S7–S9). Landscape scenario 1 covers a 2 km × 2 km area with dominating land uses of 47% arable land, 33% woods, and 15% grassland. Landscape scenario 2, also 2 km × 2 km, represents a more intense agricultural landscape of 87% arable fields and little grasslands and woods (<3%). Landscape scenario 3 consists of a 5 km × 5 km area with 42% arable land, 19% grasslands, and 17% woods. In all landscapes, the remaining areas consist of urban areas (roads, buildings) and small amounts of water and wetland (Figure 3A–D and Supporting Information: Figures S7–S9).

Case study

A case study was conducted to demonstrate the use of xOffFieldSoil, to evaluate the relative changes of xOffFieldSoil PECs compared to a local worst-case, and to preliminarily discuss results in the context of RA for off-field soil organisms. Experiments were conducted using PPPs that contain two different a.s. of contrasting environmental fate properties, such as aerobic soil half-life (DT50) and soil organic carbon sorption (Koc). The two a.s. modeled were lindane and thiacloprid. The case study comprised the use of different scenarios and mitigation options. A listing of the detailed design of the case studies' experiments is provided in Supporting Information: Tables S4 and S5. The PECsoil values were calculated for off-field soil grid cells of 1 m^2 resolution (*x*) with a one-day time step (*t*). Exposure AEs were derived from spatiotemporally explicit PECsoil(*x*,*t*). First, a temporal percentile was calculated for each individual off-field soil grid cell (1 m^2), from which, second, a spatial percentile was calculated across the 1 m^2 cells for each temporal percentile. Expectancy values and confidence bounds (lower 5th and upper 95th percentile) were calculated for the experiment (i.e., the set of MC runs). Variability was parameterized for PPP application date (uniform PDF over application period, application dates sampled by [field, day]), wind direction (uniform PDF, wind direction values sampled by [region, day]), and spray-drift deposition (gamma PDF, spray-drift deposition sampled by [1 m^2, application event], and by distance from the field; Bub et al., 2020). The variability of runoff events was driven by local precipitation patterns.

RESULTS AND DISCUSSION

The exposure components utilized in the current xOffFieldSoil approach are based on established models in regulatory exposure and RA. The scenarios either represent the edge-of-field scale established in RA or real-world agricultural landscapes. The case study experiments were set up according to real-world PPP uses and substance properties. Therefore, even if the xOffFieldSoil model and scenario developments are at early stages, the spatiotemporal exposure patterns are considered supportive for basic discussion and to draw first conclusions.

Temporal variability of exposure

Spray-drift and runoff exposure are both event based. Spray-drift events occur only on PPP application days and for off-field segments located downwind depending on wind conditions (Figure 4D). In contrast, precipitation events trigger runoff exposure depending on local conditions (e.g., soil, land use, land management; Figure 4C). Runoff due to precipitation is unconnected to spray-drift events (according to Good Agricultural Practice, farmers avoid application of PPPs before rain events). Co-occurrence of these exposure routes further depends on PPP a.s. properties (e.g., sorption to soil, degradation), which determine daily soil residues accessible to runoff. These largely random and independent processes result in local temporal variability of exposure that is reproduced in individual xOffFieldSoil MC runs (Figure 4B). Supporting Information: Figure S16 illustrates the 10-year temporal variability of a.s. depositions of a single local off-field grid cell (1 m^2) at 1 m distance from the field boundary (Experiments L-01 and T-01; Supporting Information: Table S4). As illustrated, for a persistent a.s. (such as lindane), considerable carryover between exposure events can occur, whereas for a fast-degrading a.s. (such as thiacloprid), local deposition largely corresponds to the exposure event pattern.

Spatial variability of exposure

Local habitats of off-field soil organisms are 2D (example images from agricultural landscapes in Supporting Information: Figures S3–S6), which contributes to spatial

