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One Health perspective: an integrated in-silico approach to assess the environmental fate of pesticides, the exposure of aquatic and soil organisms and the risks for human health

Nicoleta A. Suciu [a], Marco Trevisan [a], Georgios Fragkoulis [a], Lucrezia Lamastra [a], Sara Triachini [a], Nelson Abrantes [b], Trine Norgaard [c], Paula Harkes [d], Joao Pedro Nunes [d], Vera Silva [d], Irene Navarro [e], Adrián de la Torre [e], María Ángeles Martínez [e], Paul Scheepers [f], Daniel Martins Figueiredo [g,*]

[a] Università Cattolica Del Sacro Cuore, Department for Sustainable Food Process, Via Emilia Parmense 84, 29122, Piacenza, PC, Italy
[b] Centre for Environmental and Marine Studies and Department of Biology, University of Aveiro, Aveiro, Portugal
[c] Aarhus University, Department of Agroecology, Blichers Allé 20, 8830, Tjele, Denmark
[d] Soil Physics and Land Management Group, Wageningen University and Research, P.O. Box 47, 6700 AA, Wageningen, the Netherlands
[e] Unit of POPs and Emerging Pollutants in Environment, Department of Environment, CIEMAT, Madrid, Spain
[f] Radboud Institute for Biological and Environmental Sciences, Radboud University, Nijmegen, the Netherlands
[g] Institute for Risk Assessment Sciences, Utrecht University, Utrecht, the Netherlands

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ABSTRACT

Within the One Health perspective, the health of humans, animals and ecosystems is highly interconnected. This study presents an *in silico* approach to assess the environmental fate of plant protection products (PPPs) in soil and water, as well organisms and humans exposure and associated risks. The methodology integrates scenarios, models, tools and approaches recognized and used by the European Food Safety Authority and the scientific community for PPP market authorization risk assessments. Three European Member States —Portugal (PT), Denmark (DK), and the Netherlands (NL) —were selected to demonstrate = model applicability, each representing a different EU Regulatory Zone. For each country, real PPP application data and site-specific meteorological and pedological information were collected, and environmental concentrations monitored. Results showed that the predicted environmental concentration in soil (PEC_{soil}) was lower than the monitored concentrations in PT locations, whereas PEC_{soil} was overestimated in both NL and DK. The toxicity to exposure ratio (TER) indicated low risk to earthworms in all simulations. For surface water (SW), PEC_{SW} was below the environmental quality standard (EQS_{SW}) in PT, whereas significant exceedances occurred in NL and DK. However, in DK, PPP concentrations declined below EQS_{SW} within one day post-application. Comparison with reference toxicological endpoints for fish and invertebrates suggested low risks. Estimated PPP concentrations in invertebrates and fish for human consumption indicated intake would not exceed the acceptable daily intake (ADI) in PT and NL. However, at the DK location, small consumption (>13 g) of a given invertebrate would exceed the ADI for prosulfocarb (5 μg kg^{-1}). Despite limited experimental dataset and some constraints in field data collection that influenced models performance and verification, this in-silico approach can serve as a useful screening tool for assessing PPP fate and exposure in soil, aquatic organisms, and humans, supporting the integrative perspective of the One Health approach.

1. Introduction

The World Health Organization (WHO, 2021) defined One Health as an integrated, unifying approach that aims to sustainably balance and optimize the health of people, animals and ecosystems. It recognizes that the health of humans, domestic and wild animals, plants, and the wider environment-including ecosystems-is closely linked and interdependent. However, One Health is often discussed in the context of zoonotic

* Corresponding author.
E-mail address: d.m.figueiredo@uu.nl (D. Martins Figueiredo).

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disease control, with plant health and environmental concerns receiving comparatively less attention (Destoumieux-Garzon et al., 2018; Gibbs, 2014). Through its environmental dimension, One Health provides a framework for understanding the complex interaction between human well-being and plant health.

Maintaining or even increasing crop yields through healthy plants is critical to ensuring food security for a growing global population (Hofmann et al., 2022). The use of plant protection products (PPPs) plays a crucial role in this context. Indeed, a recent study of Ahvo et al. (2023) estimated that the global production of wheat would decrease by 5 % if the use of pesticides for its production decreased by 25 %. However, the PPPs application also poses significant risks to both environmental and human health (Ren et al., 2024). The fate and transport of PPPs from agricultural fields to the surrounding environment are an important cause of off-target PPPs exposure (Lonsdorf et al., 2024; Narvaez et al., 2022). As a result, terrestrial and aquatic organisms are frequently exposed to complex mixtures of PPPs, where individual compounds may interact and, sometimes produce synergistic toxic effects (Panico et al., 2022; Cantu et al., 2023).

Computer-aided simulation models can be time- and cost-effective tools for assessing the fate,transformation, and toxic effects of PPPs air, plant, soil, and water (Marín-Benito et al., 2014; Zhang and Goh, 2015; Suciu et al., 2023; Ren et al., 2024). However, these models may underestimate risk when synergistic effects occur, leading to ecosystem impacts greater than predicted (Alengebawy et al., 2021). One of the main goals of the SPRINT Project is to develop an innovative *in silico* framework that integrates PPP use with measured concentrations and exposure levels, linking environmental fate to direct and indirect toxicity and health impacts (https://sprint-h2020.eu/). Recently, Results from a monitoring campaign carried across 10 European countries revealed widespread co-occurrence of pesticide residues in soil, crops, indoor air, indoor dust, water, and sediments, covering both conventional and organic production systems (Silva et al., 2023). Overall, 86 % of the 625 tested samples presented pesticide residues, and 76 % included mixtures of different pesticides. Furthermore, hazardous assessment identified numerous hazardous compounds across environmental and household matrices, alongside data gaps, an increasing presence of lower hazard compounds and a decreasing trend in higher hazard compounds on the market. Nevertheless, the authors highlighted the need for long-term monitoring and modelling approaches to better contextualize the findings.

The main purpose of the present work was to develop, within the One Health prospective, an integrated in-silico approach able to i) verify the in-silico calculations and assumptions made during the scenarios development by comparing simulated data with monitoring data; ii) assess and better understand the fate and transport of multiple PPPs across different areas in Europe– each representing one regulatory zone according to Regulation (EC) No. 1107/2009 - in both soil and water; iii) assess the exposure of aquatic and soil organisms to the actual PPPs used in fields and their concentrations in soil, water and sediments simulated by the models and iv) define the level of risks for humans after fish and shellfish consumption. Materials and Methods.

1.1. Selected locations

To demonstrate applicability of the developed integrated in-silico approach, three locations were selected that represent different pesticide applications and pedo-climatic zones across Europe.

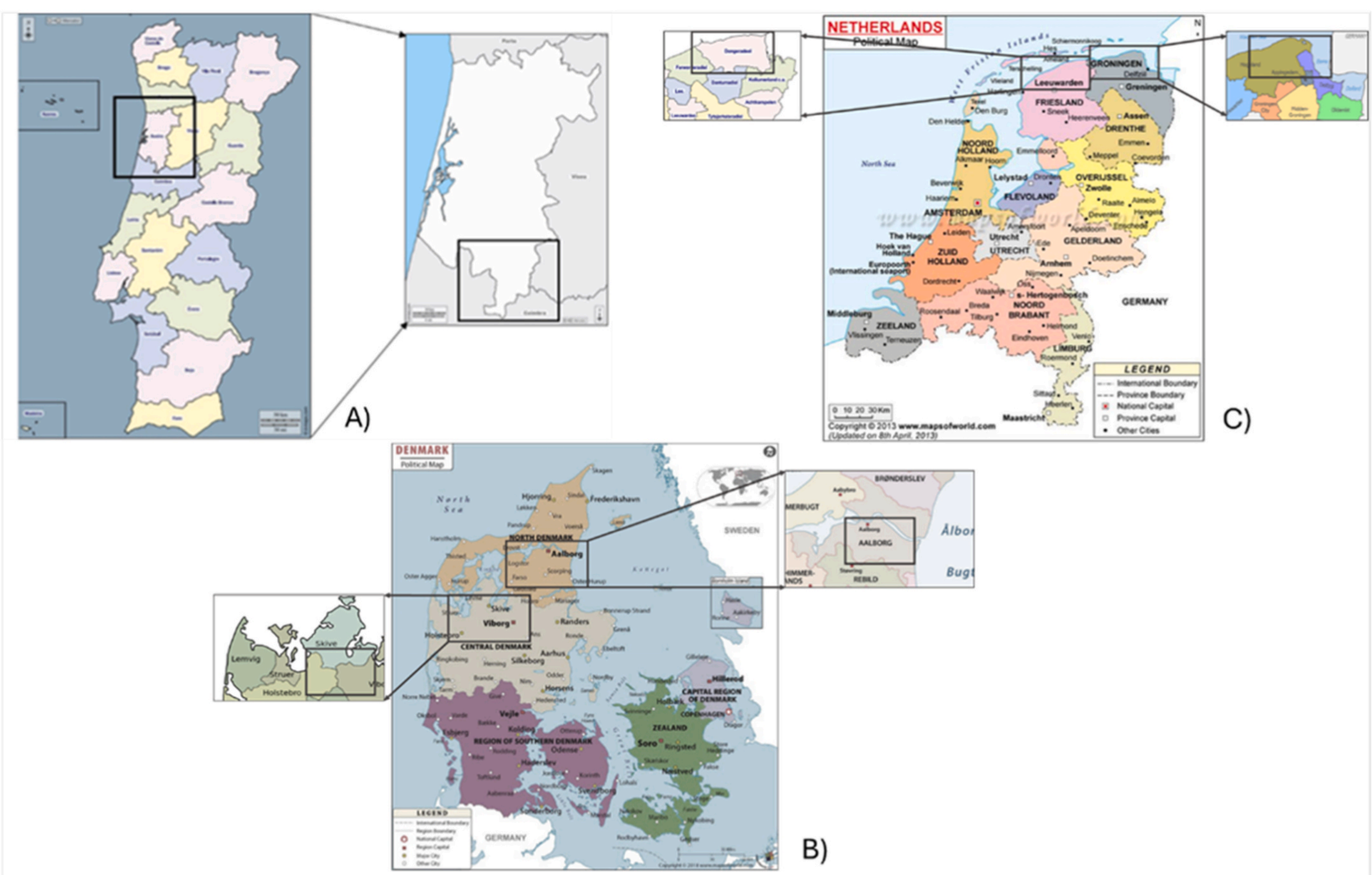

Fig. 1. Map of the study areas: A) map of Portugal divided into districts, Aveiro district and the study area; B) map of The Netherlands divided into provinces, and the two municipalities of the study area; C) map of Denmark divided into regions, and the two provinces of the study area. Note: the original maps were taken from mapsofworld.com and further elaborated to show the areas of interest.

