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Special Series

Incorporating climate projections in the environmental risk assessment of pesticides in aquatic ecosystems

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EDITOR'S NOTE:

This article is part of the special series "Integrating Global Climate Change into Ecological Risk Assessment: Strategies, Methods and Examples." The papers were generated from a SETAC Pellston Workshop held at Oscarsborg Fortress near Oslo, Norway, in June 2022. The international workshop included climate change modelers, risk assessors, toxicologists, and other specialists with a diversity of backgrounds and experience. The findings of the series demonstrate that climate change can successfully be incorporated as an integral part of risk assessment for a wide range of environments, to address the issues of long-term, adaptive environmental management.

Abstract

Global climate change will significantly impact the biodiversity of freshwater ecosystems, both directly and indirectly via the exacerbation of impacts from other stressors. Pesticides form a prime example of chemical stressors that are expected to synergize with climate change. Aquatic exposures to pesticides might change in magnitude due to increased runoff from agricultural fields, and in composition, as application patterns will change due to changes in pest pressures and crop types. Any prospective chemical risk assessment that aims to capture the influence of climate change should properly and comprehensively account for the variabilities and uncertainties that are inherent to projections of future climate. This is only feasible if they probabilistically propagate extensive ensembles of climate model projections. However, current prospective risk assessments typically make use of process-based models of chemical fate that do not typically allow for such high-throughput applications. Here, we describe a Bayesian network model that does. It incorporates a two-step univariate regression model based on a 30-day antecedent precipitation index, circumventing the need for computationally laborious mechanistic models. We show its feasibility and application potential in a case study with two pesticides in a Norwegian stream: the fungicide trifloxystrobin and herbicide clopyralid. Our analysis showed that variations in pesticide application rates as well as precipitation intensity lead to variations in in-stream exposures. When relating to aquatic risks, the influence of these processes is reduced and distributions of risk are dominated by effect-related parameters. Predicted risks for clopyralid were negligible, but the probability of unacceptable future environmental risks due to exposure to trifloxystrobin (i.e., a risk quotient >1) was 8%–12%. This percentage further increased to 30%–35% when a more conservative precautionary factor of 100 instead of 30 was used. *Integr Environ Assess Manag* 2024;20:384–400. © 2023 The Authors. *Integrated Environmental Assessment and Management* published by Wiley Periodicals LLC on behalf of Society of Environmental Toxicology & Chemistry (SETAC).

KEYWORDS: Bayesian network; Global climate model; Pesticide runoff; Precipitation intensity; Probabilistic risk assessment

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INTRODUCTION

Global climate change will significantly impact the biodiversity of freshwater ecosystems (Tonkin, 2022), both directly due to drought and heat stress (Woodward et al., 2016), and indirectly due to the interaction between climate change and other stressors (Intergovernmental Panel on Climate Change, 2022; Moe et al., 2022; Noyes & Lema, 2015; Polazzo et al., 2022). Indirect impacts are highlighted by the

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European Environment Agency as specifically important for the European environment (European Environment Agency [EEA], 2019), with an emphasis on pesticides as a prime example of chemical stressors synergizing with climate change (EEA, 2023). More frequent and extreme precipitation events will increase pesticide runoff from agricultural fields and subsequent aquatic exposures. Aquatic exposures might also change in composition, as climate-related changes in pest pressures and crop types will affect application patterns (Kattwinkel et al., 2011).

Although its importance is widely recognized, climate change has not yet been systematically embedded in prospective risk assessment practice (e.g., EEA, 2018). Prospective assessments of chemical risk are typically performed to estimate the likelihood that predicted environmental concentrations (PECs) will exceed a predefined protection level, represented by the environmental concentration below which no adverse effects are expected. As such, prospective chemical risk assessments aim to determine whether a specific chemical, given its foreseen use patterns and distribution in the environment, might present an unacceptable ecological risk. Predicted environmental concentrations are typically derived via process-based computational models that describe emissions and environmental fate of chemicals (e.g., Chiu et al., 2017; Morselli et al., 2018). For pesticides in freshwater environments, the modeling platform World Integrated System for Pesticide Exposure (WISPE) can be used (Bolli et al., 2013). The WISPE platform links models simulating pesticide transport in soils (PRZM; Young & Fry, 2014); chemical fate and transport in aquatic environments (EXAMS; Burns, 2004); and chemical dilution, partitioning, and persistence in shallow, unconfined aquifers (ADAM; Williams, 2010). The WISPE platform allows the incorporation of local climate projections with a daily time step by varying precipitation, air temperature, and solar radiation (see Mentzel, Grung, Holten, et al., 2022).

Prospective risk assessments traditionally produce a single-value risk estimate, without accounting for the uncertainty that is associated with model selection, model parameterization, or the natural variation intrinsically present in space and over time (Di Guardo & Hermens, 2013; Schmolke et al., 2010; Topping et al., 2020). Any prospective chemical risk assessment that aims to capture the influence of climate change should properly and comprehensively account for these variabilities and uncertainties, especially those inherent to projections of future climate (Moe et al., 2022). Local projections of future climate, for example, at the scale of a catchment or stream system, are particularly uncertain because they are generated via the downscaling of projections from global climate models (Benestad, 2016). Indeed, Deser et al. (2012) demonstrated that one single global climate model can produce very different regional temperature and precipitation projections on decadal scales with only tiny differences in initial conditions. As such, employing a small number of global climate models for projecting regional or local future climate is prone to result in misleading outlooks. It is possible to account for such regional internal model variability by using large ensembles of global climate model simulations (Benestad, 2021). Proper consideration of climate uncertainty and variability might be done when output from large (e.g., 30–100 member) ensembles of global climate models are downscaled to regional climate projections that are all propagated into a distribution of plausible risks that comprehensively represent the combined uncertainty and variability of future climate conditions, chemical exposures, and environmental effects (Moe et al., 2022). Unfortunately, many process-based models that predict chemical fate, including WISPE, cannot accommodate extensive multiyear and multiscenario ensembles as input because they are computationally demanding and/or graphical user interface-based. Instead, statistical approximations of the results from exposure models such as WISPE, based on distributions of its input variables, might be used to substitute their high-throughput application.

The explicit consideration of uncertainty through the incorporation of probabilistic, possibly nonlinear, relationships has already been identified as a key principle for the successful integration of climate change into chemical risk assessment practice (Landis et al., 2013). Bayesian network (BN) models can do this in an intuitive way. Bayesian networks are acyclic graphical models, built on conditional probability distributions that describe (preferably causal) relationships between model variables (Aguilera et al., 2011; Carriger & Newman, 2012; Kanes et al., 2017). One of the most beneficial features of a BN is that it can perform both predictive (forward) as well as diagnostic (backward) inference (Carriger & Barron, 2020; Moe, Wolf, et al., 2021). Furthermore, they can use various kinds of data sources for parameterization such as monitoring data, outputs from prediction models, and expert elicitation (Mentzel, Grung, Tollefsen, et al., 2022; Pitchforth & Mengersen, 2013). Bayesian network models are increasingly used in the environmental risk assessment of chemicals (Kaikkonen et al., 2021; Moe, Carriger, et al., 2021), including recently for the environmental risk assessment of pesticides under future climate (Mentzel, Grung, Holten, et al., 2022).

The work presented here lays the foundation for a BN model to estimate the synergistic impacts of pesticide pollution and climate change in a fully probabilistic manner. We apply the model to two pesticides used in pest control for winter wheat in Norway: trifloxystrobin, a fungicide typically applied in autumn, and the herbicide clopyralid, which is typically applied in spring. This case study represents one of three case studies that explore the use of BN methodology for incorporating climate model projections into environmental risk assessment, resulting from the SETAC Pellston workshop addressing this topic.