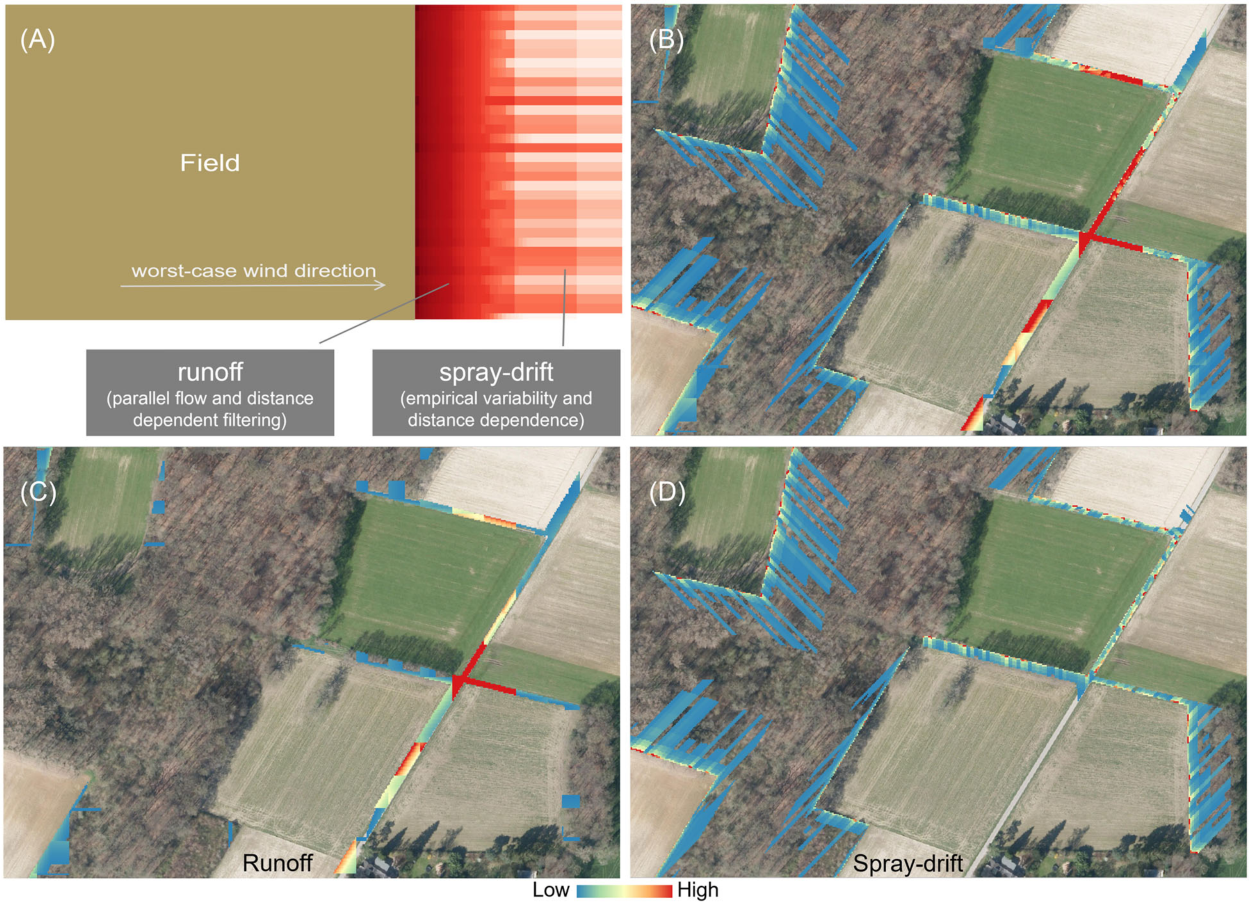

FIGURE 4 Illustration of spatial variability of edge-of-field exposure for the Schematic-1 scenario (A) and a section of Landscape-1 showing runoff and drift combined (B), runoff only (C), and spray drift only (D). Colors represent the maximum PECsoil over 10 years for each local 1 m^2 off-field grid cell based on worst-case spray-drift from westward wind and runoff event exposures (Schematic-1, A) as well as variable wind direction and realistic morphology for Landscape-1 (B). (case study: lindane L-10, no mitigation). PECsoil, predicted environmental concentration in soil

variability of off-field soil exposure and effects (see the Model design section in the Methods section). Spray-drift deposition varies along the field edge, and runoff flow varies with local landscape topography. Both exposure types decrease with distance from the field edge. This spatial variability occurs at the scale of individual off-field soil patches (e.g., over the 1 m^2 grid cells of a wood margin). Across a landscape at the regional scale, additional spatial variability occurs across the ensemble of off-field soil patches (and their grid cells), for example, for exposure of the entirety of wood margins in a landscape. The Schematic-1 edge-of-field scenario shown in Figures 3A and 4A illustrates the spatial variability of local maximum PECsoil over time. Figure 4B–D illustrates a section of the Landscape-1 scenario where the 10-year maximum PECsoil from multiple fields on surrounding locations can be observed for runoff and drift combined (B), for runoff only (C), and spray drift only (D). It should be noted that local maximum PECsoil mapping for individual 1 m^2 grid cells is for illustrative purposes of spatial variability only as this never occurs for every grid cell in a landscape at a single point in time (only for substances that do not degrade at all, i.e., DT50 = ∞).

Spatiotemporal variability of exposure

Spatial and temporal variabilities of off-field soil exposure are interrelated for individual and combined spray-drift and runoff exposure routes, resulting in spatiotemporal exposure patterns at off-field soil patch and regional scales. Spatiotemporal variability of spray-drift exposure is driven by processes of temporal and spatial variability (wind conditions, application timing and conditions, off-field soil patch dimensions, and spatial relationship to fields, etc.), whereas runoff exposure patterns depend on the temporal relationship of substance residues and precipitation pattern. In contrast to spray-drift processes, runoff exposure spatial variability comes with a deterministic component, as the spatial variability of runoff exposure largely depends on the spatial relationship of local off-field soil patches and fields with respect to landscape morphology. Off-field soil grid cells located down gradient from fields are vulnerable to

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runoff events, whereas those located up gradient of the field will not receive runoff.

We start the analysis of such complex spatiotemporal exposure patterns by stepwise calculation of percentiles along the spatial and temporal dimensions. A temporal percentile is calculated over the full simulation period for each local off-field grid cell (1 m^2), for example, a PECsoil(*x*[*t*75]) represents the spatial distribution of the 75th percentile local PECsoil over time. From these single values across 1 m^2 grid cells, a spatial percentile is calculated. A PECsoil(*x*90[*t*75]) represents the 90th spatial percentile of the local 75th percentiles over time (which can be read as "90% of off-field soil grids in 75% of time will have an exposure less than"). Such PECsoil values can be calculated to represent conservative exposure assessment endpoints (EAEs) and set in relation to ecotoxicological effect endpoints in standard RA. In contrast to realistic worst-case exposure estimates (e.g., using the Step-2 approach from FOCUS [2001]), these EAEs represent transparent temporal and spatial dimensions, their scales, the statistical groups of off-field soil patches within a maximum distance from the field, and further attributes (e.g., off-field land cover and/or use type). Thus, such explicitly derived EAEs provide improved information for the risk assessor to assess the level of protection even in lower-tier RA. A range of these PECsoil values are calculated for lindane and summarized in Table 1. According to the distance dependence of spray-drift depositions (Bub et al., 2020), as well as the runoff deposition filter functions (Runoff section) from the field edge, exposure values of off-field soil areas are highest close to the edge-of-field (Table 1, Dist = "0–5 m") and decline with distance (Table 1, e.g., Dist = "0–10 m," Dist = "2–5 m"). Consequently, large off-field soil patches like grasslands (e.g., Table 1, Dist = "0–50 m," "0–100 m") likely receive significant exposure at their margins to fields (where a PPP is applied) but have reduced exposure in other more distant areas of the grassland. Thus, the assessment of SPGs referring to large off-field soil patch areas might consider exposure heterogeneity as it relates to organism populations within the grassland and factors beyond pesticide risk, for example, off-field soil management conditions like fertilizer input. The variability of EAEs is quite robust against model input variability (Table 1, "lowerConf95" and "upperConf95"). This "variability filtering" of EAEs at the edge-of-field scale (as represented by the Schematic-1 scenario) occurs due to aggregation over many local (1 m^2) and temporal (days) exposure values. However, at the local scale, that is, for each (1 m^2, day), exposure values are quite variable according to the variability given in the spray-drift model