1.1.1. Portugal

The study area in Portugal is located in the southern part of the Aveiro district (Fig. 1A) and covers part of the Cértima River catchment. The application of PPPs took place in three main plots, one at 30 m from a tributary of the Cértima River and the other two at 150 m from the main river. The plots taken into consideration were covered by vineyards. The characteristics of the fields and of the two water sampling locations are listed in supplementary material Table SM1.

1.1.2. The Netherlands

The area in the Netherlands covers two provinces located in the North of the Netherlands, Province of Friesland, and Province of Groningen (Fig. 1B). The application of PPPs took place in three plots, cultivated with potatoes, located less than 5m from the nearest water body (stream). The characteristics of the fields and of the three water bodies are listed in Table SM2.

1.1.3. Denmark

The area in Denmark covers two regions located in North and Central Denmark (Fig. 1C). The application of PPPs took place in two plots, both at 3 m (buffer zone) from the adjacent water body (stream). The plot taken into consideration in the northern zone was cultivated with winter wheat while the plot taken into consideration in the central zone was cultivated with spring barley. The characteristics of the fields and of the two water bodies sampled are specified in Table SM3.

1.2. Integrated approach for predicting pesticides fate in soil and water bodies

1.2.1. Pesticides fate in soil

For the prediction of the PPPs concentrations in the top-soil (first 2.5 cm), the FOCUS soil calculator was used (https://www.icps.it/en/pubblicazioni/pecsoil-calculator/), following the agricultural use pattern described in Table 1 for vines, potatoes, spring barley and winter wheat. This tool allows to calculate the Predicted Environmental Concentration in soil (PEC_{soil}) for the active substances (a.s.s) of PPPs using the equations reported in the "Soil persistence models and EU registration" guideline (FOCUS, 1997).

Table 1
PPPs application patterns in the simulated fields.

Field	Substance	Application rate per treatment (g ha^{-1})	Date
PT location- vines			
Field 1	Dimethomorph	90.0	25/06/21
	Metalaxyl-M	97.5	01/05/21
	Tebuconazole	80.0	10/05/21
		80.0	25/05/21
Field 2	Dimethomorph	225.0	20/05/21
	Metalaxyl-M	97.5	01/05/21
	Tebuconazole	100.0	07/05/21
Field 3	Dimethomorph	225.0	20/05/21
	Metalaxyl-M	97.5	01/05/21
	Tebuconazole	100.0	07/05/21
NL location - potatoes			
Fields 1 and 2	Acetamiprid	12.5	July 02, 2021
		30.0	July 09, 2021
	Mandipropamid	100.0	June 25, 2021
		112.5	July 02, 2021
		112.5	July 09, 2021
Field 3	Acetamiprid	12.5	June 16, 2021
		50.0	July 02, 2021
		12.5	July 19, 2021
	Mandipropamid	100.0	June 08, 2021
		100.0	June 16, 2021
		150.0	June 24, 2021
		150.0	July 02, 2021
DK location – spring barley (field 1) and winter wheat (field 2)			
Field 1	Diflufenican	25.0	May 11, 2021
Field 2	Diflufenican	30	September 26, 2020
	Prosulfocarb	800	October 15, 2020

The soil input data requested by the FOCUS calculator are topsoil organic carbon (%) and soil bulk density (g cm^{-3}). The values considered for the simulations are reported in the supplementary material in Tables SM1, SM2 and SM3.

1.2.2. Pesticide fate in water bodies

Runoff and drift were the main contamination routes considered to estimate the PPP distribution in surface water and sediment compartment. The FOCUS PRZM 4.3.1 model was used to calculate the runoff (FOCUS, 2001) while the Drift Calculator was used to calculate the drift (Holterman and van de Zande, 2003). In the case of drift, the direct contribution of PPPs to the water stream or to the affluent water network must be considered. In the case of runoff, the PPP reaches the water stream by runoff water from rainfall. Subsequently, the FOCUS TOXSWA 5.5.3 model was used to calculate the predicted environmental concentration in surface water (PECsw), considering the output data of PRZM and the Drift Calculator and according to FOCUS surface water guidance (FOCUS, 2001, 2015).

1.2.2.1. Input data. The FOCUS PRZM and TOXSWA models require atmospheric temperature (°C), rainfall (mm) and wind speed (m/s) as meteorological data. Figure SM1 in the supplementary material presents the data collected by the closest weather stations available to the fields. For PT the water station was in Bairrada region, at 3.5 km distance from the three fields considered for the simulations, whereas for NL two weather stations were considered, located at 27 km from field 3 and 12 km from fields 1 and 2. Finally, for DK, 4 weather stations were used for collecting the meteorological data, located at a distance ranging from 8 to 73 km from the two fields considered for the simulations.

1.3. Modelled pesticides

The PPPs selected for the simulation are reported in Table 1. Their physicochemical characteristics, requested by the models, are presented in the supplementary material in Tables SM1, SM2 and SM3. The PPPs were selected based on three criteria: 1) field use, declared by farmers in the starting phase of the project, 2) presence (i.e. quantifiable) in the soil samples collected from the fields, and 3) presence in the water samples collected from the water bodies adjacent to the fields (Knuth et al., 2024; Navarro et al., 2022). In PT, the PPPs selected were dimethomorph, metalaxyl-M and tebuconazole; all three fungicides widely used against grape downy mildew and powdery mildew. In the NL CCS the PPPs selected were acetamiprid and mandipropamid. Acetamiprid is a pyridyl methylamine insecticide, used for the control of *Hemiptera spp*. especially aphids, whereas mandipropamid is a fungicide used to control oomycete pathogens on potatoes and other crops. Finally, in DK, the PPPs selected were diflufenican and prosulfocarb, both herbicides used to control grass and broad-leaved weeds.

1.4. Aquatic and soil organism's exposure

1.4.1. Predicted concentrations in phytoplankton, invertebrates, and fish

To predict concentrations in plankton, invertebrates and fish, the MERLIN-Expo Tool was applied. The equations used are thoroughly described in the MERLIN-Expo documentation (https://merlin-expo.eu/). For phytoplankton, estimated PPP concentrations in water were used as input. For invertebrates, the model incorporated PPPs concentrations estimated in phytoplankton, sediment and water. For fish, exposure was assessed using estimated concentrations in phytoplankton, invertebrates, sediment and water. The PPPs concentrations in water and sediment were based on the TOXSWA model outputs.

Necessary model parameterization includes, amongst others, the following input: PPP K_{oc} (organic carbon partition coefficient), BCF (bioaccumulation factor for a given species), metabolic half-life of chemical (dt50m) (if available); K_{OW} (octanol-water partition coefficient) (Table 2). Water temperature was assumed not to vary significantly given the available data from the closest water temperature measurement station (see https://tabuademares.com/pt/aveiro/cacia). The average value used was 15 °C.

The available BCF for fish was based on adult zebrafish (*Danio rerio*) (Alvarado-Suárez et al., 2022). Therefore, the exposure assessment focused on this species, though BCF values are likely similar in other fish species. For invertebrates, specific BCF data for the evaluated PPPs were not available, representing a limitation. However, the same BCF as for fish was applied, based on the assumption that if BCF values are greater than 1 for fish—indicating that the concentration in the organism is higher than in the medium (e.g., water)—then BCF values are likely above 1 for plankton and invertebrates as well, and conversely when BCF values are below 1 (i.e., if BCF <1) (Giulivo et al., 2018).

1.4.2. Predicted exposure of earthworms

Currently, there is no method to predict concentrations in earthworms. However, it is possible to compare PEC_{soil} with different toxicity values. The Toxicity Exposure ratios (TER) for acute and long-term exposure were calculated. Here, low risk to soil organisms is indicated if TER ≥5 (see Uniform Principles as laid down in Reg. (EU) No 546/2011 and verified by Christl et al., 2015). The formula for calculating acute and chronic toxicity to exposure ratios are:

$$TERacute = LC_{50}/PECsoil$$

$$TERchronic = NOEC/PECsoil$$

For the above equations, LC_{50} is the acute 14-day lethal concentration 50 % (mg kg^{-1}) whereas NOEC is the chronic no observed effect concentration (reproduction outcome) (mg kg^{-1}). Values were retrieved for each PPP from the PPDB (Lewis et al., 2016).