METHODOLOGY

A schematic representation of our BN model is provided in Figure 1. We adapted the existing BN (Mentzel, Grung, Holten, et al., 2022) in three ways. First, we explicitly

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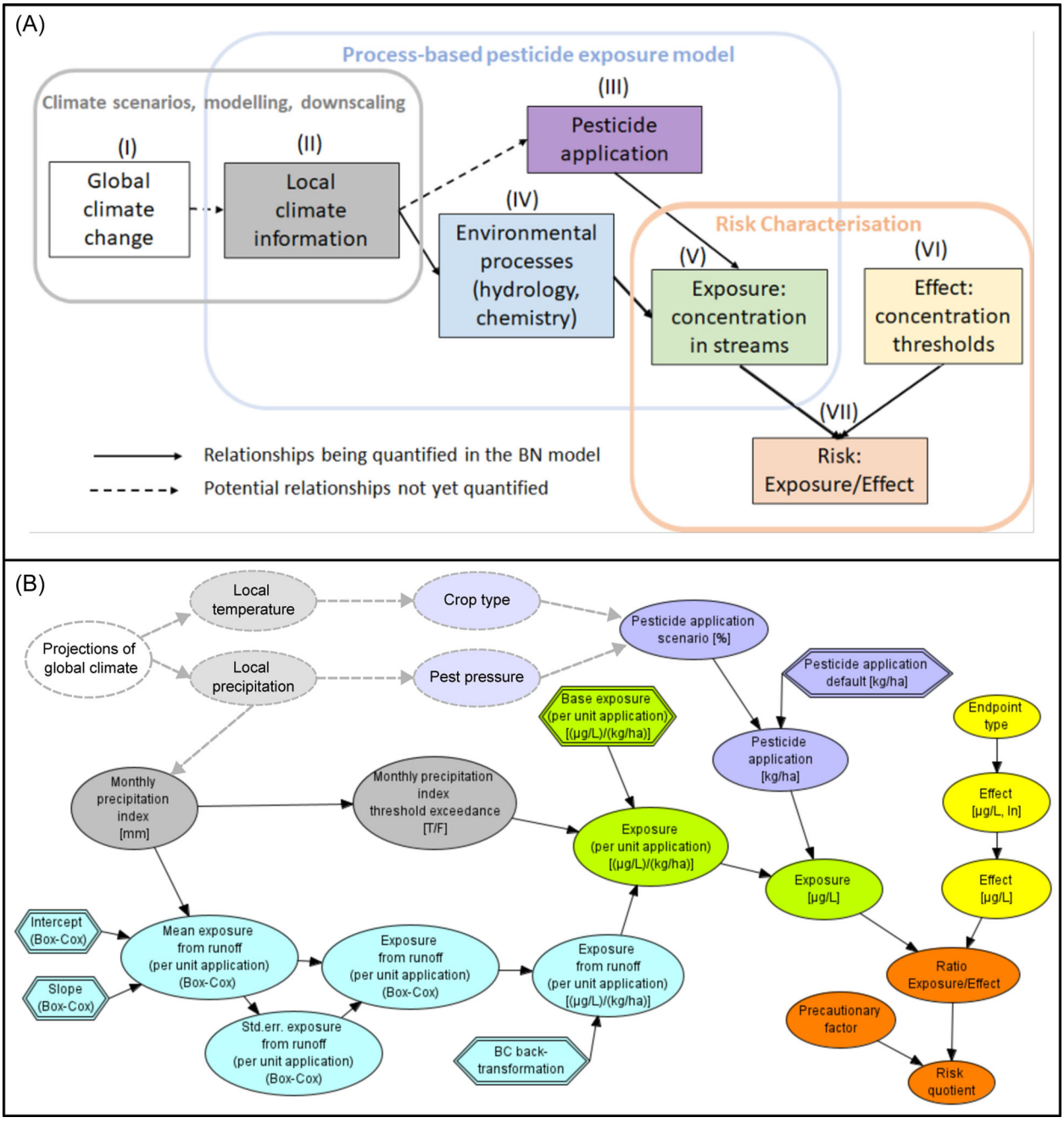

FIGURE 1 Conceptual diagram describing (A) a risk assessment approach for incorporating climate change information into exposure assessment for pesticides in freshwater ecosystems, and (B) the directed acyclic graph of its implementation as a Bayesian network model. Nodes colored according to their respective modules in the conceptual diagram. Ellipses have discrete probability distributions ("discrete chance nodes"); hexagons have fixed single values ("function nodes"); dashed arrows and node outlines represent relationships not yet quantified or implemented

accommodate the downscaling process from global climate change projections to local climate information (modules I and II in Figure 1A), to allow the propagation of ensembles of regional climate projections. Second, we included the option to account for indirect impacts of climate change on aquatic exposures, due to climate-dependent pesticide application patterns (module III). Finally, we developed a statistical methodology to circumvent the computationally laborious WISPE platform (module IV), paving the way for the high-throughput application of the model. The first two adaptations are discussed here but not yet quantified in this updated BN model (dotted arrows in the conceptual diagram in Figure 1A). The third adaptation is showcased here for the fungicide trifloxystrobin and the herbicide clopyralid.

Scenario setting

Two plant pesticides commonly used for the protection of winter wheat were selected for this study: the fungicide

trifloxystrobin, applied in autumn (early October), and the herbicide clopyralid that is applied in spring (early May). The physicochemical and fate properties that determine their environmental behavior are shown in Table 1 and are required as input to the WISPE model. Both pesticides are approved for agricultural use in Norway, the focus of our case study. The field site Syverud, located in Ås (southeast Norway), is considered representative of Norwegian conditions. It is a former meadow, and its soil structure is classified as loam/silt, which has high infiltration capacity, saturated hydraulic conductivity, and aggregate stability (Bolli et al., 2013; Mentzel, Grung, Holten, et al., 2022).

Statistical modeling of the climate-exposure relationship

We adapted and expanded the BN model described in detail previously (Mentzel, Grung, Holten, et al., 2022). It uses the WISPE platform to quantify the relationship between regional climate conditions and in-stream pesticide concentrations (Bolli et al., 2013). World Integrated System for Pesticide Exposure requires as input daily time series of various climate variables, that is, precipitation (cm), air temperature (°C), evapotranspiration (cm), solar radiation (Langley), and wind speed (cm/s), as well as the pesticide application rate (kg/ha) and the day(s) of spraying. For single application events, WISPE generates a series of declining daily in-stream exposure concentrations from the day following pesticide application to 60 days after. Mentzel, Grung, Holten et al. (2022) ran WISPE twice for the period 2001–2099, each run using a different local climate scenario. These scenarios were based on the same emissions scenario (A1B; Nakicenovic et al., 2000) and the same regional climate model for downscaling (RCA3; Samuelsson et al., 2011), but different global climate models, that is, ECHAM5-r3 (Roeckner et al., 2004) and HADCM3-Q0 (Gordon et al., 2000). Since WISPE does not carry over calculations and variables between years, this yielded a total of 198 independent exposure estimates for both trifloxystrobin and clopyralid across the 99 simulation years and the two global climate model runs.

TABLE 1 Physicochemical and fate properties of trifloxystrobin and clopyralid, as used as input to the WISPE model platform

	Trifloxystrobin	Clopyralid
CAS-RN	141517-21-7	1702-17-6
Molecular weight (g/mol)	408.37	192
Solubility (mg/L)	0.61	7850
Vapor pressure (kPa)	3.4	1.36×10^{-6}
K_{OC} (L/kg)	2287	5
Freundlich exponent 1/*n* (–)	0.96	N/A[a]
Plant uptake factor (–)	0	0.5
$DT_{50,soil,lab}$ (days)	0.34	23.2
$DT_{50,water,aerobic}$ (days)	1.1	148
$DT_{50,sediment,anaerobic}$ (days)	1000	1000
$DT_{50,photolysis,direct}$ (days)	2.7	271

Note: Values obtained via Lewis et al. (2016).
Abbreviation: WISPE, World Integrated System for Pesticide Exposure.
[a]No Freundlich exponent available, default assumption of concentration-independent sorption (i.e., Freundlich exponent = 1).

We used these data to evaluate the statistical relationship between local climate variables and the concentrations on the day after a single pesticide application. For many of the simulated years, climate conditions did not vary enough to instigate differences in exposure concentrations, that is, WISPE simulated the same trifloxystrobin exposure concentration of 0.498 µg/L for 170 out of 198 years and the same clopyralid exposure concentration of 0.167 µg/L for 131 out of 198 years. For all other years, simulated concentrations exceeded these values. We were able to relate this pattern to the antecedent precipitation intensity, showing that typically pesticide applications that are preceded by relatively dry periods result in minimum exposure, while the probability of higher exposures increases with more precipitation preceding the day of application (Figure 2). We assume that this behavior can be explained by the presence or absence of surface runoff and found that the best distinctive power was achieved by a monthly precipitation index (I_m; mm) that aggregates all precipitation over the 30-day period up until and including the day of application, as follows:

$$I_m = \sum_{d=1}^{30} \left(\frac{I_d}{d^2} \right). \quad (1)$$

In which I_d is the precipitation intensity at day d (mm), with d defined as the number of days prior to the day of application (at which $d = 1$). This weighted summation of daily precipitation amounts preceding application is conceptually similar to the established hydrological antecedent precipitation index (e.g., Ali et al., 2010). Indeed, the mean I_m is significantly different between WISPE simulations resulting in minimum exposure and those exceeding minimum exposure, for both trifloxystrobin (Figure 2C) and clopyralid (Figure 2D).