TABLE 1 Spatial percentiles from the local 75th percentile temporal PECsoil(*x*[*t*75])

Dist (m)	Min	1%	5%	10%	25%	50%	75%	90%	95%	99%	Max	
0–5	0.044	0.046	0.049	0.052	0.057	0.067	0.081	0.134	0.151	0.178	0.193	LowerConf95
	0.045	**0.046**	**0.050**	**0.052**	**0.058**	**0.067**	**0.082**	**0.136**	**0.152**	**0.181**	**0.197**	**Mean**
	0.046	0.047	0.050	0.053	0.058	0.068	0.083	0.137	0.154	0.183	0.201	UpperConf95
2–5	0.044	0.046	0.048	0.050	0.054	0.059	0.066	0.074	0.078	0.083	0.088	LowerConf95
	0.045	**0.046**	**0.049**	**0.050**	**0.054**	**0.060**	**0.067**	**0.075**	**0.078**	**0.084**	**0.089**	**Mean**
	0.046	0.047	0.049	0.051	0.055	0.060	0.067	0.075	0.079	0.085	0.090	UpperConf95
0–10	0.026	0.028	0.030	0.032	0.037	0.052	0.067	0.091	0.134	0.168	0.193	LowerConf95
	0.026	**0.028**	**0.031**	**0.033**	**0.038**	**0.052**	**0.068**	**0.092**	**0.136**	**0.170**	**0.197**	**Mean**
	0.027	0.029	0.031	0.033	0.038	0.053	0.068	0.093	0.137	0.171	0.201	UpConf95
0–20	0.010	0.012	0.013	0.014	0.017	0.031	0.052	0.072	0.091	0.157	0.193	LowerConf95
	0.011	**0.012**	**0.014**	**0.015**	**0.017**	**0.031**	**0.052**	**0.072**	**0.092**	**0.159**	**0.197**	**Mean**
	0.011	0.012	0.014	0.015	0.018	0.031	0.053	0.073	0.093	0.161	0.201	UpperConf95
0–50	0*	0*	0*	0.001	0.003	0.009	0.021	0.052	0.067	0.134	0.193	LowerConf95
	0*	**0***	**0.001**	**0.001**	**0.003**	**0.009**	**0.021**	**0.052**	**0.068**	**0.136**	**0.197**	**Mean**
	0*	0*	0.001	0.001	0.003	0.009	0.021	0.053	0.068	0.137	0.201	UpperConf95
0–100	0*	0*	0*	0*	0*	0*	0.009	0.031	0.052	0.090	0.193	LowerConf95
	0*	**0***	**0***	**0***	**0***	**0***	**0.009**	**0.031**	**0.052**	**0.091**	**0.197**	**Mean**
	0*	0*	0*	0*	0*	0*	0.009	0.031	0.053	0.093	0.201	UpperConf95

Note: The arithmetic mean represents the expectation values over MC runs ($n = 30$), for example, the 90th percentile spatial PECsoil (PECsoil[*x*90{*t*75}]) for off-field soil segments occurring within the 0–10 m distance from fields is shaded in gray (experiment lindane, Schematic-1 [L-01], PECsoil in [mg a.s./kg soil]). Abbreviations: Max, maximum; MC, Monte Carlo; Min, minimum; PECsoil, predicted environmental concentration in soil.

(Bub et al., 2020) as well as by conditions affecting local runoff depositions, which are a composite of random (e.g., weather) and locally deterministic conditions (e.g., spatial morphological relationship of a 1 m^2 off-field soil cell to a neighboring field).

Contour plots provide insight into the relationship between the spatial and temporal exposure patterns that are essential to assess the protection level of off-field soil organisms using EAEs in standard-tier RA. Figure 5 shows contour plots of temporal (*x*-axis) and spatial (*y*-axis) PECsoil