As an additional exploratory step, literature review on earthworm toxicity for all seven PPPs studied were performed. The aim was to identify whether existing studies reported adverse effects at lower exposure levels. In parallel, exposure-toxic effects, considering the predicted concentrations, were also examined. PEC_{soil} values were based on estimates from the FOCUS calculator.

Table 2
Key properties used in MERLIN-Expo model simulations for the PPPs of interest in PT, NL and DK.

PPPs	Log K_{OW}	Log K_{OC}	BCF (L kg^{-1})	DT_{50m} (days)
Dimethomorph	2.63 (EFSA, 2023)	2.62 (EPA, 1998)	27 (Pubchem, 2024c)	0.458 (EFSA, 2023)
Tebuconazole	3.70 (ECHA, 2013)	2.88 (Xu et al., 1999)	78 (PPDB, 2024)	24 (Andreu-Sánchez et al., 2012)
Metalaxyl-M	1.7 (EPI,2024)	1.60 (Nguyen, 2023)	15 (PPDB, 2024)	0.86 (Zhou et al., 2023)
Acetamiprid	0.80 (Pubchem, 2024a)	2.30 (PPDB, 2024)	3.98 (Ma et al., 2022); 3.00 (Pubchem, 2024a) *	1 (Zhou et al., 2023; Guo et al., 2022)
Mandipropamid	3.20 (RIVM, 2016)	2.92 (Pubchem, 2024b)	48 (PPDB, 2024)	70 (Palawski et Knowles, 1986)
Prosulfocarb	4.65 (APVMA, 2007)	3.19 (BVL, 2017)	700 (PPDB, 2024)	0.1053 (EFSA, 2007)
Diflufenican	3.74 (PPDB, 2024)	3.53 (Bayer, 2019)	1650 (ECHA, 2018	10.1 (Lazartigues et al., 2013)

2. Results and discussion

2.1. Predicted environmental concentrations of PPPs in soil

Fig. 2 shows the PEC_{soil} values of the seven PPPs applied in the three locations (PT, NL and DK). Fig. 2a) reports PEC_{soil} values for the three fungicides applied in the three Portuguese fields, with values up to 430 μg kg^{-1} for dimethomorph and to 190 μg kg^{-1} for metalaxyl-M, in field 3, and up to 230 μg kg^{-1} for tebuconazole in field 1. Notably, tebuconazole was applied twice in field 1, reaching its highest PEC_{soil} value (230 μg kg^{-1}) 15 days after the second application.

Fig. 2b) reports the PEC_{soil} values for the insecticide acetamiprid and of the fungicide mandipropamid in the three NL fields, with concentrations up to 55 μg kg^{-1} and 822 μg kg^{-1}, respectively, in field 3. Higher PEC_{soil} values in field 3 compared with fields 1 and 2 occurred immediately after the last application (day 17 for acetamiprid and day 24 for mandipropamid), likely due to the greater number of applications.

Fig. 2c) reports the PEC_{soil} for the two herbicides applied in the DK location, reaching 2415 μg kg^{-1} for prosulfocarb in field 2 and 113 μg kg^{-1} for diflufenican in field 1. The higher application rate of diflufenican in field 2 (17 % higher than in field 1) resulted in soil concentrations approximately 1.5 times higher.

2.1.1. Model fits and comparison

The simulated results were compared with the monitored/measured concentrations to verify the models' performance and the influence of the assumptions made during the scenario development/design (Fig. 3). Information on LOD, LOQ, Rec (%) RSD (%) for soil measurements can be found in annex 13 from Knuth et al. (2024). The model evaluation metrics indicate mixed performance. The mean error (ME = 3.1) suggests that the model has only a small systematic bias, meaning predictions are not consistently over- or underestimated. However, the large mean absolute error (MAE = 84.8) shows that individual predictions often deviate substantially from measured values, particularly for mandipropamid in PT. The very large root mean square error (RMSE = 123) further indicates the presence of some extremely inaccurate predictions. This is likely driven by the absence of information on the background or baseline values in the dataset, which reduces the model's ability to anchor predictions and leads to large outliers. The detailed monitoring results for the presence of the selected PPPs in soil were previously reported by Knuth et al. (2024) and are presented in Table SM4, providing also the simulation day and value to which this date corresponds. For metalaxyl-M, used in PT CSS, the models predicted a complete degradation at the date of sampling whereas the monitoring values were up to 136.8 μg kg^{-1}.Significantly higher monitoring values were reported for field 2 and 3 with respect to field 1. Without having PPPs concentration values in the soil before application, it is difficult to completely explain these discrepancies between the simulated and the monitored results for metalaxyl-M. However, the DT_{50} value of 6.5 days considered for the simulations could have influenced the simulation values as metalaxyl-M has low to medium persistence in soil (DT_{50} 1–100 days) (EFSA, 2015).

Considering the first sampling date, the PEC_{soil} for dimethomorph in field 1 was lower than the monitored values, similar for field 2 (60.0 μg kg^{-1} PEC_{soil} vs 64.3 μg kg^{-1} monitored) and almost 5 times higher in field 3. A similar trend was observed for tebuconazole, with PEC_{soil} lower than the monitored for field 1, similar for field 2 and almost 3-times higher values for field 3. Considering the second sampling date, dimethomorph for fields 1 and 2 showed PEC_{soil} values 3 to 4 times lower than the monitored values while two times higher for field 3. In the case of tebuconazole, PEC_{soil} values were up to 4.7 times lower than the monitored for field 1 and 2 during the second sampling and similar for field 3 (10 μg kg^{-1} simulated vs 14.1 μg kg^{-1} monitored). As fields 2 and 3 have identical soil characteristics (Table SM1), meteorological data (Figure SM1) and application patterns (Table 1), these differences cannot be correlated to PPPs physicochemical and soil properties or

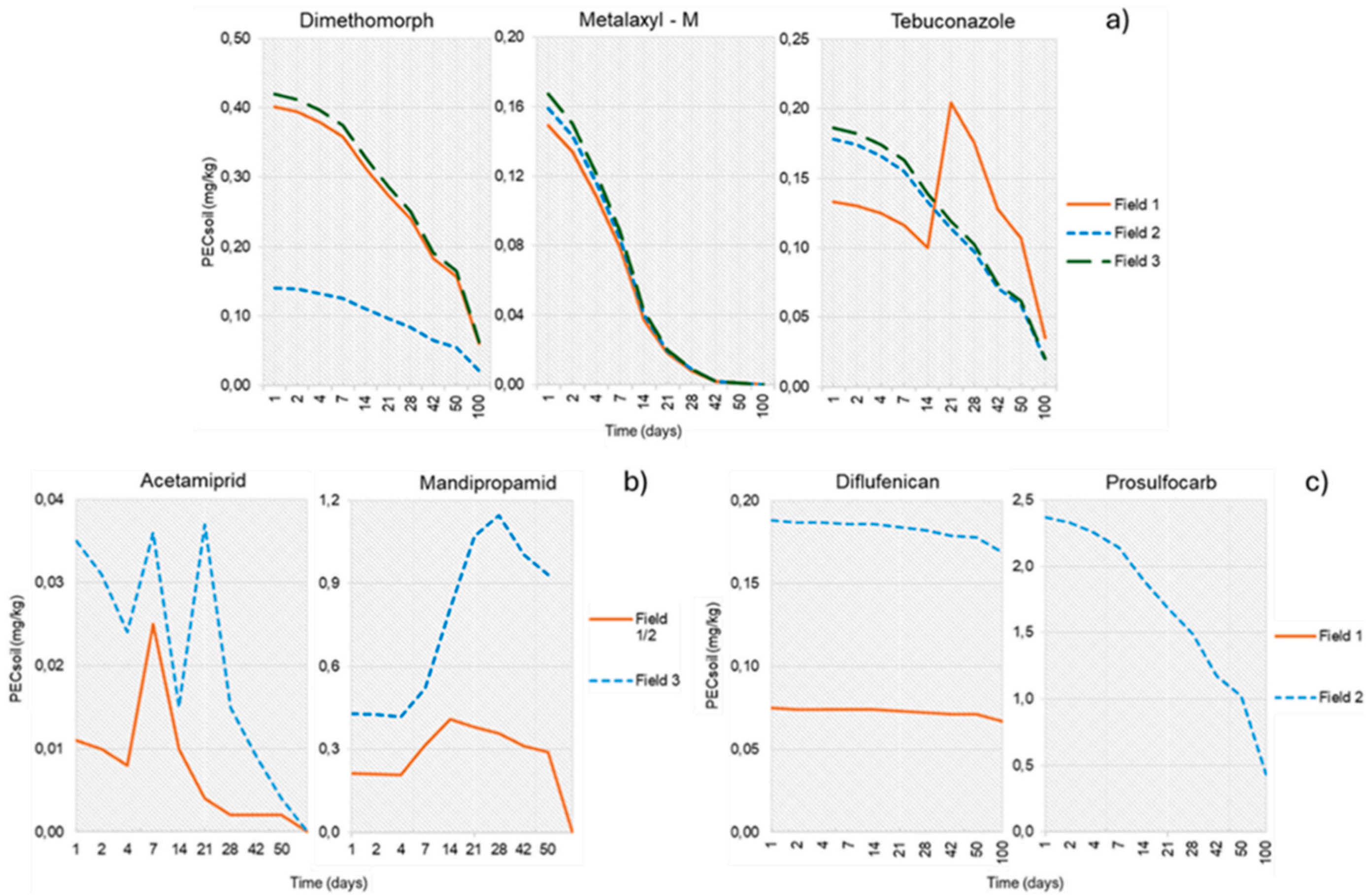

Fig. 2. PECsoil following application of a) Dimethomorph, Metalaxyl – M and Tebuconazole in PT, b) Acetamiprid and Mandipropamid in NL and c) Diflufenican and Prosulfocarb in DK, at a mixing depth of 2.5 cm. Prosulfocarb was not applied in field 1.