Based on this threshold behavior, we constructed pesticide-specific statistical models on the relationship between I_m and exposure concentration $C_{exposure}$ consisting of two phases: a binary probability function that decides whether the base exposure concentration (C_{base}; 0.498 µg/L for trifloxystrobin and 0.167 µg/L for clopyralid) is exceeded at a specific value of I_m (shaded areas in Figure 2A,C), and a linear regression estimating the excess exposure C_{delta} (µg/L) for all instances where C_{base} is indeed exceeded. Binary probability functions were based on nonparametric logarithmic kernel density estimators of the I_m values in each distinct group of observations. The linear regressions were performed on Box–Cox transformed C_{delta} values and were subjected to global validation for normality, heteroskedasticity, linearity, and independence. The Supporting Information contains the annotated R model code for these

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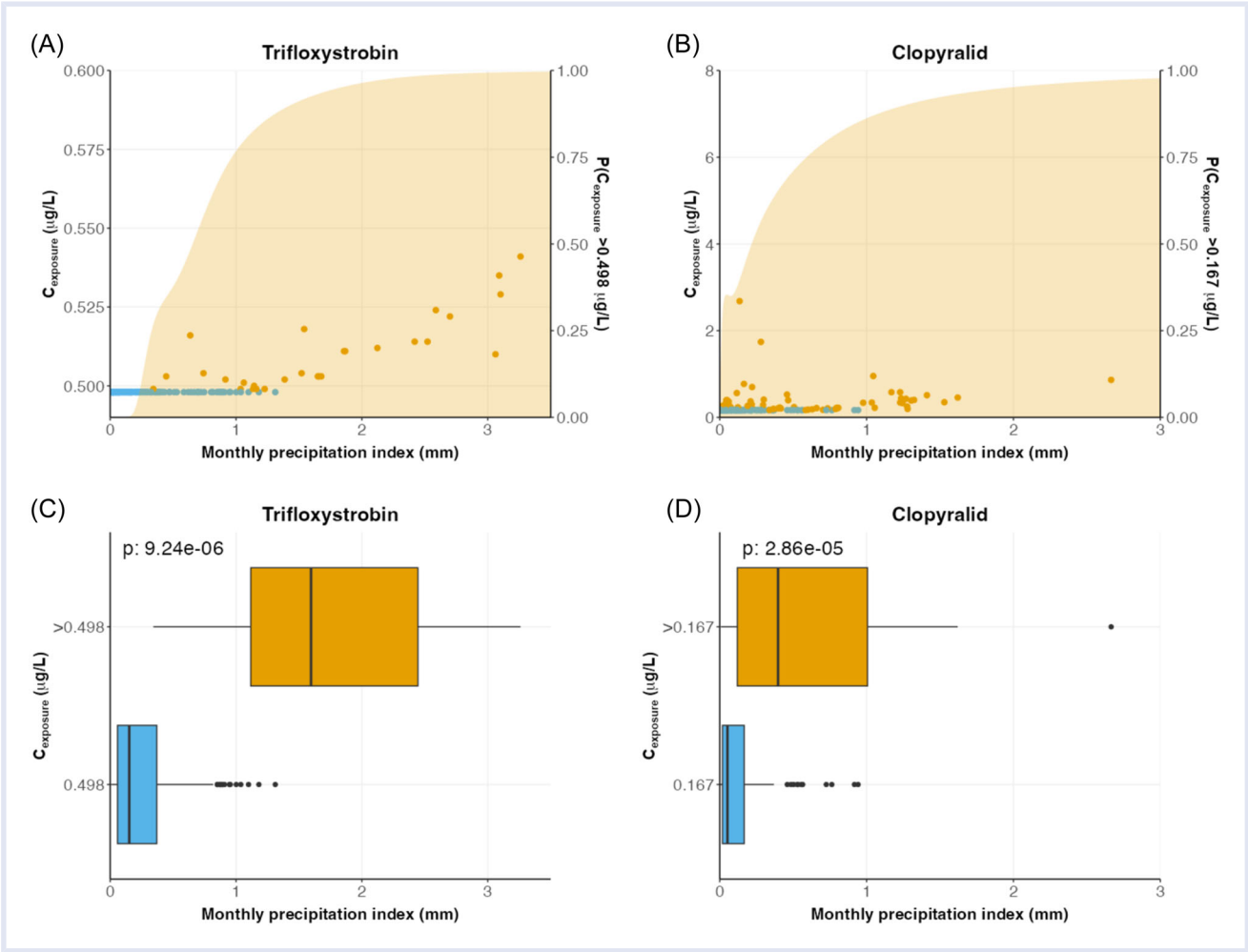

FIGURE 2 Monthly precipitation index and exposure concentrations ($C_{exposure}$) for (A, C) trifloxystrobin and (B, D) clopyralid. Blue dots and boxes: 198 independent WISPE simulations (period 2001–2099; two local climate scenarios as described in Mentzel, Grung, Holten, et al. [2022]) resulting in a base exposure of 0.498 µg/L (trifloxystrobin), or 0.167 µg/L (clopyralid); orange dots and boxes: WISPE simulations resulting in a concentration exceeding base exposure. Shaded orange area in A and B: probability that base exposure is exceeded (secondary *y*-axis). Boxplots in C and D show the distribution of monthly precipitation indices for which WISPE simulations result in base exposure (blue box) or higher than base exposure (orange box), with mean monthly precipitation indices being significantly different in both cases (Welch's *t*-test). WISPE, World Integrated System for Pesticide Exposure

calculations. The resulting statistical models can be used to generate possible future observations of $C_{exposure}$ for either trifloxystrobin or clopyralid (Figure 3). We added a stochastic term to the best estimate of $C_{exposure}$ as returned by the model, reflecting the sampling uncertainty (i.e., the standard error of the prediction) due to the suboptimal fit of the regression line to the data. Figure 3 displays the regressions for both pesticides—with their respective 95% confidence and 95% prediction intervals—including sample draws of possible future observations of $C_{exposure}$.

Bayesian network implementation

The BN was structured as a set of modules or subnetworks (Figure 1A). The original BN (Mentzel, Grung, Holten, et al., 2022) had links from the climate and application scenarios directly to pesticide exposure. The BN model structure presented here has two additional modules: local climate information (II) and environmental processes (III). The pesticides have an identical model structure in terms of nodes, arcs, number of states, and equations; the differences are in the ranges, discretization, values, and parameters of certain nodes (described in Table 2). The full set of states and posterior probability distributions are shown for selected nodes in Figure 4. The models were implemented in the software HUGIN Expert, from which a complete model documentation is generated (Supporting Information). An open online user interface for the two models has been developed to allow for public exploration of the model (https://demo.hugin.com/example/PesticidesInStreams).

The BN consists of 21 nodes of five different types (Table 2): interval, numbered, labeled, Boolean, and constant (single value). Continuous variables such as precipitation, concentrations, and risk quotients (RQ) were discretized into intervals, which is a common procedure for BN nodes. The interval nodes had a relatively high resolution (10 states), which was possible since the conditional probability tables (CPTs) for all