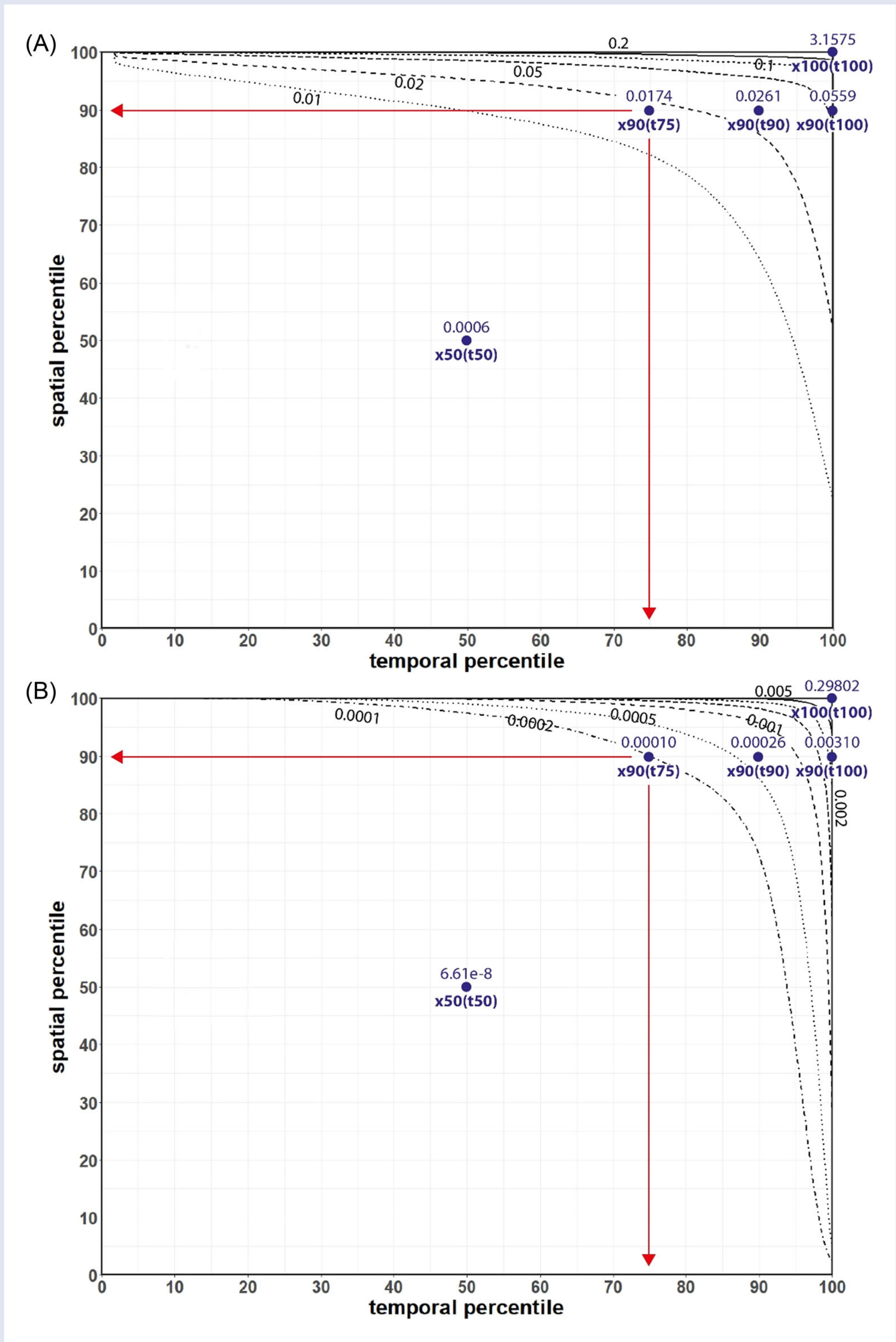

FIGURE 5 Contour plot of edge-of-field (0–10 m) off-field PECsoil (upper 5 cm [mg/kg]) for lindane (A) and thiacloprid (B) using Landscape-1 scenario, variable wind, and a 5 m in-crop buffer (Experiments L-25 and T-14); abbreviations "x_*t*" stand for calculated PECsoil percentiles, for example, the red arrows at *x*90*t*75 = PECsoil(*x*90[*t*75]) that represent the 90th spatial percentile over the 75th temporal percentile PECsoil. PECsoil, predicted environmental concentration in soil

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percentiles for lindane (Figure 5A) and thiacloprid (Figure 5B). For example, the point *x*90(*t*75) in the charts (red arrows) indicates that in 75% in time (of the simulation days, *x*-axis) and for 90% in space (the off-field grid cells, *y*-axis), the PECsoil was <0.0174 mg/kg for lindane and 0.0001 mg/kg for thiacloprid. The contours demonstrate the different spatiotemporal PECsoil patterns for the two a. s. of different soil degradation properties (DT50 of 148 vs. 18 days for lindane and thiacloprid, respectively).

In Figure 6, selected spatiotemporal PECsoil percentiles are presented (i) to gain first insights into the spatiotemporal exposure pattern for spray-drift and runoff (Collection 1), (ii) for a comparison between scenarios (Collection 2), and (iii) to learn about the effect of mitigation measures (Collection 3). The definitions of all the experiments conducted in the case study are listed in Supporting Information: Tables S4 and S5 and outcomes are provided in the Supporting Information tables (Supporting Information: Section S1.5 and Supporting Information).

The contour plots (Figure 5) and the bar graphs (Figure 6, e.g., Collection 1) show a high variability of off-field exposure within 10 m of the field, with PECsoil values ranging over orders of magnitudes in space and time. Local maximum PECsoil over time and space (PECsoil[*x*100{*t*100}], the upper right corner of charts in Figure 5) represent singular extremes occurring for one 1 m^2 cell once in 3650 days. Most off-field soil areas receive considerably lower PECs, as illustrated by a spatial 90th percentile of the temporal 75th percentile (PECsoil[*x*90{*t*75}], Figure 6, Collection 1, *x*90_*t*75). The temporal variability is more pronounced for the faster-degrading thiacloprid. This can be seen in the steep decline in PECsoil temporal percentiles at the same spatial percentile *x*90(*t*100, *t*90, *t*75). Temporal variability becomes even higher when moving from a permanent worst-case wind direction (Figure 6, Panel 2A) to a more realistic variable distribution (Figure 6, Panel 2D). For both a. s., the singular local maximum PECsoil(*x*100[*t*100]) is primarily driven by spray-drift exposure (Collection 1, comparing Panels 1B,C and 2B,C). Graph 1D (Collection 1) illustrates that an a.s. with a longer DT50 in soil like lindane (148 days) is present on the surface of arable fields for a longer time and thus more prone to become mobilized by runoff. The fast degradation of thiacloprid (DT50 = 18 days) reduces both the temporal availability for runoff discharges and the accumulation of the deposited compound in the off-field area. This results in a PECsoil(*x*90[*t*90]) about an order of magnitude below PECsoil(*x*90[*t*100]), even though it is applied twice per year. The comparison of exposure pattern between an edge-of-field (0–10 m; Figure 6, Panels 1D and 2D) and a larger off-field soil habitat (0–100 m, e.g., a grassland patch, Figure 6, Panels 1E and 2E) shows that protection goals referring to larger habitats of soil organisms are basically met, as significant exposure likely affects only parts of such habitats. In general, the spatiotemporally explicit exposure patterns show that spray-drift and runoff are not simply additive. Even for lindane with slow degradation, a PECsoil(*x*90[*t*75]) from the spatiotemporally explicit approach is about two orders of magnitude below a local realistic worst-case approach, resulting in a PEC_FOCUS-STEP2 = 0.72 mg a.s./kg.