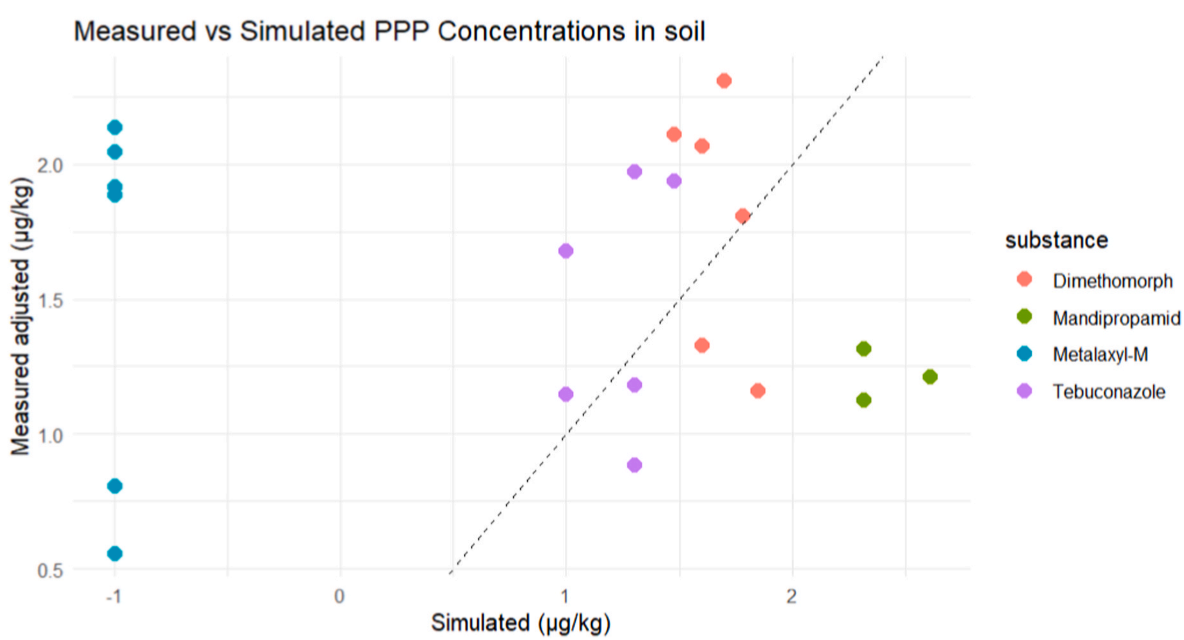

Fig. 3. Simulated vs measured concentrations for pesticides measured across the three locations.

application doses but rather to incomplete information collected from the field.

At the NL location, soil was sampled i once per field. Overall, the models tended to overestimate measured concentrations. Acetamiprid was below the LOD (1.3 μg kg^{-1}) in the soil sample from field 3, whereas the models predicted 14 μg kg^{-1} for the same date. No comparison was possible for fields 1 and 2, as acetamiprid applications began after sampling. For mandipropamid, modelled concentrations exceeded measured values by up to 15-foldin fields 1 and 2 and up to 25-foldin field 3.

The PEC_{soil} values were calculated using the FOCUS Soil Calculator; which considers only soil degradation and excludes other losses (mainly leaching), representing a worst-case scenario. Acetamiprid has a low K_{oc} (106.5 mL g^{-1}), so soil leaching is also a route by which it dissipates from the soil. However, mandipropamid was applied to field 3 on 16 June, and sampling took place on 21 June. The model predicts a concentration of almost 200 μg kg^{-1} (at a mixing depth of 2.5 cm) in the soil, considering 15 % crop interception and only losses from degradation. Even assuming higher interception (60 %, as in later applications), the PEC_{soil} would have been 50 μg kg^{-1}, still four times higher than measured. Additional information on crop development stage (BBCH scale) at the time of application would improve interpretation.

Another key factor is the soil DT_{50}. The assessment used the geometric mean DT_{50} from laboratory studies, consistent with regulatory practice and a realistic worst-case assumption. However, lower DT_{50} values in field soils could explain discrepancy, as PEC_{soil} five days after application would then be substantially lower.

For DK, as well as in NL, just one sampling time was undertaken and an overestimation of the concentrations simulated by the models was observed. Indeed, diflufenican showed a measured concentration of 3.2 μg kg^{-1} in field 1, whereas for the same date the models simulated up to 23 times more (75 μg kg^{-1}). This may be due to several factors such as different soil layers considered for the modelling and sampling (2.5 cm vs 5 cm) (Silva et al., 2021), high DT_{50} in soil considered in the modelling (645 days, Table SM3), as suggested in the renewal assessment report for diflufenican (EC, 2011), even if other studies (EFSA, 2008) reported a faster degradation, up to 245 days. Prosulfocarb was not applied in field 1. No comparison was possible for prosulfocarb and diflufenican in filed 2 as the application of the PPPs were done several months (≈11 months for diflufenican and ≈10 months for prosulfocarb) before the monitoring campaign.

2.2. *Earthworm exposure*

Results for TER_{acute} and $TER_{chronic}$ are shown in Fig. 4 and Table SM5 in supplementary material. In general, in all three locations the TER values were well above 5, indicating low risk.

However, several studies have reported toxicity effects at low concentrations for metalaxyl-M, a PPP used in PT location. For example, Zhu et al. saw that even at concentrations of 0.1 mg kg −1, metalaxyl-M “greatly increased ROS levels, which led to lipid peroxidation in earthworms and the antioxidize system in earthworms was dramatically affected when the concentration of metalaxyl-M was higher than 0.1 mg kg^{-1}, which resulted in irreversible oxidative damage in cells.” (cited

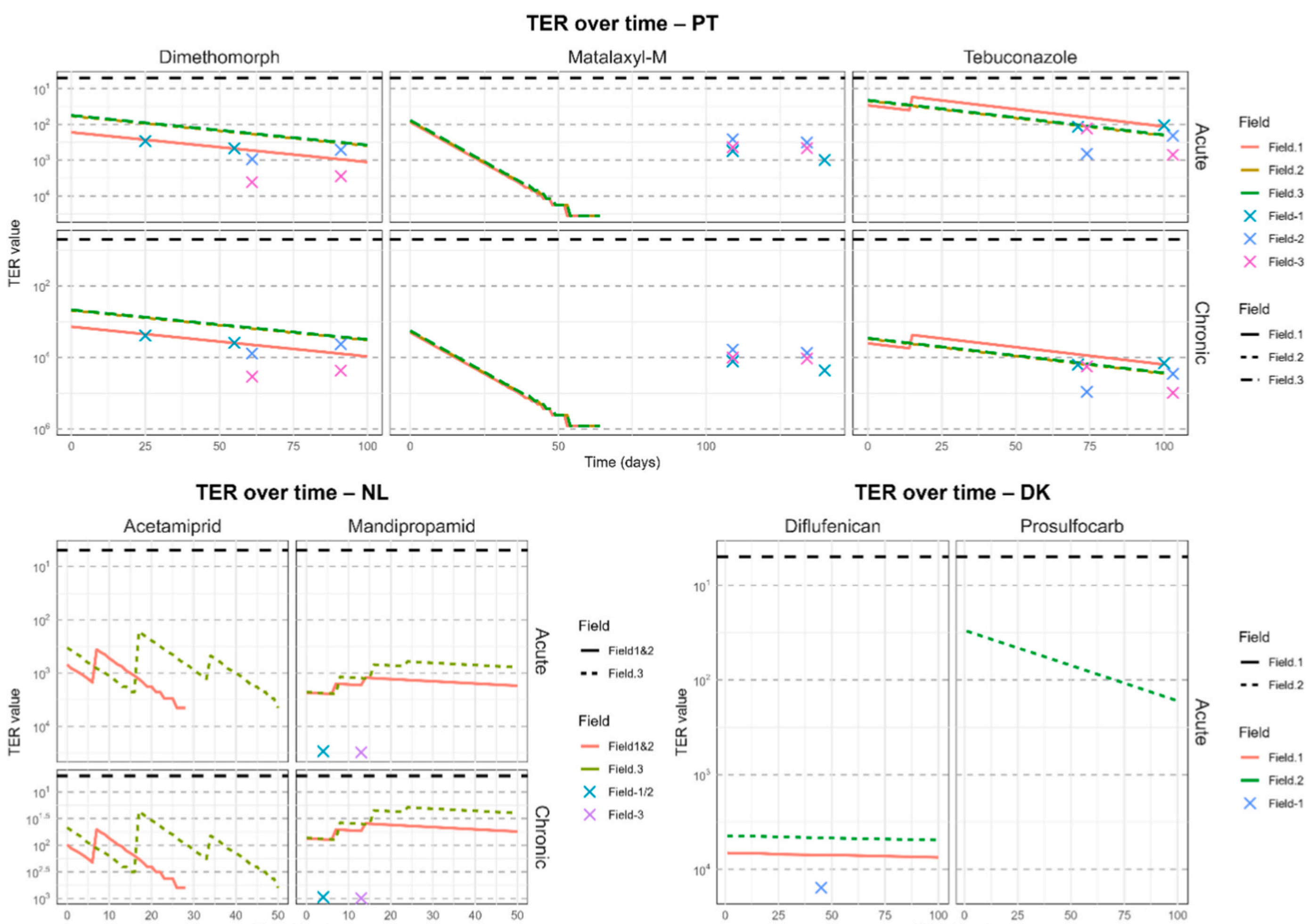

Fig. 4. Earthworms TER_{acute} and $TER_{chronic}$ based on modelled and measured soil concentrations for locations: a) PT, b) NL, c) DK. In the x axis the simulated days; in the y axis the log10 (TER). Each panel is a combination of a Pesticide and a TER outcome (acute or chronic). The black dotted line indicates TER = 5 (above this value there is risk). Each line is a different field (legend on the right). The X mark represents the TER calculated based on the measured (at that time point) soil concentration. For NL, we took the average of field 1&2. TER was not calculated for values < LOD.

from Liu et al., 2014). In the light of these findings, the exposure-toxicity ratio (TER) with genotoxic effect as an outcome was recalculated and it resulted below 5 in several instances. This means that continuous exposure to metalaxyl-M at the predicted levels would likely lead to DNA damage. For tebuconazole, other studies (Li et al., 2022; Zhang et al., 2020) found lower acute LC50 than the one reported in PPDB. Nevertheless, when recalculating TER_{acute} for tebuconazole all values were still well above 5. Finally, for dimethomorph, no studies were found that showed largely different values than those used from PPDB. For example, Wang et al. showed that low to intermediate (1–10 mg kg^{-1}) concentrations of dimethomorph had no significant effect on earthworm toxicity (Wang et al., 2017). No studies were found that looked at mixture exposure to two or three of the PPPs used in PT fields combined.