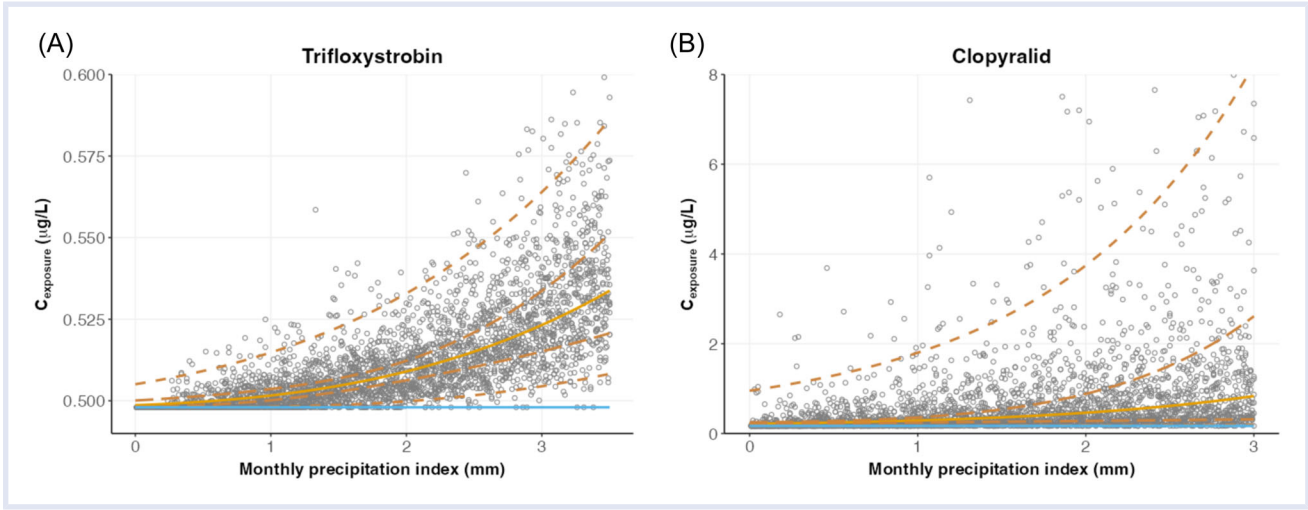

FIGURE 3 Results of our two-step statistical model on the relationship between monthly precipitation index and exposure concentrations ($C_{exposure}$) for (A) trifloxystrobin and (B) clopyralid. Solid lines represent base exposures (blue) and linear regressions on excess exposure C_{delta} (orange). Darker orange lines represent the bounds of the 95% confidence intervals (inner, long-dashed) and 95% prediction intervals (outer, short-dashed). Gray circles are simulated (future) $C_{exposure}$ values, of which 10 were randomly drawn per monthly precipitation index along a gradient with intervals of 0.01 mm

these nodes were generated from expressions such as equations or statistical distributions (either built into HUGIN or generated from the statistical model in R; see Table 2). The range of the exposure and other interval nodes were set to capture the observed or simulated values and included an open upper interval (inf) if requested by the respective expression. Within the given range, the discretization of exposure and effect concentrations as well as I_m was set to be equidistant in the natural logarithm (ln-)scale (these variables typically follow a lognormal distribution). For example, for clopyralid, the node *Expo_from_runoff_per_appl* had an interval width increasing with a factor of 1.65 (corresponding to a constant width of 0.5 at ln-scale), while the node *Expo_per_appl* had an interval width increasing with a factor 2.72 (corresponding to the width of 1 at ln-scale). Variables in the ln-transformed or Box–Cox-transformed scale were discretized by equidistant intervals.

The statistical relationship between local antecedent precipitation intensity and exposure was incorporated as a series of nodes in modules II and IV (Figure 1B). The monthly precipitation index I_m and the intercept and slope of the regression were included as parent nodes of the (Box–Cox-transformed) excess exposure C_{delta}. This best estimate of C_{delta} and the sampling uncertainty associated with the regression were combined into a node reflecting the variation between future observations of C_{delta}. Because this sampling uncertainty varies along the regression curve, that is, it is larger at relatively low and at relatively high values of I_m (Figure 3), its size directly depends on the best estimate of C_{delta}. Finally, Box–Cox-transformed estimates of C_{delta} were first back-transformed before being added to the base exposure, conditional to whether surface runoff occurs at the specific I_m.

To accommodate the future incorporation of alternative pesticide application levels into our model (module III in Figure 1A), we split application rates into a fixed value node reflecting the default rate under current practice (0.150 and 0.050 kg/ha for trifloxystrobin and clopyralid, respectively), and a five-state numeric node representing a multiplicative factor. This factor can be made dependent on local climate conditions (gray and purple dashed-border nodes in Figure 1B). A prerequisite of this approach is that our statistical models on $C_{exposure}$ are independent of the actual rate of application. Analysis of the WISPE model outputs generated before at different application rates (100%, 50%, and 150% of the current default) (Mentzel, Grung, Holten, et al., 2022), showed this prerequisite was met. Indeed, concentration outputs by WISPE are completely and linearly dependent on the input rates of application, for both pesticides (Supporting Information). This linearity allowed us to adjust our statistical models by expressing both C_{base} and C_{delta} on a "per unit application"-basis (µg/L/kg/ha) (Figure 1B). In our BN, these application-independent estimates of C_{delta} are added to the application-independent and constant base concentration C_{base}, to derive application-independent exposure concentrations (module V). Finally, these are multiplied with the variable application rates (module III) to derive actual concentrations for the exposure characterization.

The remaining nodes in modules V–VII (effect and risk) have an identical set-up as the original model (Mentzel, Grung, Holten, et al., 2022) and are not further described here.

Sensitivity analysis

We performed a value of information (VoI) analysis of the BN model to assess the sensitivity of the target nodes (response variables) exposure and RQ to evidence in their respective parent nodes (predictor variables) (Figure 1) (HUGIN EXPERT, 2019). In this, sensitivity is expressed as the mutual information between each combination of target node and parent node. The sensitivity analysis integrates

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TABLE 2 Overview of nodes in the Bayesian network model (Figures 1B and 4)

Node group	Node no.	Node label	Node type	No. of states	Range, trifloxystrobin	Range, clopyralid	Information source for node table or value
Climate information	1	Monthly precipitation index (mm)	Interval	7	[0, 20]	[0, 20]	Scenario
	2	Monthly precipitation index threshold exceedance (T/F)	Boolean	2	[T, F]	[T, F]	Table generated by simulation from the statistical model
Pesticide application	3	Pesticide application scenario (%)	Numbered	5	[50%, 150%]	[50%, 150%]	Scenario
	4	Pesticide application default (kg/ha)	Constant	1	[0.15]	[0.05]	Table 2 in Mentzel, Grung, Holten et al. (2022)
	5	Pesticide application (kg/ha)	Numbered	5	[0.075, 0.225]	[0.025, 0.075]	Scenario
Hydrology and chemistry	6	Intercept (Box–Cox)	Constant	1	−2.67491	−0.0863395	Parameter estimate from the statistical model
	7	Slope (Box–Cox)	Constant	1	0.431408	1.01412	Parameter estimate from the statistical model
	8	Mean exposure from runoff (per unit application) (Box–Cox)	Interval	10	(−Inf, −3, …, 1, Inf)	(−Inf, 0, …, 7, Inf)	=Node_6 + Node_7 × Node_1
	9	Standard error exposure from runoff (per unit application) (Box–Cox)	Interval	10	[0.3, …, 0.75, Inf)	[1.5, …, 3.75, Inf)	Table generated by simulation from the statistical model
	10	Exposure from runoff (per unit application) (Box–Cox)	Interval	10	(−Inf, −1.5, …, 1, Inf)	(−Inf, 0, …, 8, Inf)	~N(Node_8, Node_9)
	11	BC back-transformation	Constant	1	[0.3]	[0.1]	Parameter estimate from the statistical model
	12	Exposure from runoff (per unit application) (μg/L/kg/ha)	Interval	10	[0, …, 67, Inf)	[0, …, 54.6, Inf)	$=(\max(\text{Node\_10}, -3.3) \times \text{Node\_11} + 1)^{(1/\text{Node\_11})}$
Pesticide exposure	13	Base exposure (per unit application) ([μg/L]/[kg/ha])	Interval	1	[3.32]	[3.34]	Parameter estimate from the statistical model
	14	Exposure (per unit application) (μg/L)	Interval	10	[0, …, 15.6, Inf)	[0, …, 403, Inf)	=If (Node_2 = TRUE), then (Node_13 + Node_12), else (Node_13)
	15	Exposure (μg/L)	Interval	10	[0, …, 2.12, Inf)	[0, …, 20.1, Inf)	=Node_14 × Node_5

(*Continued*)

TABLE 2 (*Continued*)

Node group	Node no.	Node label	Node type	No. of states	Range, trifloxystrobin	Range, clopyralid	Information source for node table or value
Pesticide effect	16	Endpoint type	Labeled	2	[EC50, NOEC]	[EC50, NOEC]	Scenario
	17	Effect (µg/L, ln)	Interval	10	(–Inf, –2, …, 8, Inf)	(–Inf, –2, …, 8, Inf)	Trif.: If (Node_16 = EC50), then (~N(4.48, 1.72)), else (~N(3.18, 1.77)) Clop.: If (Node_16 = EC50), then (~N(11.45, 1.99)), else (~N(7.73, 3.67))
	18	Effect (µg/L)	Interval	9	[0, …, 1097, Inf)	[0, …, 362222, Inf)	=Exp(Node_17)
Risk	19	Ratio exposure/effect	Interval	8	[0, 3]	[0, 3]	=Node_15/Node_18
	20	Precautionary factor	Numbered	7	[1, 1000]	[1, 1000]	Scenario
	21	Risk quotient	Interval	8	[0, …, 3, Inf)	[0, …, 3, Inf)	=Node_19 × Node_20

Note: A complete model documentation including all states, expressions, and conditional probability tables is given in the Supporting Information. The effect distributions are taken from table 4 in Mentzel, Grung, Holten, et al. (2022). ~N(µ, SD) means distribution normal (mean, standard deviation).

the signal and the "noise" of all CPTs between a target node and the predictor node. This means that a stronger relationship (e.g., a higher slope) will increase the sensitivity, while higher uncertainty (e.g., a higher standard error) will decrease the sensitivity. Variables with higher mutual information should be prioritized for additional information gathering over those with lower mutual information when the aim is to reduce uncertainty in the target node. In other words, new information on these nodes will most improve the confidence in the exposure and risk estimates.