Schematic versus landscape scenarios

Real-world landscape compositions, structure, and morphology are likely to affect off-field soil exposure. Thus, differences of the spatiotemporal exposure pattern are expected between the schematic and the real-world landscape scenarios. As the edge-of-field scale plays a prominent role in SPGs in off-field soil RA (EFSA PPR Panel, 2017), the comparison of off-field soil EAEs between the schematic and the real-world landscape scenarios focused on off-field soil areas occurring in the first 10 m vicinity of fields (e.g., of wood, grassland, and natural areas). Thus, the comparison is actually an edge-of-field analysis at the landscape scale. Furthermore, the evaluation of the exposure pattern needs to take into account that off-field soil habitats in real-world landscapes are frequently represented by field margin strips of smaller width than the full 0–10 m considered in the Schematic-1 edge-of-field scenario analysis. For SPGs referring to the landscape scale (e.g., for biodiversity endpoints), analysis can be done taking all off-field soil into account occurring at any distance from the fields.

Results for both lindane and thiacloprid show that local maximum PECsoil values over entire space and time are higher for the real-world landscapes than for Schematic-1 (Supporting Information: Section S2.4, e.g., PECsoil(*x*100[*t*100]) Schematic-1 ≈ 0.6 mg/kg, PECsoil(*x*100[*t*100])_Landscape-1/-2/-3 ≈ 2 mg/kg). Such local extremes are driven by runoff concentration in local off-field soil areas due to landscape morphology, as typically runoff occurs only along one field boundary or even on local "hot-spots"; Figure 4 and Supporting Information: Section S2.3), and can possibly occur for exceptional local spray-drift depositions because the total edge-of-field boundary is much larger in real-world landscapes, hence causing a higher chance that extremes from the spray-drift distribution might occur. These maximum PECsoil values are exceptional local hot-spots in space is shown by the 99th spatial percentiles (*x*99[*t*100]), which are in the same order of magnitudes for the schematic and the landscape scenarios (PECsoil[*x*99{*t*100}] ≈ 0.4–0.6 mg/kg across all scenarios).

For slowly degrading lindane, the 90th percentile spatial PECsoil of upper end temporal percentiles (*x*90[*t*100], *x*90[*t*90], *x*90[*t*75]) are similar for the schematic and landscape scenarios (Figure 6, Collection 2, Supporting Information: Section S2.4, Table S8, and Supporting Information: PECsoil(*x*90[*t*100]) ≈ 0.2 mg/kg, PECsoil(*x*90[*t*90]) ≈ 0.1 mg/kg, PECsoil(*x*90[*t*75]) ≈ 0.06 mg/kg). For 75% of off-field soil areas and upper end temporal percentiles, PECsoil values are lower for the real-world landscapes than for the schematic (PECsoil[*x*75{*t*90}]_Schematic-1 = 0.072 mg/kg, PECsoil[*x*75{*t*90}]_Landscape-1 = 0.045 mg/kg, PECsoil[*x*75{*t*90}]_Landscape-2 = 0.044 mg/kg, PECsoil[*x*75{*t*90}]_Landscape-3 = 0.052 mg/kg). For half of the off-field soil