For acetamiprid and mandipropamid, both used in NL, a comprehensive study on multiple outcomes (Saggioro et al., 2019) reported that acetamiprid concentrations at 0.5 and 1 mg kg −1 may lead to earthworm avoidance responses and that reproduction (outcome used as chronic NOEC guideline in the present study) was also affected, with fewer cocoons and hatchlings per cocoon observed at 0.05 and 0.1 mg kg −1. As indicated by the authors, these results were statistically significant for chronic (i.e. long-term) exposure. Hence, the NOEC chronic from 1.26 mg kg −1 (PPDB database) to 0.05 mg kg −1 was adjusted, but all TER values were still above 5, indicating low risk even at these low dosages. For mandipropamid only one study was found but did not contain relevant data. The focus of this study was on mandipropamid isomers and detoxification mechanisms of earthworms (*Eisenia fetida*) (Fang et al., 2021). Finally, no mixture studies were found, using both acetamiprid and mandipropamid combined, however, it is important to point out that Teng and colleagues (2022) found that acetamiprid joint effects with another PPP, namely abamectin, were synergistic, meaning that the impact is more significant than both could have shown by themselves. So, TER values for this mixture are likely lower than those presented here.

For DK location the TER values were calculated only for acute exposure (see Fig. 4), since there were no reports on chronic NOEC for prosulfocarb and since the reported values of NOEC for diflufenican were like those of acute LC50 (>500 mg kg^{-1}) (Lewis et al., 2016). For diflufenican and prosulfocarb, herbicides used in DK locations, the literature search indicates one study that reported acute LC50 of 12.464 μg cm^{-2}. When re-calculated from μg cm^{-2} to mg kg^{-1}, by assuming values for common earthworm: 12 cm length; 0.64 cm width and 3.7 g weight, the value of 25 mg kg^{-1} was obtained, which is lower than the one registered in PPDB (=71.8 mg kg^{-1}). Independently, the TER_{acute} with the lowest LC50 value as input is still well above the threshold of five. No chronic effect studies on Prosulfocarb in earthworms were found. Also, for diflufenican no additional studies besides the one reported by PPDB were found.

2.3. *Predicted environmental concentrations of PPPs in water and sediments*

Fig. 5 shows the PEC_{SW} and PEC_{sed} of the seven PPPs applied in the three locations, PT, NL and DK.

For PT location the PEC_{SW} values in the first three days after the application were very high but decreased below 0.1 μg L^{-1} after day 21. The main route of water contamination is drift due to spraying, although the three plots are far away from the nearest water body (30–150 m) and the drift due to spraying is mitigated by more than 90 % (compared to the predetermined distance in the FOCUS scenarios, 4 m between the treated plot and the nearest water body). PEC_{SW} values have resulted higher for the "field 1″ plot due to its greater proximity to the nearest water body (30 m, tributary) compared to the "fields 2 and 3″ plots (150 m from the water body, Cértima river). When the nearest body of water is located more than 20 m away from the treated plot, surface runoff is reduced by 80 %. The reduction of runoff with increasing distance is less than that of drift. However, based on the results obtained for the period taken into consideration during the simulation, the PT location was not subject to surface runoff, since PPPs applications were done at the beginning of the dry season and 2021 was a particularly dry year. In fact,

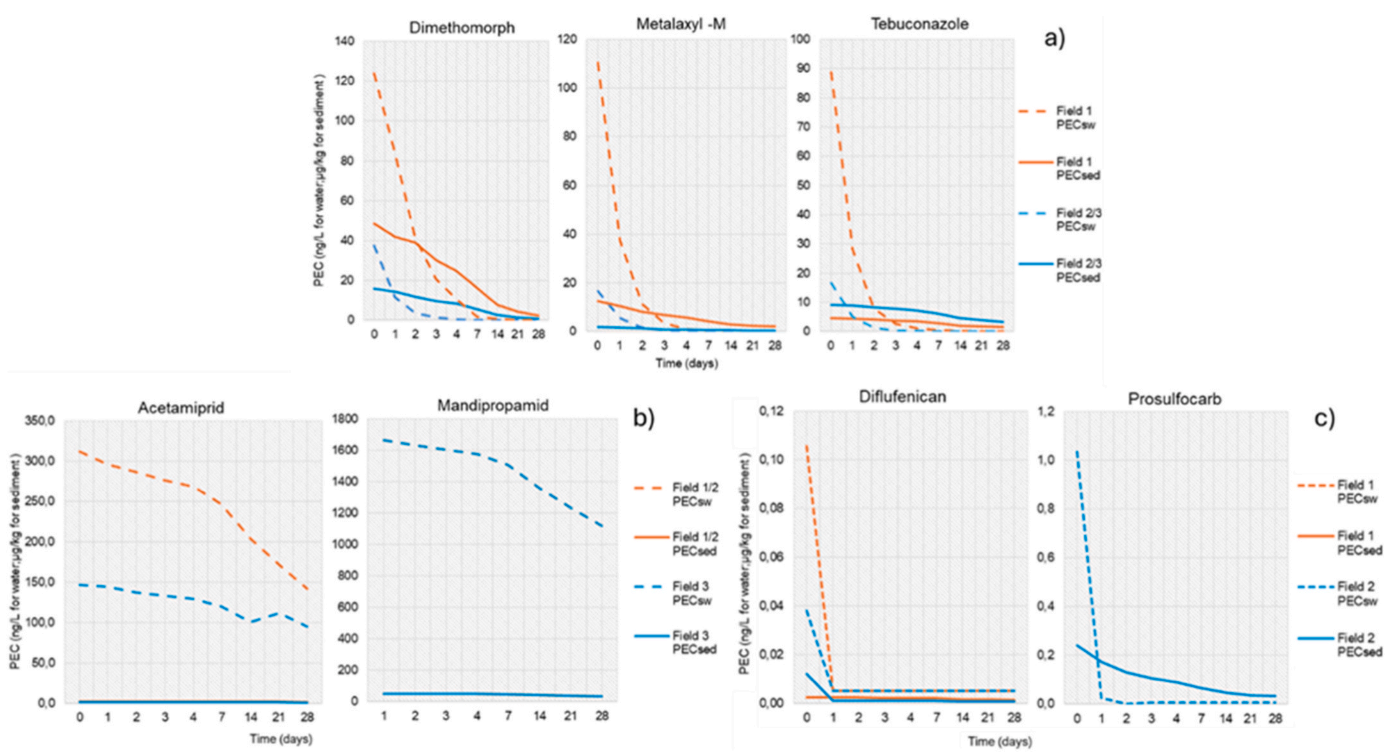

Fig. 5. PECsw and PECsed following application of a) Dimethomorph, Metalaxyl–M and Tebuconazole in PT, b) Acetamiprid and Mandipropamid in NL and c) Diflufenican and Prosulfocarb in DK.

the total annual rainfall for the year 2021 was only 419 mm. For runoff events, the distribution of precipitation is more important than the amount of total annual rainfall. Especially important is the precipitation occurring a few days after the application of the PPPs. In the PRZM model, a precipitation event of at least 20 mm/day is required to have a runoff event. For the Portuguese location, the first significant rainfall event after the application of the three fungicides occurred on October 17 (22 mm of rain), therefore long after the dates of application of the three fungicides, which were done in the May–June period. As a result, no significant runoff events have occurred near the period of application of the three fungicides and drift resulted as the main route of surface water contamination. However, 2021 was a dry year, and should not be considered representative of pedoclimatic characteristics for PT.