RESULTS

Precipitation intensity and predicted pesticide exposures

Pesticide concentrations, simulated by the WISPE model under varying climate conditions, show threshold behavior related to precipitation intensity (Figure 2). That is, simulated concentrations increase with increasing precipitation, but seemingly only when some precipitation threshold is exceeded. Otherwise, simulated exposure concentrations stay at minimum base concentrations C_{base} of 0.498 µg/L (trifloxystrobin) or 0.167 µg/L (clopyralid). This behavior is more distinct for trifloxystrobin (Figure 2A) than clopyralid (Figure 2B), for which a few outlier values can be observed at very high exposure concentration $C_{exposure}$ values (>1 µg/L) but low monthly precipitation index I_m values (<1 mm). Indeed, the difference in mean monthly precipitation index I_m is highly significant between simulations resulting in C_{base} and simulations exceeding C_{base} for both pesticides (Figure 2C,D), but most for trifloxystrobin ($p = 9.24 \times 10^{-6}$ compared to $p = 2.86 \times 10^{-5}$ for clopyralid). The more distinct threshold behavior for trifloxystrobin is also reflected by its kernel density distribution on $C_{exposure}$ exceeding C_{base} (shaded area in Figure 2A), which is narrower than for clopyralid (Figure 2B). At an I_m value of 0.66 mm, there is a 50% probability that $C_{exposure} > C_{base}$ for trifloxystrobin, while for clopyralid this 50% probability was already reached at an I_m of 0.22 mm.

While the relationship between precipitation intensity and exposure concentrations was less distinct for clopyralid, the range of concentrations simulated by WISPE (0.167–2.68 µg/L) was much wider than the range of trifloxystrobin concentrations (0.498–0.541 µg/L). Consequently, the prediction interval around its two-step regression model is much wider as well (short-dashed orange lines in Figure 3B). This in turn affects the extent to which the magnitude of exposure is influenced by precipitation intensity relative to the pesticide application scenario (100% = current default) (Figure 5). For both trifloxystrobin (Figure 5A) and clopyralid (Figure 5B), exposures logically increase with higher application rates and higher precipitation intensities. However, the influence of precipitation is more profound for clopyralid. For trifloxystrobin, a clear influence of I_m on the exposure concentration (e.g., exceeding 0.78 µg/L) is evident only for values above 0.37 mm in combination with the highest application scenarios (125%–150%). For clopyralid, on the

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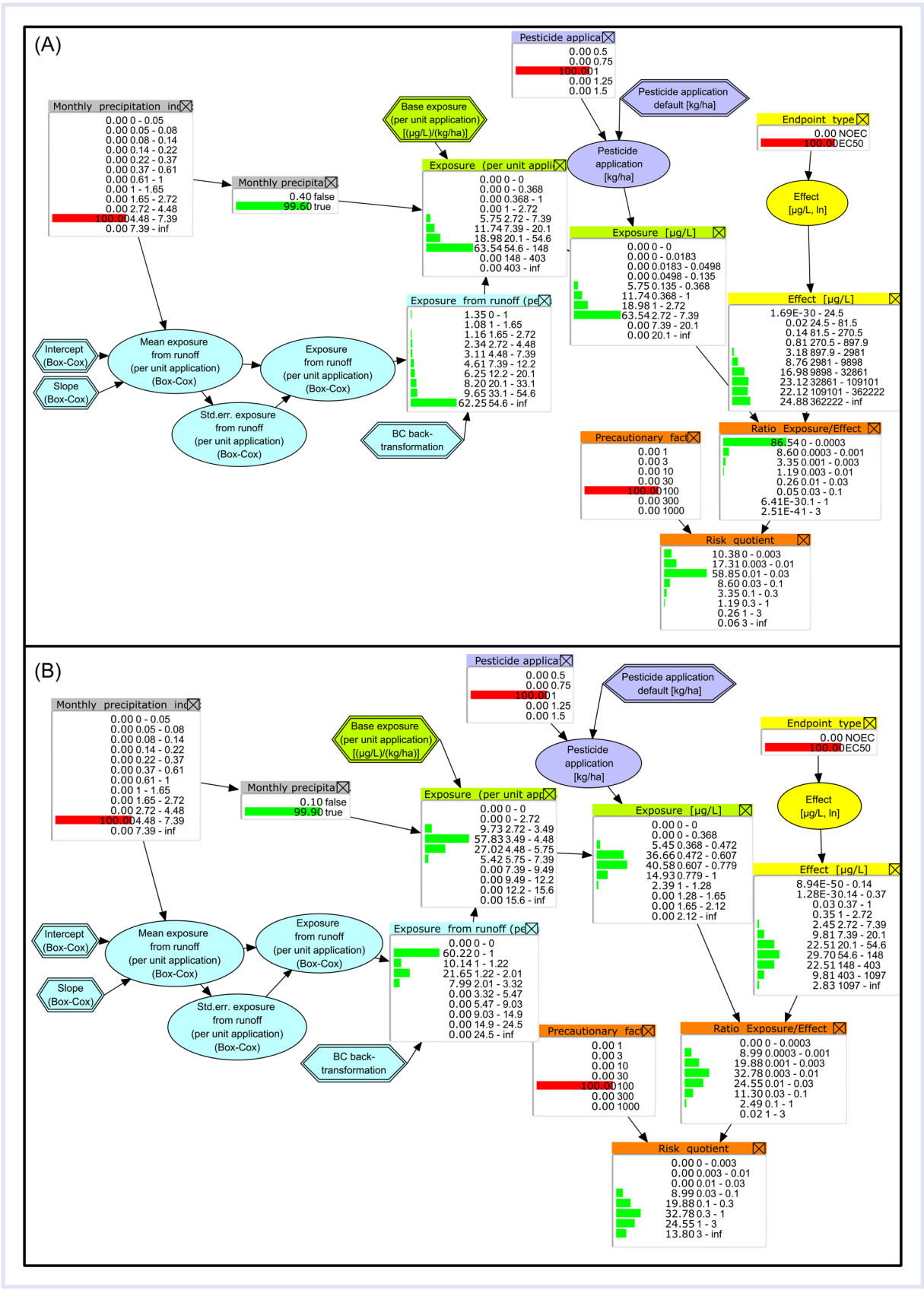

FIGURE 4 Display of Bayesian network model run for selected scenario combination and posterior probability distributions displayed for a selection of nodes, for (A) trifloxystrobin and (B) clopyralid. Model settings: Monthly precipitation index = (4.48 – 7.39) mm, pesticide application = 100%, endpoint type EC50, precautionary factor = 100