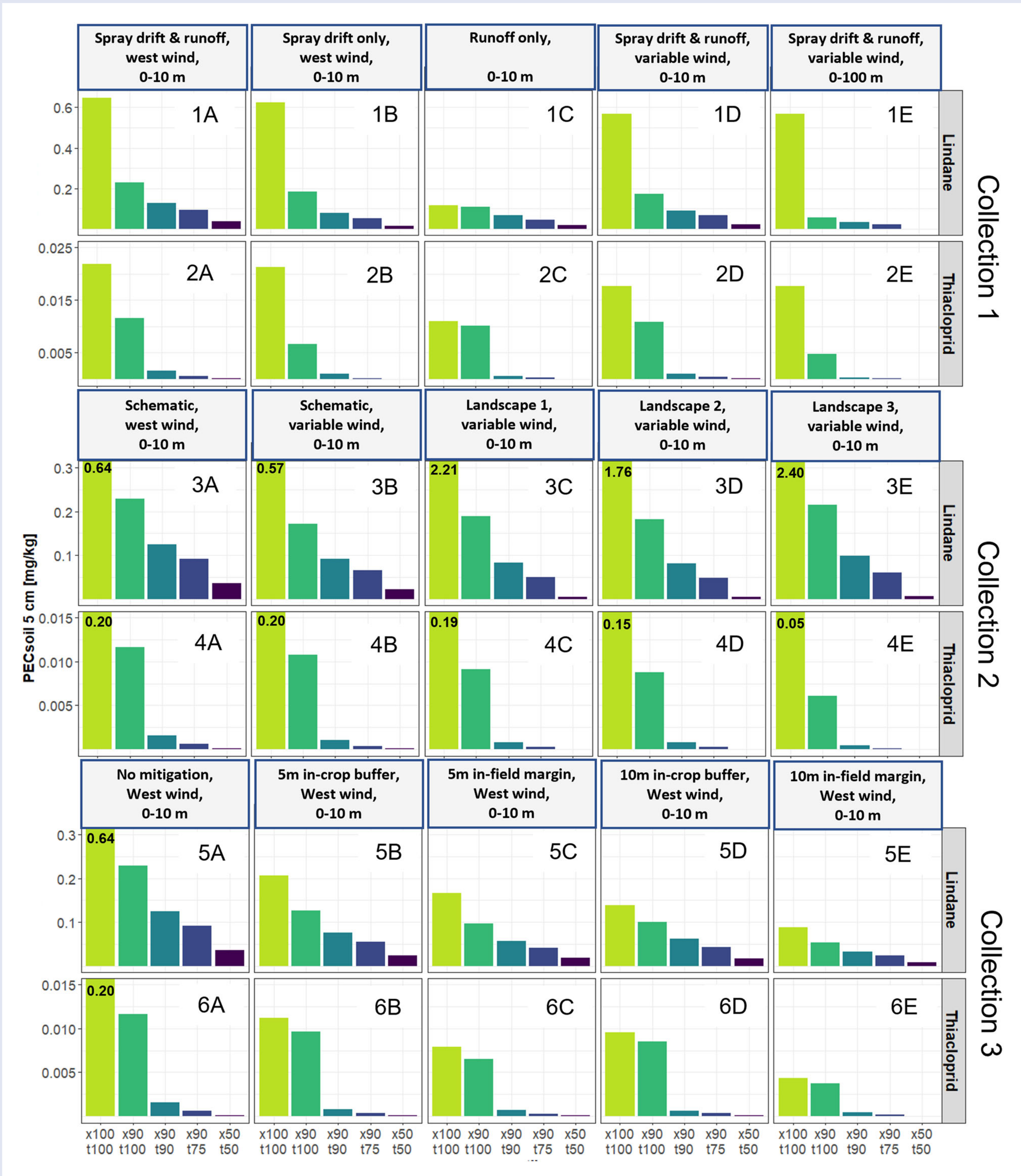

FIGURE 6 Spatiotemporal PECsoil percentiles for lindane and thiacloprid (rows). *X*-axis abbreviations "*x*_*t*" stand for spatial (*x*) percentile over local temporal (*t*) percentiles, for example, PECsoil(*x*90[*t*75]) represents the spatial 90th percentile over the 75th percentile PECsoil over time (10 years). "0–10 m" defines the maximum distance of off-field soil from field edge. Labels are supplied at the top of the bar for *x*100(*t*100) PECsoil values that exceed the *y*-axis. Collection 1 provides results for the analysis of individual exposure routes using the Schematic-1 scenario; Experiments: (A) L-01, T-01; (B) L-02, T-06; (C) L-05, T-20; and (D, E) L-08, T-23. Collection 2 illustrates results from using different scenarios, Schematic-1, Landscape-1, -2, and -3; Experiments: (A) L-01, T-01; (B) L-08, T-23; (C) L-10, T-02; (D) L-11, T-03; and (E) L-31, T-04. Collection 3 focuses on effects of mitigation measures using the Schematic-1 edge-of-field scenario; Experiments: (A) L-01, T-01; (B) L-22, T-10; (C) L-12, T11; (D) L-39, T-31; and (E) L-13, T-21. PECsoil, predicted environmental concentration in soil

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areas and the entire simulation time period (of 10 years), PECsoil values are lower in real-world landscapes than in the schematic scenario (*x*50[*t*100], *x*50[*t*90], *x*50[*t*75]; Supporting Information: Table S8).

For fast-degrading thiacloprid, results for the landscape scenarios were slightly below those for the schematic scenario at the 90th spatial percentile (Supporting Information: Section S2.4 and Table S9): PECsoil(*x*90[*t*100])_Schematic-1 ≈ 0.01 mg/kg, PECsoil(*x*90[*t*100])_Landscape-1/-2/-3 ≈ 0.006 –0.009 mg/kg, PECsoil(*x*90[*t*90])_Schematic-1 ≈ 0.001 mg/kg, PECsoil(*x*90[*t*90])_Landscape-1/-2/-3 ≈ 0.0004–0.0007 mg/kg. At the 75th spatial percentile PECsoil, the landscape scenarios are about half of that of the schematic (Supporting Information: Table S9): PECsoil(*x*75[*t*100])_Schematic-1 ≈ 0.01 mg/kg, PECsoil(*x*75[*t*100])_Landscape-1/-2/-3 ≈ 0.003–0.005 mg/kg, PECsoil(*x*75[*t*90])_Schematic-1 ≈ 0.0007 mg/kg, PECsoil(*x*75[*t*90])_Landscape-1/-2/-3 ≈ 0.0002–0.0004 mg/kg. As thiacloprid shows fast degradation in soil, the 90th temporal percentile (PECsoil_*x*[*t*90]) for the entire off-field soil area (i.e., for all spatial percentiles) is ≤0.01 mg/kg in the real-world landscapes. These results for thiacloprid were obtained for a twofold application that comes with a correspondingly higher chance for increased and broader local spray-drift depositions.

Supporting Information: Table S4 presents the parameterization for the experiments discussed here, while Supporting Information: Table S5 includes additional experiments not discussed herein. xOffFieldSoil model input files (i.e., *experiment*.xrun) are provided in the Supporting Information as well as with the model provision on GitHub (https://github.com/xlandscape/xOffFieldSoilRisk).

In summary, landscape composition and structure clearly affect exposure to off-field soil organisms. Spatiotemporal PECsoil patterns depend on landscape composition and structure, percentile ranges (spatial and temporal), substance properties (DT50), and application (e.g., single vs. multiple). Further studies are required for additional insights, for example, to quantify the protection level of a single edge-of-field off-field soil area compared to a collection of edge-of-field off-field soil areas as present in real-world landscapes. Beyond the EAEs discussed herein, consequences of spatiotemporal exposure patterns to off-field soil organisms become visible and transparent when linking soil exposure models directly with effect models.

In case an SPG refers to the spatial scale of larger off-field soil units like grasslands, as expected, the results show (Supporting Information) that the majority of the areas of larger off-field soil patches do not receive significant loadings, leading to correspondingly lower PECsoil values for the entire patch scale.

Mitigation

The bar graph Collection 3 in Figure 6 shows the effects of mitigation measures for the Schematic-1 edge-of-field scenario utilizing a permanent worst-case wind direction. Imposing a 5 m (10 m) in-crop buffer as spray-drift mitigation to the use of lindane cut selected spatiotemporal PECsoil percentiles by ≈30% to 50% (Figure 6, Panels 5A, 5B, 5D). Using an in-field margin reduces spray-drift and runoff entries and adds a significant reduction of exposure due to runoff filtering (Panels 5A, 5C, 5E). PECsoil reductions due to mitigation effects for thiacloprid are somewhat lower due to its twofold application, resulting in a higher likelihood that larger areas receive significant spray-drift input. All results are available in the Supporting Information, including mitigation analysis for the real-world landscapes. As indicated in Figure 4B, in real-world landscapes, runoff follows the landscape morphology, resulting in local runoff hot-spots (Supporting Information: Sections S1.5, S2.3 and Figure S17). This deterministic exposure characteristic provides a means for generic landscape-scale mitigation measures (e.g., vegetated filter strips, contour-ploughing; Alix et al., 2013; Wendland et al., 2016, 2023).