In the NL location a significant exposure of the water bodies to the two a.s.s acetamiprid and mandipropamid was observed, with values during the entire simulation period (up to 28 days after PPPs application) higher than the environmental quality standard for surface water (EQS_{SW}) of 0.037 μg L^{-1} for acetamiprid (EC, 2009) and of 0.1 μg L^{-1} for mandipropamid (DL, 2015). The highest concentrations for acetamiprid were simulated in the ditches located at 1m from fields 1 and 2 while 2.1 times lower concentration was simulated in the stream adjacent (1m distance) to field 3. Despite the higher number of applications in field 3, the higher stream flow relative to the ditch result in lower concentrations. The same trend was observed for the concentration of mandipropamid, with 1.2 lower values in the stream adjacent to field 3. The main route of entry is spraying drift. In FOCUS models, runoff only occurs when daily precipitation is higher than 2 cm (20 mm). Since no significant precipitation occurred the first days after applying the two pesticides, the runoff contribution was negligible. However, the PEC_{sw} results obtained should be considered as preliminary, indicating a certain exposure of water bodies to the PPPs used in agricultural fields in the area under study. In the assessment, only three fields were considered, and the complex hydrographic scheme of the polder was not taken into account. It is also possible that other fields in the polder were treated. The results obtained for DK simulations showed significant exposure of the water bodies to diflufenican and prosulfocarb, right after the application, with values higher than the EQS_{SW} of 0.1 μg L-1. Nevertheless, from the first day after the application the concentration decreased below the standard value. The highest concentration of diflufenican (0.11 μg L-1) was simulated in the water body adjacent to field 1 (3 m distance) while 3 times lower concentrations were simulated in the water body located at 3 m from field 2. Even if the application dose of Diflufenican was higher in field 1 than in field 2, the dilution effect in the water body adjacent to field 2 determines its lower concentration there. Prosulfocarb was applied just to field 2 and its concentration was 10 times higher than the EQS right after the application, but it decreased by 40 times in 24 h. The main route of entry in surface water was spray drift at the date of application. Loadings from surface runoff were negligible as the runoff events in PRZM model can be triggered only if the daily rainfall is above 20 mm. The Danish meteorological files used for field 1 and 2 show no heavy rainfall event during the 15–20 days after the application of the two studied pesticides in the fields.

The PPPs concentrations in the sediment in all three countries showed a similar trend as for surface water, with a significant decrease over time. The lowest dissipation rate in time was observed for acetamiprid, mandipropamid and tebuconazole. Acetamiprid and tebuconazole have high DT_{50} (1000 days, Tables SM1, SM2) whereas mandipropamid and tebuconazole have high K_{ow} (log P > 3.2, table). High K_{ow} and DT_{50} values mean higher accumulation capacity and persistence in sediments (Peris et al., 2022).

2.3.1. *Model fits and comparison*

To assess the performance of the models and the influence of the assumptions made during the scenario development, a comparison was made between the simulated and the monitoring results. The PPP measured concentrations for the water surface bodies were previously reported by Navarro et al., and are presented in detail in Table SM6. Information on LOD, LOQ, Rec (%) RSD (%) for surface water measurements can be found in annex 2 from Navarro et al.,).

The comparison in PT was possible just for the Tributary of Cértima river, as the other points samples in the SPRINT campaign were irrelevant to this scope. The models predicted lower concentrations (up to two orders of magnitude) at the sampling date than the monitored concentrations. This may be explained by the fact that the tributary "collects" the residues from the upstream fields. Indeed, taking as an example dimethomorph, its concentration in water the day before the application (24th of June) was already 19.6 ng L^{-1} and on 16th of July was 8.1 ng L^{-1}. Its PEC_{SW} on the same day, the 16th of July, 21 days after the application taken into consideration by the model, was 0.04 ng L^{-1}, 20 times lower than the concentration monitored. Furthermore, for the entire assessment constant streamflow of the water bodies was considered. This represents a limitation of the assessment considering that for Cértima river in the dry season the streamflow starts at 1 m^3 s^{-1} in May and declines to 0.1 m^3 s^{-1} at the end of August, temporarily increasing when it rains. In a very dry year, like the one taken into consideration in the present assessment (Figure SM1A), it can decline to below 0.01 $m^3 s^{-1}$. This lower streamflow decreases the stream's dilution capacity, leading to higher contaminant concentrations for the same load. So, modelling with constant streamflow is not realistic in this site and may explain why the simulated values are lower than the observed values, considering also the high stability of dimethomorph in water (DT_{50} of 1000 days). A similar behavior was observed for tebuconazole, which is also highly stable in water (DT_{50} of 365 days)

For NL, in Table SM6 are presented the monitoring results for the water bodies adjacent to fields 1 and 3 over 6 months period, the time before the start of PPPs application and the harvest of the crops (April–October 2021). Higher simulated concentrations were observed for water and sediment for both fields 1 and 3. For water for both fields and both pesticides, from 2.5 to 24 times higher concentrations were calculated by the models. However, the monitoring date used for comparison was at least 8 days later than the last day of simulation and a higher decay could have been seen on the day of monitoring. Indeed, the only monitoring dates useful for the comparison were26th of August 2021 for field 1 and August 25, 2021 for field 3 even if also these dates do not correspond to the simulation dates but are the closest. The last day of simulation for field 1 in water was the 6th of August and in sediment was the 21st of August, whereas for filed 3 was the 30th of July for water and the 9th of August for sediment. The concentrations in the sediment for both compounds were below LOD, resulting in much lower values than the simulated values. Also here, the watershed characteristics may have influenced the monitoring results as the hydrographic scheme is very complex with ditches separated by sluice gates.

In DK, one single monitoring campaign was undertaken in May 2021. Comparing the results of the simulations with the monitored results, higher simulated values were observed for diflufenican in the water body adjacent to field 1 compared to the monitored values (105 ng L^{-1} simulated vs < LOD of 0.7 ng L^{-1} monitored). However, in less than 24 h the simulated concentration decreased below 1 ng L^{-1}. For this field the date of the application of diflufenican corresponds with the date of monitoring. No comparison between simulated and experimental results was possible for field 2 as both a.s.s were applied several months (≈14 months for diflufenican and ≈13 months for prosulfocarb) before the monitoring campaign.

2.4. *Aquatic organisms' exposure*

To assess the impact of water contamination on aquatic organisms in the three countries, both simulated and monitored concentrations of PPPs were compared with acute (LC_{50}) and chronic (NOEC) toxicological endpoints for fish (mainly *Oncorhynchus mykiss*) and invertebrates (*Daphnia magna*) (Table SM7). Toxicological values for each PPP were retrieved from the PPDB (Lewis et al., 2016). In general, the toxicological values were between one and eight orders of magnitude higher than the PEC_{sw} and the monitored concentrations. Specifically, LC_{50} values were at least two orders of magnitude higher than the simulated concentrations, and four orders of magnitude higher than the monitored ones, while the NOEC is at least one order of magnitude higher than the simulated and three orders of magnitude higher than the monitored concentrations for all locations.

For the risk assessment of the active substance metalaxyl-M, used in PT, EFSA reported two different studies on *O. mykiss*, one indicating an LC_{50} of 100 mg L^{-1} (as indicated in Table SM4) and the other a higher value of 121 mg L^{-1} (EFSA, 2015). For dimethomorph, no relevant LC_{50} studies were found for *O. mykiss*; instead, toxicity data are primarily available for zebrafish (*Danio rerio*), a tropical freshwater species not representative of the three countries (OECD, 2019). Nevertheless, zebrafish is considered a valuable model organism due to its transparent body, rapid development, and well-characterized genetics-features it shares with *D. magna* (Hussain et al., 2020). Sancho et al. (2016) reported a NOEC of 0.41 mg L^{-1} for the intrinsic rate of natural increase in *D. magna* exposed to tebuconazole for 21 days—higher than the NOEC reported in the PPDB. Furthermore, an EC_{50} (effective concentration of the toxicant at which the value of a given parameter is reduced of 50 % with respect to the control) of 0.62 mg L^{-1} was calculated for the number of neonates per female over the same exposure period, indicating a 50 % reduction compared to the 14-day experiment. Despite this value being higher compared to the simulated and monitored ones in the PT, the decreasing trend of the EC_{50} over time suggests that a continuous chronic exposure to tebuconazole may impair the reproductive function of *D. magna*.

For acetamiprid, applied in NL, there is at least a four orders of magnitude difference between the PECsw and the monitored PPP concentrations, both of which remain well below the toxicological thresholds. In the case of mandipropamid, however, EFSA reported a 21-day NOEC for reproduction and body length in *D. magna* of 0.076 mg L^{-1}, which is one order of magnitude higher than the PEC_{sw} values and two from the monitored ones (EFSA, 2012).

The toxicological data of diflufenican and prosulfocarb, as reported in Table SM4, were derived from the corresponding EFSA risk assessments (EFSA, 2007 and 2008). For diflufenican, simulated values were at least five orders of magnitude lower than the lowest toxicological value (a 21-day chronic NOEC of 15 μg L^{-1} for fish). In the case of prosulfocarb, EFSA adopted a conservative approach in selecting the acute toxicity threshold for *O. mykiss*, using an LC_{50} of 0.84 mg L^{-1}, despite another cited study reporting a higher value of 4.3 mg L^{-1} (EFSA, 2007). Nevertheless, the PEC_{sw} of prosulfocarb is just one order of magnitude lower than the NOEC for *D. magna*.

No studies were found that analyzed the exposure of aquatic organisms to a mixture of more than one of the PPP considered. Therefore, based on the results obtained, there is no significant risk to fish and invertebrates considering the simulated and monitored concentrations in any of the three locations. However, potential synergistic effects arising from combined exposures cannot be ruled out and warrant further investigation.

2.5. Predicted concentrations in invertebrates and fish and human consumption risks

Results for all studied water bodies in PT, NL and DK and separated by aquatic organisms were calculated. For most cases, concentrations in both fish and invertebrates followed a log-normal distribution, with concentration decreasing with increase in time after exposure (see Fig. 6, example for NL).

For PT, the overall results for invertebrates show maximum concentrations around 1 mg kg $^{-1}$ body weight for tebuconazole, a relatively low value in terms of risk for human consumption. For example, if an invertebrate with these predicted concentrations were consumed as part of a human diet (e.g. crustaceans), it would be needed to consume 2 kg to exceed the current acceptable daily intake (ADI) of 0.03 mg kg $^{-1}$ body weight (assuming body weight of 70 kg).