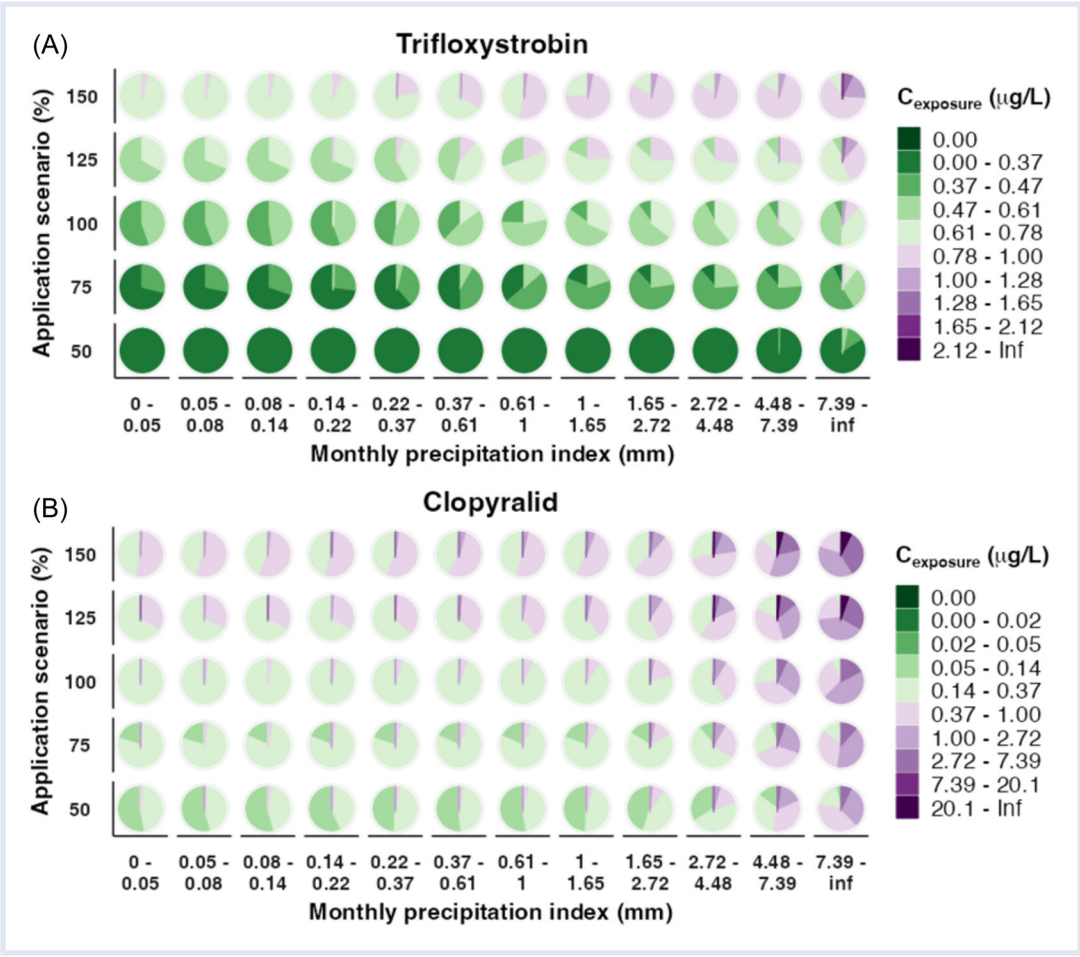

FIGURE 5 The influence of monthly precipitation index and application scenario on the distribution of aquatic exposures to (A) trifloxystrobin and (B) clopyralid. Additional fixed nodes were endpoint type (instantiated at "EC50") and the precautionary factor (instantiated at 100)

other hand, the influence of I_m on exposure concentration is visible along the whole gradient of I_m values. Note that the color coding in both panels is not directly comparable due to the differences in concentration ranges and discretization for the two pesticides. Finally, the results of our sensitivity analysis provide further support (Table 3). Comparing the two pesticides, clopyralid in-stream concentrations were more sensitive to the monthly precipitation index, while trifloxystrobin exposure was more sensitive to the pesticide application scenario.

Predicted environmental risks

In environmental risk assessment, predicted pesticide concentrations are evaluated in relation to the expected toxic effects. Following traditions in environmental risk assessment, we calculated the exposure/effect ratio to derive an RQ as a measure of environmental risk. The standard calculation of RQ uses a single value for the effect threshold, the predicted no-effect concentration (PNEC). A PNEC is typically based on a distribution of no observed effect concentration (NOEC) values (alternatively EC50 values), from which a lower quantile (5% hazard concentration) is derived, which is further reduced by the application of assessment factors of value 1–100. In our approach, instead, the whole distribution of NOEC or EC50 values is used in the calculation of the exposure/effect ratio (Mentzel, Grung, Tollefsen, et al., 2022). To obtain an RQ in line with the traditional calculation, the BN includes a scaling factor labeled precautionary factor, to account for both the derivation of the 5% quantile and further reduction by the assessment factor. However, to keep this subjective assessment value separate from the exposure and effect assessment steps as far as possible, we applied the precautionary factor only after the calculation of the exposure/effect ratio.

Applying our BN, we calculated RQ distributions based on an EC50 effect distribution, for three different states of the monthly precipitation index I_m, spread at the lower end (0–0.05 mm), middle (0.61–1 mm), and upper end (4.48–7.39 mm) of its value range (Figure 6). In Figure 6, the influence of the choice of precautionary factor is visualized, with Figure 6A,B showing the distribution of RQs under a precautionary factor of 30 and Figure 6C,D the same distribution but then under a precautionary factor of 100. We consider the latter value of 100 as default, building on the work of Mentzel, Grung, Holten, et al. (2022). In these bar plots, green, orange, and red bars

TABLE 3 Results of the value of information analysis, expressed as mutual information between target nodes and predictor nodes

	Trifloxystrobin		Clopyralid	
	Exposure (μg/L) ($H = 1.67$)	Risk quotient ($H = 2.02$)	Exposure (μg/L) ($H = 1.37$)	Risk quotient ($H = 1.72$)
Monthly precipitation index (mm)	0.11	2.09×10^{-3}	0.36	6.22×10^{-3}
Pesticide application scenario (%)	0.71	0.02	0.17	1.13×10^{-3}
Exposure (μg/L)	N/A	0.03	N/A	0.01
Effect (μg/L)	N/A	0.16	N/A	0.20
Endpoint type	N/A	0.03	N/A	0.06
Precautionary factor	N/A	0.47	N/A	0.56

Note: The mutual information I (Y, X) is a measure of the information shared by X and Y, that is, the reduction in entropy (*H*) of Y from observing X. The target nodes (response variables) are exposure (i.e., peak in-stream concentration) and risk quotient for both pesticides (trifloxystrobin and clopyralid).

represent RQ values < 0.1, 0.1–1, and >1, respectively. From these plots, it becomes clear that, although clopyralid exposures are substantially higher than trifloxystrobin exposures (e.g., Figure 5), this does not propagate into a substantial probability of RQs exceeding 1 or even 0.1 (Figure 6B,D). Only at the highest precipitation intensity and precautionary factor of 100, there is a small probability of ~1% that a future environmental risk due to clopyralid exposure exceeds 0.1.

For trifloxystrobin, we predict higher environmental risks. Under a precautionary factor of 30, there is an approximate 64%–67% probability that a future environmental risk due to trifloxystrobin exposure exceeds 0.1 (Figure 6A). The variation in these probabilities is due to the (limited) influence of precipitation intensity on the output risk distribution. Moreover, the probability that a future RQ exceeds 1 is approximately 8%–12%, indicating an unacceptable environmental risk. These percentages further increase to 87%–90% (probability that RQ > 0.1) and 30%–35% (probability that RQ > 1) when a precautionary factor of 100 is applied (Figure 6C).

For both pesticides, the calculated RQ had low sensitivity to the pesticide exposure and its upstream nodes (e.g., monthly precipitation index I_m and the pesticide application scenario) (Table 3). The RQ was more influenced by the effect node, which has a much wider concentration range (species sensitivity distribution [SSD] based on NOEC or EC50 values) than the concentration range of exposure (simulated exposure concentrations). Although the effect distributions had a slightly higher mean for EC50 than for NOEC (Table 2), the choice of endpoint type (NOEC or EC50) had a low influence on the RQ (Table 3).

DISCUSSION

The comprehensive incorporation of local climate projections in the environmental risk assessment of pesticides requires consideration of the full breadth of the uncertainty associated with these projections. Because they are generated via downscaling of projections from global climate models, this uncertainty is substantial (Deser et al., 2012). Previous studies modeling the effect of future climate on local aquatic fate and risks of pesticides typically employed one or a few global climate models (e.g., Chen, 2007; Kattwinkel et al., 2011; Martínez-Megías et al., 2023; Mentzel, Grung, Holten, et al., 2022). The resulting local climatic patterns, for example, long-term fluctuations in precipitation, might be reasonable for the individual model(s) but difficult to interpret as a general expected future trend. Because our BN model uses statistical regressions to quantify the relationship between precipitation intensity and exposure, it allows the propagation of many downscaled projections covering extensive ensembles of global climate models.

Here, we reflect on the feasibility of our approach and discuss the next steps that we envision, related to the actual incorporation of climate model projections and climate-dependent pesticide applications. This is followed by a description of the practical applicability of our approach specifically and BN modeling in general.