Exposure endpoints in RA

Spatiotemporal percentiles, like PECsoil(*x*90[*t*75]) values, can be quantitatively introduced in standard RA. EAEs from the case study of lindane were used in a standard RA. A lower- and a higher-tier RAC RAC_Lindane-lowerTier = 0.041 mg/kg and a RAC_Lindane-higherTier = 0.1 mg/kg (Supporting Information: Section S2.3) were used to calculate RQs: RQ = PEC/RAC. In a standard RA, acceptable risk is indicated for RQ < 1.

Results from using the RAC_Lindane-higherTier show that the local realistic worst-case *PECsoil_FOCUS-STEP2* = 0.72 mg/kg equates to a RQ ≈ 7 (using RAC_Lindane-higherTier), which is >1, that is, indicating unacceptable risk. In contrast, from the case study using the spatiotemporally explicit approach (Supporting Information: Table S4), the EAEs located at the upper ends of the spatial and temporal exposure distributions of PECsoil(*x*90[*t*75]) result in RQs < 1 for all scenarios using RAC_Lindane-higherTier (Supporting Information: Table S6). For the edge-of-field scenario Schematic-1, using variable wind conditions and an even more conservative EAE represented by the PECsoil(*x*90[*t*90]), the RQ = 0.91 (Experiment L-08). Imposing a 5 m in-crop buffer as a mitigation measure results in RQs < 1 for the PECsoil(*x*90[*t*90]) for all scenarios.

A single RAC was derived for the RQ calculation of thiacloprid (RAC_Thiacloprid = 0.037 mg/kg; Supporting Information: Section S2.3). For the local realistic worst-case, *PECsoil_FOCUS-STEP2* = 0.034 mg/kg equates to an RQ < 1, that is, indicating no unacceptable risk. Likewise, from the case study using the spatiotemporally explicit approach (Supporting Information: Table S4), EAEs of the spatial and temporal exposure distributions of PECsoil result in RQs < 1 for all scenarios (Supporting Information: Table S6).

Such ranges of RQs and their transparent relationship to the protection of off-field soil organisms in space and time demonstrate that a more realistic spatiotemporally explicit approach provides an improved information basis for risk assessors to decide upon acceptable risk levels. In the same way, the approach supports the identification of effective and efficient mitigation measures balancing between the range of ecosystem services requested from cultivated landscapes. Mapping of potentially critical areas (e.g., of RQ > 1; Supporting Information: Figure S17) can support the identification of landscape-scale mitigation measures (e.g., installing vegetated filter strips or designing more favorable structural relationships between fields and off-field soil).

The definition of certain spatial and temporal exposure percentiles (e.g., PECsoil[*x*90{*t*75}]) as EAEs to be used in a RA for soil organisms is not trivial. Depending on the ecological characteristics (e.g., species occurrence, movement, life cycle, and species sensitivity), the protection level of the same EAE can be different for different species. Further work is needed to define EAEs for different species (groups, traits). Ultimately, the spatiotemporally explicit exposure outcomes should be directly fed into effect models (see the Outlook section).

CONCLUSION

In this work, we present an initial spatiotemporally explicit model approach to assess exposure (and risk) of off-field soil organisms due to spray-drift and runoff entries of pesticides from nearby fields. The approach is flexible and able to operate at any desired spatial and temporal resolution to propagate variability of relevant processes (e.g., PPP use, spray-drift deposition, rainfall-induced runoff) into off-field soil exposure (and effect) patterns. This is achieved by a combination of discretizing spatial and temporal variability, together with defining scale-dependent PDFs utilized within a MC approach. The spatiotemporally explicit raw outcome can be transparently aggregated into exposure patterns for scientific insights and to build meaningful AEs for regulatory RA. The impact of risk mitigation options can be analyzed in detail, for example, comparing PPP use-specific mitigations like drift-reducing nozzles against generic landscape design options such as runoff filter strips. The model is scalable and can be used with any scenario ranging from simple schematic edge-of-field to larger real-world landscapes. The architecture of the framework underlying the xOffFieldSoil model is modular. This is a key design principle that allows the use of individual process components of different complexity (and reality) levels and validation status, and hence to build models that operate at different regulatory tiers. To enhance transparency and development, the model and example scenarios are open source.

The case study demonstrates the applicability of xOffFieldSoil for the intended purposes. It reveals details about the spatiotemporal dynamics of spray-drift and runoff exposure to off-field soil areas for two substances with different properties. Exposure percentiles are derived from the raw spatiotemporally explicit outcome, for example, in a stepwise way, first along the temporal dimension for each spatial grid cell and then along the spatial dimension for all grid cells. These PECsoil percentiles are introduced as EAEs into RQ calculations within current regulatory RA approaches. A 90th spatial percentile taken over the 75th temporal percentile of local exposure values (PEC[*x*90{*t*75}]) protects 90% of the off-field soil populations for 75% of the time. Visualization of such percentiles in contour plots supports an understanding of protection levels with respect to different soil organisms' traits and soil functions. However, targeted assessment of effects with respect to SPGs requires the use of effect models. Direct linking of exposure and effect models in appropriate spatial and temporal resolution is a core value of the spatiotemporally explicit xOffFieldSoil approach.