For fish, the maximum concentration of tebuconazole was 0.0050 mg kg $^{-1}$. Overall, the values for the three PPPs for these aquatic organisms near the Portuguese location do not seem to pose a risk for human consumption.

Contrarily to the PT location, in NL, predicted concentrations were lower for all species (Fig. 6). Overall, results for invertebrates show maximum concentration of 6.5 mg kg^{-1} body weight for mandipropamid and 1.25×10^{-5} mg kg^{-1} for acetamiprid. The concentrations in fish were even lower, indicating that consumption of fish would not lead to values above the ADI established for humans.

For DK, for invertebrates, maximum predicted concentration was close to 1 mg kg^{-1} bw for diflufenican and 29 mg kg^{-1} bw for prosulfocarb. The concentrations in fish were significantly lower for both

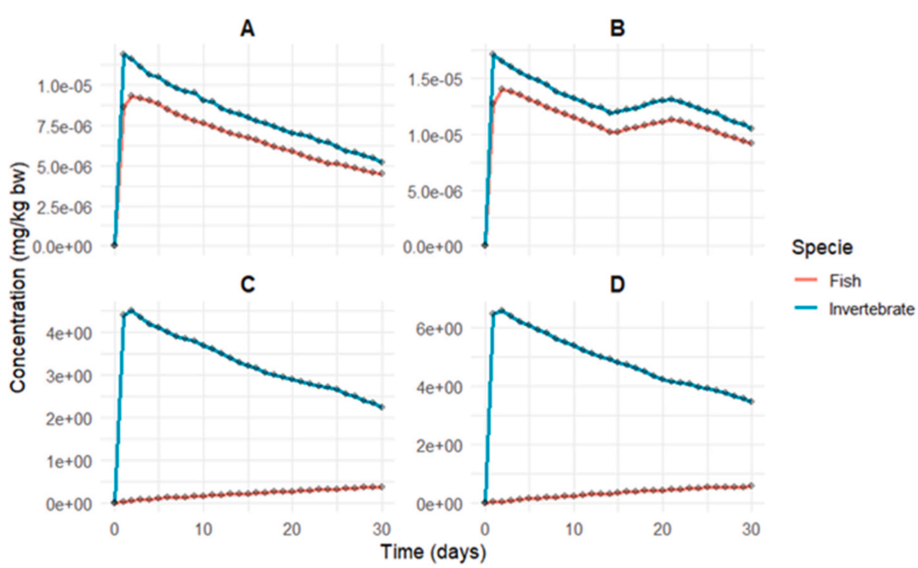

Fig. 6. Concentrations of pesticides in invertebrates and fish for NL location. a) Acetamiprid - contribution from Fields 1 + 2; b) Acetamiprid – contribution from Field 3; c) Mandipropamid - contribution from Fields 1 + 2; d) Mandipropamid - contribution from Field 3. X axis the simulated days and y axis the concentration (mg kg −1 bodyweight). Each line represents different species.

PPPs, likely due to bodyweight used in model predictions. The current established ADI for prosulfocarb is 0.005 mg kg^{-1} bw day, which means that a small consumption (above 13 g) of a given invertebrate (e.g. crawfish or sea urchin) at the predicted concentration would lead to an estimated daily intake over the ADI (assuming human bodyweight of 70 kg). It is important to stress that the model assumes an average invertebrate weight, which may affect predicted concentration based on each species weight. For diflufenican, no risk for human consumption is foreseen at these concentrations.

It was possible to compare the predicted concentrations across the three countries against available PPP measured data for fish items across EU for the year 2020, using the EFSA monitoring databases (EFSA, 2020). Although fish commodities are not mandatory to be analyzed (according to Regulation (EC) No 396/200), 962 fish samples were analyzed during the 2020 EU-coordinated control program. Fish search strings, FoodExCodes, number of samples analyzed and percentage of samples below LOQ can be found in Table S5. Fig. 7 shows variability in pesticide concentrations (in ug/kg) across different fish species, including freshwater and marine species. Mandipropamid, metalaxyl-m, prosulfocarb and tebuconazole were always found below limit of quantification. Maximum concentrations of 1.32 μg/kg were measured in in European plaice for trans-nonachlor (a organochlorine pesticide, component of chlordane). This pesticide was not measured or predicted in our locations, but the orders of magnitude measured in the EU monitoring campaign align with those predict by us. No risk for human consumption is foreseen at these concentrations, however specifically for trans-nonachlor no safe threshold could be confidently identified and with a ADI set anywhere between 0 and 0.0005 mg kg^{-1} bw/day, risk cannot be excluded.

Beyond implications for human consumption, these results highlight the strong interconnectedness between ecosystem health and human health through shared exposure pathways and food-web-mediated transfer of contaminants. We simulated pesticides entering surface water bodies and being taken up by primary producers and aquatic invertebrates, subsequently transferring to higher trophic levels such as fish and, ultimately, to humans via dietary intake. Even when predicted concentrations in fish remain below human health thresholds, elevated concentrations in invertebrates may indicate ecological stress at lower trophic levels, potentially altering community structure, biodiversity, and ecosystem functioning. Such disruptions can indirectly influence human health by affecting the availability, quality and safety of aquatic food resources, as well as ecosystem services such as fisheries productivity and water quality regulation.

Furthermore, the results demonstrate that risk signals may emerge earlier in aquatic organisms than in humans, particularly in scenarios where invertebrate concentrations approach or exceed levels of concern while fish concentrations remain low. This underscores the value of aquatic organisms as sentinels of environmental contamination and reinforces the importance of considering cross-species exposure and feedbacks rather than isolated endpoints. By explicitly linking environmental concentrations to organism-level uptake and potential human exposure within the same modelling framework, this study illustrates how integrated fate–exposure approaches can support a One Health perspective, in which risks to ecosystems and humans are assessed jointly, enabling earlier identification of emerging hazards and more informed risk management decisions.

2.6. Strengths and limitations of the modelling exercise

While the individual models used in this framework (FOCUS, PRZM, TOXSWA and MERLIN-Expo) are EFSA-recognized and well established, the innovation of this work lies in their systematic and comprehensive integration into a single, coherent modelling chain. To date, such integration has typically been limited to coupling no more than two models, often for specific regulatory purposes. Here, for the first time, these tools are linked sequentially to simulate the full continuum from pesticide

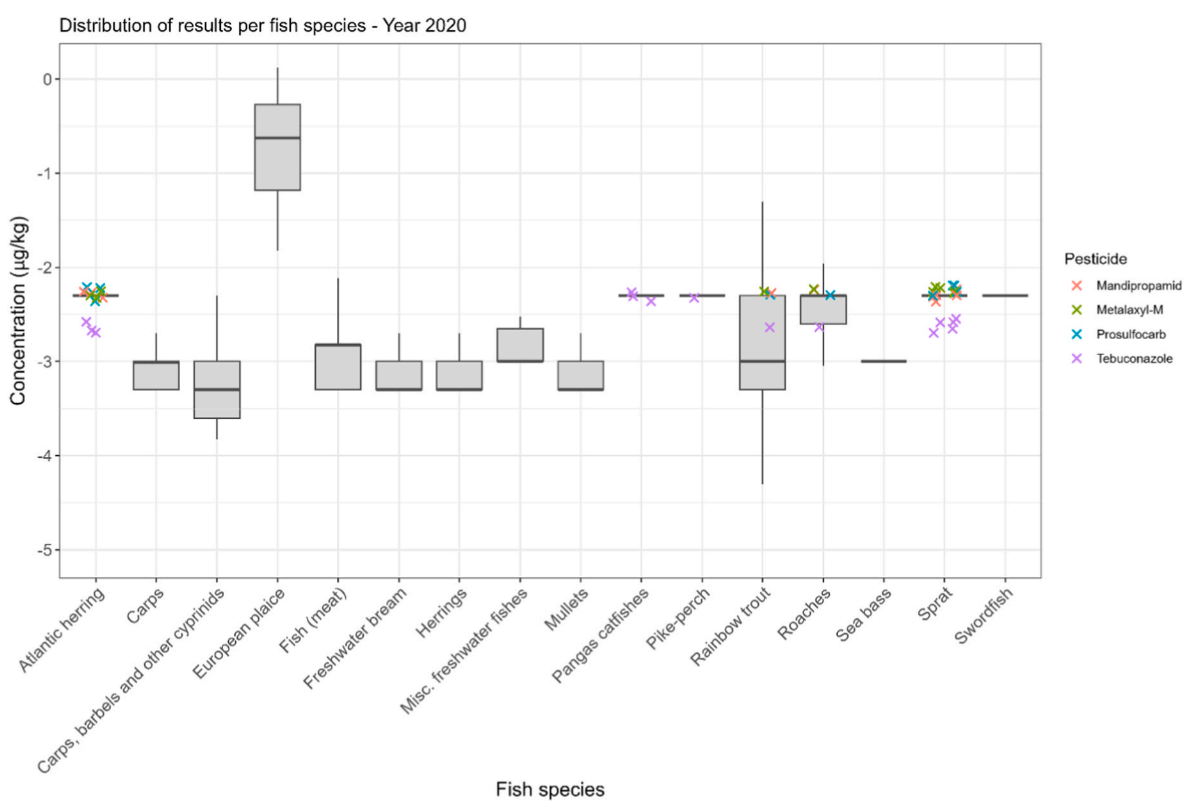

Fig. 7. Concentrations of pesticides in fish species measured across the EFSA 2020 EU-coordinated control program. Highlighted are the pesticides measured and predicted across the studied locations X-axis the different fish species and y axis the concentration (ug kg −1 bodyweight). Values below LOQ, were set to LOQ/2. Samples with LOQ equal or higher than 10 μg/kg were excluded from this visualization.

application in agricultural fields through environmental fate and transport to exposure and risk assessment. This integrated framework enables the calculation of pesticide concentrations in surface water bodies that are directly applicable to ecotoxicological risk assessment and further extended to plankton–invertebrate–fish uptake as well as potential human exposure, thereby supporting a cross-species, One Health risk perspective. In addition, the framework advances current practice by moving beyond scenario-based assessments towards a more realistic representation of agricultural landscapes. Existing regulatory approaches typically focus on simplified, conservative scenarios (e.g. a single treated field adjacent to a water body under predefined conditions). In contrast, the proposed system explicitly accounts for multiple co-existing fields within the same spatial domain, heterogeneous soil properties and textures, varying hydrological conditions, and multiple adjacent water bodies with different flow regimes. By capturing these interacting processes simultaneously, this framework represents a substantive methodological step towards simulating real-world pesticide use patterns and their consequent fate, exposure and risks for both ecosystems and humans, rather than isolated worst-case scenarios.