Feasibility of the presented approach

The application of our BN model to trifloxystrobin and clopyralid showed that, at least for these two pesticides, a statistical regression approach can be feasibly employed to circumvent the computationally laborious WISPE platform. However, replacing the extensive WISPE calculations with a single univariate correlation of precipitation and exposure does come with some drawbacks.

First, this model's simplicity introduces uncertainty and as a result a nonperfect regression fit. We accounted for this via the explicit future sampling from this regression, propagating this uncertainty into the downstream distributions of exposure and risk. This was especially relevant for clopyralid, for which the regression model was less robust and the range of possible exposures large (Figure 3). A possible explanation for the difference in model fit between trifloxystrobin and clopyralid relates

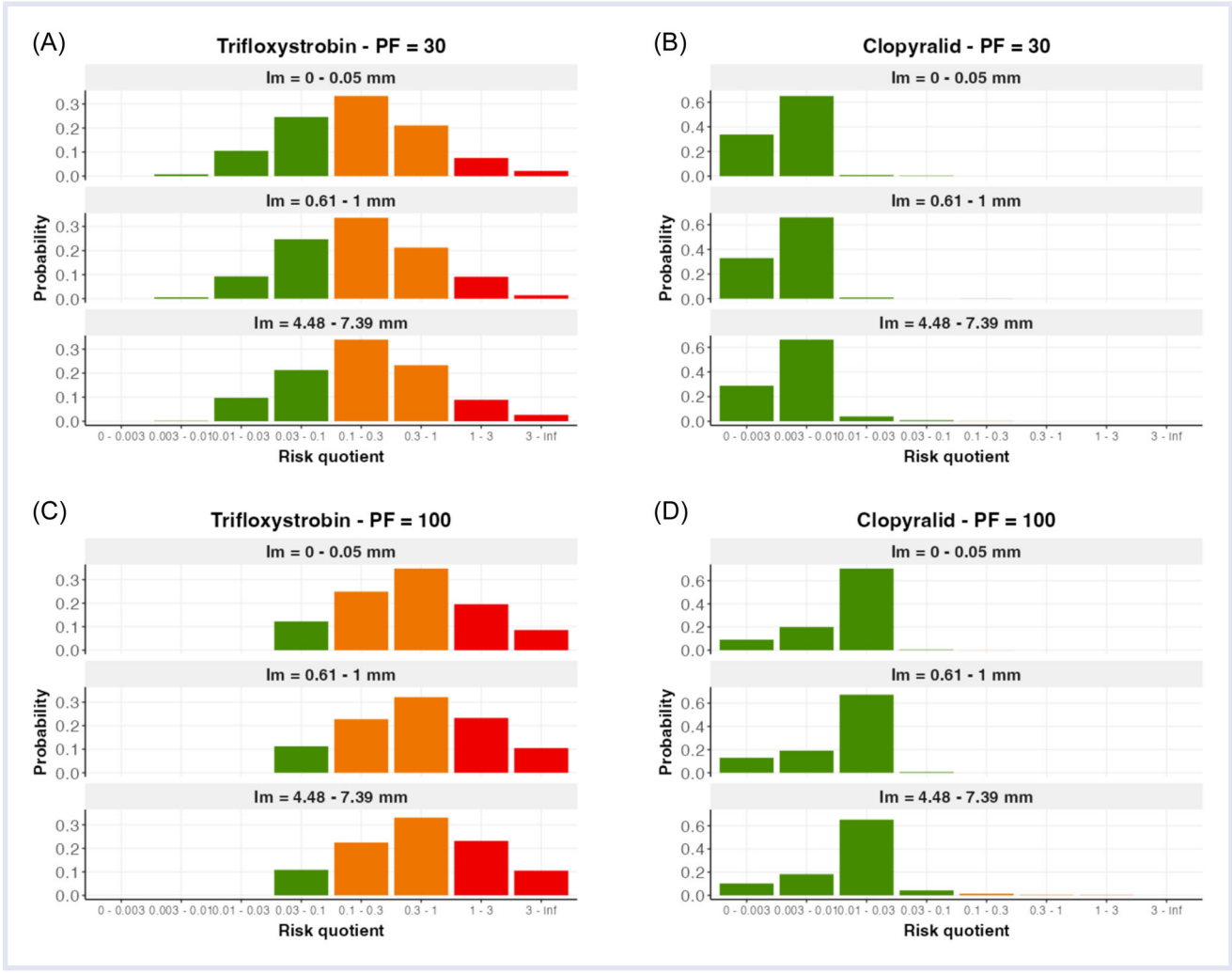

FIGURE 6 The influence of monthly precipitation index (I_m) and choice of the precautionary factor on risk quotient distributions due to aquatic peak exposures to (A, C) trifloxystrobin and (B, D) clopyralid. Fixed nodes were, in addition to I_m, the endpoint type (instantiated at "EC50") and application scenario (instantiated at 100%). Green: risk quotients RQ < 0.1; orange: 0.1 < RQ < 1, red: RQ > 1. RQ, risk quotient

to the fact that clopyralid is a herbicide applied in spring and trifloxystrobin is a fungicide applied in autumn. As autumn is a season with more rainfall, the data underlying the statistical model for trifloxystrobin covered a wider range of I_m values (Figure 2A). Especially at higher I_m values, fewer data were available for clopyralid (Figure 2B), limiting model quality in this upper region of precipitation intensity. This also introduces a second drawback of our approach: it has limited applicability beyond the range of the case study data. As such, our predictions for clopyralid at high values of I_m should be interpreted with caution. The training of our models with additional WISPE outputs generated along a larger gradient of precipitation indices is a logical next step to improve their applicability. However, our approach does not yet reach beyond the current case study setting. Analysis of other geographical contexts, other pesticides, or other agricultural practices (related to crop selection, pesticide application frequency, or tillage practice) would require a redoing of the model development and validation as described in this study.

Incorporation of climate model projections

While future climate projections were already incorporated in the BN model on which the present model is based (Mentzel, Grung, Holten, et al., 2022), the use of climate information in that study had several shortcomings identified by the authors: it was based on a single Intergovernmental Panel on Climate Change (IPCC) scenario (A1B, which is now outdated), only two global climate models, and only one downscaling method. The BN model presented here paves the way for the high-throughput propagation of ensembles of regional climate projections (modules I and II in Figure 1A). Here, we outline the next steps that will be feasible with the current BN.

First, climate projections should be obtained from a global climate model ensemble, for a selection of IPCC climate scenarios or storylines and time horizons (e.g., 2040–2060).

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For the current case study, climate projections for the relevant region can be obtained from a climate service provider such as the Norwegian Centre for Climate Services (https://klimaservicesenter.no/). Regional climate projections should be further downscaled to the appropriate spatial scale (see below). For each climate scenario, the monthly precipitation index can then be characterized by statistical properties, taking into account the variability among the climate models as well as among the years. The resulting probability distribution can be incorporated into the BN model as an expression or as a derived CPT.

Considering the methodology for downscaling, it has been recommended to make a synthesis based on both dynamical (e.g., the Euro-CORDEX ensemble) as well as empirical–statistical downscaling, since these two approaches are based on different assumptions and associated with different strengths and weaknesses (Benestad et al., 2023). At least one of the downscaling approaches should compare a selection of global climate model simulations with multimodel ensembles provided by the Coupled Model Intercomparison Project 6th phase (CMIP6, under the auspices of the World Climate Research Programme). It is not necessary to use every simulation as input in an impact model if the information about the ensemble spread can be described by statistical properties. Benestad et al. (2023) reported that for a sufficiently large ensemble, the spread of seasonally aggregated data is often close to being normally distributed.

Our study focused on precipitation since this was identified as the most important climate variable influencing the WISPE-simulated exposure concentrations. However, other climate variables might also contribute to the pesticide exposure profile more generally. For example, higher temperatures might increase the bio- and photodegradation rates and thereby reduce exposure durations. For example, Table 1 shows that trifloxystrobin has lower biodegradation and photodegradation half-lives than clopyralid, and is more rapidly degraded in both soil and water (Table 1). The BN model can be expanded to consider other climate variables with impacts on the exposure assessment, and any relevant interactions (e.g., synergistic or antagonistic effects) between the climate variables.

Climate-dependent pesticide applications

The application-independent manner in which we incorporated the relationship between climate and exposure allows for the inclusion of climate-dependent pesticide application patterns (module III in Figure 1A). Our results show this to be relevant for both case study pesticides. Especially for trifloxystrobin, varying application rates had a relatively large influence on exposure concentrations compared with precipitation intensity (Table 3 and Figure 5).