As the percentiles and their distribution in the case study indicate, a PECsoil based on FOCUS-Step 2 represents a realistic worst case due to its range of conservative assumptions. Their relationship to protection levels is not transparent. Risk management decisions drawn from exceptional worst-case occasions can lead to biased labeling of crop protection measures. An indication of unacceptable risk from an off-field soil RA perspective using unrealistic assumptions can be an impediment to the use of a PPP of a positive RA profile from other risk perspectives (e.g., aquatic, plants). The presented approach can be used to transparently identify effective and efficient combinations of PPP application-specific mitigation with generic (local) landscape-scale risk management options (e.g., Wendland et al., 2016, 2023).

We believe that a discussion with all stakeholders on the use of more realistic and landscape-scale RA approaches for off-field-soil organisms within the regulatory scientific community would be of high value. This should include topics of appropriate exposure AEs for lower-tier RA, the development of landscape scenarios that can be used in RA, and the modular integration of exposure and effects models to directly address SPGs.

OUTLOOK

The xOffFieldSoil model, scenarios, and the case study presented are intended to make a step forward toward more realistic RA for off-field soil organisms. xOffFieldSoil can now be used to gain in-depth insights into systems' behavior to support the conceptual and technical development of future tiered exposure approaches, scenarios, and RA tiers. The work presented here is provided as open-source software to feed discussions in the regulatory scientific community (GitHub https://github.com/xlandscape/xOffFieldSoilRisk).

Additional model components are being developed to enhance the functionality of xOffFieldSoil as well as to improve its processing efficiency. These include a US-based version of the PRZM module (PRZMus), a "lite" version of PRZM with a focus on core runoff calculations and more flexible runtime control (PRZMlite), a refined soil concentration module based on the PRZM leaching model (PECsoil_przm), a VFSMOD-based runoff filtering module (Vegetative Filter Strip MODeling system, Muñoz-Carpena et al., 1999, 2015), and a module to enable simulation of real-world multiple pesticide uses in a landscape (xPProtection). xPProtection allows the definition of PPP application sequences to multiple crops in a landscape, taking tank mixes and mitigation into account. Furthermore, a spray-drift component based on AgDRIFT® used by USEPA (Teske et al., 2002) is being implemented. Alternative empirical or mechanistic models can be used as components to calculate PECsoil within xOffFieldSoil, and so to further improve the exposure calculation of off-field soil organisms (e.g., PERSAM, PEARL, PELMO; EFSA, 2017) as can be seen in Supporting Information: Figure S1, which shows the recent xOffFieldSoil model scheme.

The EAEs introduced here can be used to refine standard RA, and yet should be regarded as an interim solution as SPGs for soil organisms are concerned with biological entities, and hence require corresponding modeling endpoints like the population level (EFSA PPR Panel, 2017). As effect models are also becoming increasingly more available for RA purposes (Bart et al., 2021; Forbes et al., 2020; Gergs et al., 2022; Johnston et al., 2014a, 2014b, 2018; Meli et al., 2013; Raimondo et al., 2021; Rakel et al., 2020; Reed et al., 2016; Roeben et al., 2020), an important next step is to integrate effect models into xOffFieldSoil, and so directly link them to the exposure module in required spatial and temporal resolutions. The outcome of xOffFieldSoil then provides biological AEs and their spatiotemporal scales directly addressing SPGs of off-field soil organisms.

The validation status of the xOffFieldSoil model needs detailed analysis and documentation. As a composition of individual models, the validation of xOffFieldSoil can be derived, to some extent, from the validation of its individual components and employed scenarios. In this context, systematic monitoring and its integration with modeling into "systems-based approaches" are considered to play an important role (EFSA, 2021). A 2D MC extension is under development to allow for uncertainty and sensitivity analysis.

The concepts and model development presented here addressing RA of off-field soil organisms can also be applied to "off-field" nontarget terrestrial plant RA in the EU and US (e.g., Plant Assessment Tool utilized for endangered species RA, USEPA, 2022, and modeling population and community effects of herbicide drift, Reeg et al., 2014).

In order to account for harmonization, transparency, and reproducibility in regulatory RA, a conceptual framework for off-field soil scenarios should be developed covering aspects such as the definition and identification of off-field soil types, potential data sources and data processing, and documentation and publication.

AUTHOR CONTRIBUTION

Thorsten Schad: Conceptualization; data curation; funding acquisition; investigation; methodology; project administration; resources; software; writing—original draft; writing—review and editing. **Sascha Bub**: Data curation; formal analysis; investigation; methodology; software; visualization. **Magnus Wang**: Methodology; software; validation; writing—review and editing. **Christopher M. Holmes**: Investigation; visualization; writing—original draft; writing—review and editing. **Joachim Kleinmann**: Methodology; software; validation. **Klaus Hammel**: Methodology; validation; writing—review and editing. **Gregor Ernst**: Funding acquisition; supervision; writing—review and editing. **Thomas G. Preuss**: Funding acquisition; supervision; writing—review and editing.

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OPEN DATA BADGE/OPEN MATERIAL BADGE

This article has earned an Open Data Badge and Open Material Badge for making publicly available the digitally shareable data necessary to reproduce the reported results. The data and material are available at https://github.com/xlandscape/xOffFieldSoilRisk. Learn more about the Open Practices badges from the Center for Open Science: https://osf.io/tvyxz/wiki.

DATA AVAILABILITY STATEMENT

Data and associated models for this manuscript are available as the Supporting Information, online via GitHub (https://github.com/xlandscape/xOffFieldSoilRisk).

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SUPPORTING INFORMATION

5a Off-field soil risk Supporting Information.pdf—Additional information on model design, scenarios utilized, input parameters for all simulations and case study results (summarized).

5b SuppInfo Off-Field Soil Risk FOCUSsw-Step2.xlsx - FOCUS Step 2 PEC calculation worksheet.

5c SuppInfo Off-Field Soil Risk Lindane_PecSoil percentiles.xlsx - full table of spatiotemporal results for lindane simulations presented in the article.

5d SuppInfo Off-Field Soil Risk Thiacloprid_PecSoil percentiles.xlsx - full table of spatiotemporal results for thiacloprid simulations presented in the article.

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