The outputs of the present modelling exercise were highly influenced by the limited data available as input for the models, collected from the three countries' locations, and in some cases by the miss of important processes in the calculation approach.

One of the most important limitations related to the data used as input for surface water and soil assessments is the availability of suitable weather data. Indeed, for NL and DK, we have used for the assessments data collected by weather stations located at 7, 12, 27 and 73 km away. This made the prediction of drift during the application and of run-off events after application highly questionable and influenced the predicted PEC_{SW} and PEC_{sed} in the water bodies. Additionally, for PT, the weather data collected did not covered the entire application period of PPPs and for some months data from the most recent available months was used. This may have also influenced the PEC_{SW} and PEC_{sed} values in PT. The use of proper climatic conditions may also have influenced the PEC_{soi}l values, as processes such as degradation are highly dependent on the temperature.

Still, for the scenario development very limited data about the surface water bodies hydrology and structures were available. Indeed, in most of the cases one single streamflow measurement was available. Therefore, using a single streamflow value in a highly variable stream which dries up in summer, like in PT, or in a human-managed drainage ditch system, like in NL, may have significantly influenced the predicted water concentrations, even if the loads from fields or during application were correctly predicted. Continuous streamflow measurements would have been useful to properly assess the performance of the used models.

However, in some cases important processes influencing the fate and transport were not considered in the models. This is the case of FOCUS Soil calculator that does not consider losses by leaching.

Concerning the evaluation of models' prediction performance, several limitations were individuated. Firstly, we could not account for PPPs used in other fields during the simulated periods. This would account for model underestimation when compared with measured data. Secondly, a very low amount of experimental data (one single sampling time) was available and useful for comparison between predicted and monitored results. The appropriateness of the model calculation can be either assessed by modelling statistics or simulation graphics. When both system output and model output are deterministic, the arithmetic difference between the measured and calculated output is the most straightforward measure of the model deviation. However, the large amount of data enhances the use of more comprehensive model deviation indicators. Vanclooster et al., 2000 proposes a selection of statistical indicators, but in our case the very low amount of experimental data, one sampling time, does not allow a proper evaluation of model performance. Indeed, in most of the cases the sampling campaigns did not follow the real PPPs application, even if a specific monitoring plan was developed to support modelling exercise. Indeed, a full coordination between farmers and monitoring bodies is mandatory for these studies but it is quite complex to achieve. A higher awareness of the famers concerning the importance of their behaviour should be pointed out already from the beginning of the study. Finally, no useful background values were available.

We acknowledge that the modelling approach involves several simplifying assumptions that introduce uncertainty into the estimated pesticide concentrations. First, the assumption of constant flow neglects short-term hydrological variability, such as storm-driven runoff or low-flow conditions, which can substantially affect in-stream pesticide concentrations through dilution during high-flow events or concentration during stagnant periods. Consequently, peak concentrations may be underestimated or overestimated depending on actual flow dynamics. However, this information was not available for the studied locations. Second, the use of meteorological data from stations located outside the immediate catchment introduces uncertainty related to spatial variability in precipitation, temperature, and evapotranspiration, which influence pesticide transport and degradation. However, this uncertainty is likely limited because the selected stations are within the same climatic region and long-term average conditions, rather than event-scale extremes, are the primary drivers of the simulated processes. Finally, the neglect of pesticide leaching to groundwater represents a conservative simplification for surface-water assessments, as leaching can act as a loss pathway from the soil surface, potentially reducing direct runoff-related inputs to surface waters, while delayed subsurface contributions were outside the temporal scope of the model. This could lead to overestimation of pesticide concentrations in soil; however our results showed that the model bias was low.

However, beside all these limitations, overall, the models performed well considering that in most of the cases the differences between the simulated and the monitored concentrations were of maximum two orders of magnitude and that the largest differences were in the order of nanograms. Indeed, an over- or underprediction of monitored results by two orders of magnitude is considered reasonable, and the models are deemed suitable for supporting regulatory decisions on pesticides (Winchell et al., 2017, 2018).

3. Conclusions

In this study, the fate and the transport of seven PPP applied under real conditions across different crops in locations from three countries, namely Portugal, the Netherlands and Denmark, were assessed in soil, surface water and sediment. The simulated concentrations were compared with monitoring data to assess the reliability and appropriateness of the modelling approach and then used to evaluate the exposure and potential risks to aquatic and soil organisms, as well as to humans.

Counting the soil assessment, the simulated PEC_{soil} was lower than the monitored values in PT, whereas an difference of approximately one-order of magnitude was observed for NL and DK locations. The calculated TER values indicated a low risk to earthworms. However, for metalaxyl-M, applied in PT, several studies have reported toxicity effects at low concentrations. Indeed, when recalculating the TER using genotoxicity as the endpoint, the results suggest that a continuous exposure to metalaxyl-M could lead to DNA damage in earthworms.

For the surface water assessment, the PEC_{SW} values were lower than the EQS_{SW} in the PT location, indicating low exposure of water bodies. In the NL location, however, the modelled PEC_{SW} values showed a significant exposure of the water bodies to acetamiprid and mandipropamid, with concentrations remaining above the EQS_{SW} throughout the entire simulation period (up to 28 days after PPP application). A similar scenario was observed in the DK, where PEC_{SW} values for diflufenican and prosulfocarb also exceeded the EQSsw. In all three locations, when comparing simulated with monitored data, an overestimation of up to two orders of magnitude was observed. When simulated or monitored surface water concentrations are used to assess toxicity to fish and invertebrates, comparisons with reference toxicological endpoints indicate that actual water contamination levels generally remain at least three orders of magnitude below toxicological thresholds. This margin is reduced to one order of magnitude when simulated concentrations are considered. Nevertheless, further investigation is required to account for the combined exposure of aquatic organisms to mixtures of PPPs, which is not currently addressed and is essential for a more robust risk assessment.

Conversely, when simulated surface water concentrations were used to estimate PPPs levels in aquatic invertebrates and fish intended for human consumption, the predicted values indicate that ingestion would not exceed the acceptable daily intake established for humans in PT and NL locations. However, in DK, for the herbicide prosulfocarb, the predicted concentrations suggest that consuming even small amounts (above 13 g) of certain invertebrates (e.g., crawfish or sea urchin) could lead to an estimated intake exceeding the established ADI (assuming a 70 kg body weight). It is important to stress that the model takes an average invertebrate weight, which may influence predicted concentrations depending on each species body mass. For diflufenican, no risk for human consumption is foreseen at simulated concentrations.

Overall, despite the limited experimental and field data that influenced model performance and verification, the in-silico approach presented here provides a useful screening-level framework for assessing PPP fate and exposure in soil, aquatic organisms, and humans. The discrepancies observed between simulated and monitored concentrations—particularly in soil and surface water—reflect both the inherent uncertainty of environmental fate modelling and the constraints of the available field data. Most deviations occurred at very low (nanogram-level) concentrations, where both measurements and simulations are subject to higher variability. Within these limitations, the modelling framework remains a valuable tool for integrating environmental and human health considerations, supporting the One Health perspective by highlighting the interconnectedness of soil, aquatic ecosystems, and human exposure pathways.

CRediT authorship contribution statement

Nicoleta A. Suciu: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Marco Trevisan:** Writing – review & editing, Project administration, Funding acquisition, Conceptualization. **Georgios Fragkoulis:** Writing – review & editing, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation. **Lucrezia Lamastra:** Writing – review & editing, Methodology, Conceptualization. **Sara Triachini:** Writing – review & editing, Writing – original draft, Investigation, Conceptualization. **Nelson Abrantes:** Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Trine Norgaard:** Writing – review & editing, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Paula Harkes:** Writing – review & editing, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Joao Pedro Nunes:** Writing – review & editing, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Vera Silva:** Writing – review & editing, Data curation, Conceptualization. **Irene Navarro:** Writing – review & editing, Methodology, Formal analysis, Data curation, Conceptualization. **Adrián de la Torre:** Writing – review & editing, Validation, Methodology, Formal analysis, Data curation, Conceptualization. **María Ángeles Martínez:** Writing – review & editing, Validation, Formal analysis, Data curation, Conceptualization. **Paul Scheepers:** Writing – review & editing, Methodology, Conceptualization. **Daniel Martins Figueiredo:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envres.2026.123805.

Data availability

Data will be made available on request.

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