Apart from the direct effects climate change is likely to have on pesticide fate, transport, and exposure, changes in climate are also likely to have indirect effects on pesticide emissions, due to changes in pest pressures and thus the amount (and timing) of pesticides applied to crops (e.g., Bloomfield et al., 2006; Grünig et al., 2020; Hader et al., 2022). As the derivation and implementation of different climate change scenarios into the current BN were beyond the scope of this study, so too was the development of corresponding climate-dependent pesticide emissions scenarios and resulting distributions of possible pesticide application masses. However, since the current BN calculates pesticide exposures and risks on a per-unit mass application basis, climate change-dependent scenarios of pesticide emissions could be developed and readily implemented into the current BN structure in a future study.

Two distinct methods have been identified throughout the literature that investigated how pesticide emissions may change in response to climate change, namely (1) empirical-based analysis between pesticide application and climate variables, and (2) mechanistically relating climate variable changes to changes in pest pressures and thus pesticide emissions. For the empirical-based analysis method, data on historical climate conditions are analyzed with data on previous pesticide applications to generate relationships between the amount of pesticide applied over a defined area and measures of climate variables such as temperature and/or precipitation (Chiu et al., 2017; e.g., Kattwinkel et al., 2011). These climate–pesticide relationships are then paired with projections of the climate variables to estimate the corresponding changes in pesticide emissions that would be expected under climate change conditions. For the mechanistic climate change-pest pressure analysis method, projected changes in climate variables are directly related to the physiological impacts such environmental changes would have on pests of interest (e.g., Gagnon et al., 2016; Stöckle et al., 2010). Given guidance on pesticide application mass and timing relative to pest pressures, the likely resultant response in pesticide usage under climate change conditions can then be estimated. This method has been applied, for example, estimating increases in the number of codling moth generations due to warmer temperatures under climate change and the expected increase in pesticide sprays (Stöckle et al., 2010) as well as how changes in temperature and precipitation may shift the emergence of seasonal plant, fungus, and insect pests and the resultant changes in pesticide application timing and/or amounts (Gagnon et al., 2016).

For incorporation into the current BN, the probabilistic climate parameter results from a range of climate change scenarios, models, and downscaling approaches (i.e., module II; Figure 1A) could be paired with either the empirical-based or mechanistic-based methods described above to derive probabilities of pesticide applications across the different climate scenarios and models incorporated into the BN. These pesticide application probabilities could be used to scale the results of the per-unit mass application results presented here, and thus arrive at probabilistic estimates of aquatic exposures to and risks from pesticides that more comprehensively capture the possible impacts of climate change.

Implications for future research

The case study with trifloxystrobin and clopyralid presented here shows that weather conditions and application rates, both influenced by climate change, might impact environmental exposures to varying degrees. The VoI analysis points toward two focus points for improvement of exposure estimates (Table 3). For trifloxystrobin, it would be most informative to get a good understanding of what constitutes realistic climate-dependent application scenarios. For clopyralid, a better characterization of its environmental fate following application would be more beneficial, for example, through the exploration of additional climatic variables as independent predictors in the regression model.

When considering environmental RQs as target nodes instead of exposures, the VoI analysis was dominated by predictor nodes related to ecotoxicological effects (Table 3). In order of decreasing influence, these were the precautionary factor, the effect node, and the endpoint type. It should be realized that, while the precautionary factor is most influential for the distribution of RQs for both pesticides, its size is normally not uncertain but driven by (regulatory) instructions and guidelines. As such, for improvement of the presented environmental risk assessment, a better understanding of actual effects would be most beneficial. This should also extend to other climate-related stressors that might combine with pesticide exposure in additive or even synergistic ways (Topping et al., 2020). An example is the incorporation of additional SSDs on mortality due to acute heat stress (e.g., De Vries et al., 2008). Where possible, pesticide and temperature sensitivity distributions might be integrated, acknowledging that the aquatic toxicity of most chemicals is directly temperature-dependent (Wang et al., 2019). Similarly, our current pesticide-by-pesticide BN models could be expanded to allow the simultaneous modeling of (relevant mixtures of) multiple pesticides. This could be done via the integration of SSD-ensembles for multiple chemicals (Oldenkamp et al., 2015; Posthuma et al., 2019), and would be specifically relevant for plant protection products that comprise multiple pesticides and allow climate-dependent application scenarios that not only vary in magnitude but also in types of pesticide sprayed.

Practical application of the presented approach

The use of BN modeling as a probabilistic method for environmental risk assessment has various advantages over other (nonprobabilistic) alternatives (Moe et al., 2022). Most importantly, the calculation of full probability distributions of RQs provides more information and possibilities for interpretation than the generation or extraction of a single value of risk. For example, the probabilities that relevant risk thresholds are exceeded (e.g., 0.1 or 1) can be computed under various climatic, agricultural, or regulatory conditions (see Figure 6). Moreover, BNs can make use of climate information that is expressed by statistical properties, and nonlinear responses or interactive effects can easily be incorporated. A typical drawback of the BN approach is the discretization of continuous variables (e.g., concentrations), which implies a loss of precision and model sensitivity when ranges have little overlap. In our case study, this holds for the exposure and effect concentration ranges of clopyralid, as evidenced by its distributions of negligible risk in Figure 6. The model could potentially be improved by further development into a hybrid BN containing both discrete and continuous variables (Moe et al., 2020).

Despite their advantages, BNs have not been applied frequently in regulatory environmental risk assessment thus far (Kaikkonen et al., 2021). Nevertheless, they are considered an effective tool when dealing with a variety of research fields and are able to better communicate risk (Chen & Pollino, 2012; Kaikkonen et al., 2021; Landis et al., 2013; Moe, Carriger, et al., 2021; Sperotto et al., 2017). Other probabilistic approaches are often associated with constraints while communicating results to decision-makers (Dreier et al., 2021; Giddings et al., 2000). Unlike other probabilistic approaches, BNs derive probability density distributions as outputs in place of cumulative probability distributions and are considered more straightforward to interpret than many of the conventional probabilistic approaches (Moe, Carriger, et al., 2021). Also, some BN software allows for a web interphase (e.g., HUGIN) that enables better visualization and communication of the models, and their in and outputs.

In conclusion, the BN model we have presented here opens the door for the high-throughput propagation of regional climate information in chemical risk assessments. As such, we believe it provides a timely and suitable method for the climate-inclusive probabilistic environmental risk assessment of pesticide products as demonstrated in a case study with the fungicide trifloxystrobin and the herbicide clopyralid applied to an agricultural field in Norway.

AUTHOR CONTRIBUTION

Rik Oldenkamp: Conceptualization; formal analysis; methodology; visualization; writing—original draft; writing—review and editing. **Rasmus E. Benestad**: Conceptualization; methodology; writing—original draft; writing—review and editing. **John D. Hader**: Conceptualization; Methodology; writing—original draft; writing—review and editing. **Sophie Mentzel**: Conceptualization; methodology; writing—review and editing. **Rory Nathan**: Conceptualization; formal analysis; methodology; writing—review and editing. **Anders L. Madsen**: Methodology; software; visualization; writing—review and editing. **S. Jannicke Moe**: Conceptualization; formal analysis; funding acquisition; methodology; project administration; supervision; visualization; writing—original draft; writing—review and editing.

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CONFLICT OF INTEREST

The authors declare no conflicts of interest.

DISCLAIMER

The peer review for this article was managed by the Editorial Board without the involvement of S. Jannicke Moe.

DATA AVAILABILITY STATEMENT

A complete specification of the two Bayesian network (BN) models is available from the Supporting Information as a PDF file generated by the software (HUGIN). The R code used for the statistical modeling is available from the Supporting Information as an annotated PDF generated by R Markdown, including an MS Excel spreadsheet with WISPE input and output data. In addition, an online user interface has been developed for public access to running the BN model (https://demo.hugin.com/example/PesticidesInStreams).

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SUPPORTING INFORMATION

SI1_Trifloxystrobin_model_specification.pdf: Complete specification of BN model for trifloxystrobin, except its largest conditional probability tables.

SI1_Trifloxystrobin_large_CPTs.xlsx: Specification of the largest conditional probability tables for the BN model for trifloxystrobin.

SI1_Clopyralid_model_specification.pdf: Complete specification of BN model for clopyralid, except its largest conditional probability tables.

SI1_Clopyralid_large_CPTs.xlsx: Specification of the largest conditional probability tables for the BN model for trifloxystrobin.

SI2.pdf: R Markdown describing the code for the statistical modelling.

SI3.xlsx: All input and output data from the BN model runs reported in this publication.

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