Pesticide exposure assessment for surface waters in the EU. Part 2: Determination of statistically based run-off and drainage scenarios for Germany

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Abstract

BACKGROUND: In order to assess surface water exposure to active substances of plant protection products (PPPs) in the European Union (EU), the FOCUS (FOrum for the Co-ordination of pesticide fate models and their USE) surface water workgroup introduced four run-off and six drainage scenarios for Step 3 of the tiered FOCUSsw approach. These scenarios may not necessarily represent realistic worst-case situations for the different Member States of the EU. Hence, the suitability of the scenarios for risk assessment in the national authorisation procedures is not known.

RESULTS: Using Germany as an example, the paper illustrates how nationals soil–climate scenarios can be developed to model entries of active substances into surface waters from run-off and erosion (using the model PRZM) and from drainage (using the model MACRO). In the authorisation procedure for PPPs on Member State level, such soil–climate scenarios can be used to determine exposure endpoints with a defined overall percentile.

CONCLUSION: The approach allows the development of national specific soil–climate scenarios and to calculate percentile-based exposure endpoints. The scenarios have been integrated into a software tool analogous to FOCUS-SWASH which can be used in the future to assess surface water exposure in authorisation procedures of PPPs in Germany.

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1 INTRODUCTION

Regulation (EC) No 1107/2009 governs not only the procedures for European Union (EU) approval of active substances of plant protection products (PPPs), but also the authorisation of PPPs themselves. With the EU approval of active substances harmonised endpoints such as toxicity values or parameters on their fate and behaviour in the environment are established. For the authorisation of PPPs zonal assessment procedures strengthening the principle of the mutual recognition of authorisations are implemented. Once a PPP has been authorised by a Member State, its authorisation should also be accepted by all other Member States with similar agricultural, plant health and environmental (including climatic) conditions. Individual risk mitigation measures for each country may nonetheless be applied. This approach requires harmonised assessment schemes between Member States. On condition national specific agricultural, environmental (including climatic) conditions may be considered,

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the harmonised assessment schemes should recognise national specific spatial and temporal environmental (including climatic) elements as well. Conditions for authorisation may therefore differ from Member State to Member State as a consequence of specific environmental situations rather than due to specific national risk assessment approaches considering country-specific exposure conditions or simulation models. For EU approval of active substances the FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe) Surface Water (sw) workgroup developed a tiered approach to assess exposure of organisms to active substances in edge of field water bodies. This approach is based on the principle of demonstrating ‘one safe use’ throughout Europe. The intention of FOCUSsw was not to perform a specific national exposure assessment but to provide a certain range of possible conditions that could occur. However, FOCUSsw is also used in many Member States to assess national exposure in the context of authorising PPPs. Although the FOCUSsw approach is routinely used for national regulatory decision-making, the overall level of protection is unclear. This lack of clarity is mainly related to the level of protectiveness of FOCUSsw soil–climate scenarios for national specific agro-environmental conditions.

The German Federal Environment Agency (Umweltbundesamt, UBA) has initiated the development of a new approach in order to address the risk resulting from run-off, erosion and drainage entries into surface waters for national authorisation in Germany, to adapt Germany’s national exposure and risk assessment procedure to the FOCUSsw approach as the harmonised exposure assessment approach within the EU, and to overcome some of the limitations of FOCUSsw. The new approach would bring Germany’s assessment procedure in line with the established FOCUSsw procedure, while allowing for the consideration of agro-environmental conditions specific to Germany. The approach for spray drift in Germany is similar to the FOCUSsw approach. Therefore changes on the drift scenarios were not considered.

An exposure assessment approach should first identify the full range of soil and climate conditions in the area of interest. These conditions should then be classified into a manageable number of unique soil–climate combinations for calculating predicted environmental concentrations (PECs). The SEISMIC information system for assessing the fate and behaviour of pesticides in the environment represented an early attempt to achieve this. SEISMIC was based on knowledge of the soil, hydrological, climatic and hydro-geological factors that determine the vulnerability of land and water resources in a given geographic area. Herrchen et al. presented a concept for regionalising the ecological risk of pesticide application with respect to groundwater contamination. Centofanti et al. parameterised 16 climates, 264 soil types and 42 crops for the purpose to facilitate GIS-based pesticide risk assessment for the whole of Europe. These agro-environmental scenarios were developed in the context of the FOOTPRINT project to support pesticide risk assessment in Europe. However, they were never implemented. Representative surface and groundwater scenarios were developed for simulations using the MACRO and PRZM models for Norway; however, the surface water scenarios have not been used for the authorisation procedure. The GIS-based Proziris tool went a step further by facilitating spatially distributed and probabilistic pesticide exposure assessment at the national and zonal levels in Europe. Burns et al. assessed the protectiveness of the national and FOCUS leaching scenarios for the Northern zone by comparing the modelling results of the FOCUS and the national scenarios with spatial cumulative distribution functions (CDFs) produced by Proziris. Tiktak et al. derived an exposure scenario for the Netherlands which corresponds to the 90th spatio-temporal percentile of annual maximum concentration by probabilistic and geostatistical modelling of concentration distribution in all ditches that receive input from spray drift and drainpipes. In terms of the risk assessment for soil organisms the European Food Safety Authority (EFSA) developed two exposure scenarios for each of the three European regulatory zones which satisfy the 90th percentile of exposure concentration in total soil and in liquid phase, respectively. The reliable assessment of a statistically based exposure of a PPP generally involves calculating the basic population of the substance concentrations in all surface water bodies with entire soil–climate combinations in a given regulatory area of interest and for a long weather time series. This results in an overall spatio-temporal cumulative distribution function (CDF) of PECs for a PPP. The level of protection of the aquatic environment is then defined from a regulatory perspective, resulting in an exposure endpoint PEC which represents a specific percentile of the CDF. However, this approach continues to be hampered in practice by limited processing power. In the FOCUSsw Step 3 procedure, the models PRZM and MACRO are used to simulate edge-of-field substance loss by run-off/erosion and drainage, respectively, and subsequently the TOXSWA model to assess substance concentrations in surface water bodies. That means in FOCUSsw, for a basic population of 1000 soil–climate combinations, each with a 30-year time series, a quad-core PC would take around 120 h to run MACRO 5.2 simulations for one PPP (PRZM 4.51 is much faster); consecutive TOXSWA runs would take even longer. This workload continues to be unrealistic for routine use by notifiers and regulators.

For this reason, in order to assess exposure assessment for the authorisation procedure in Germany, a less computationally demanding, but nevertheless spatially and temporally probabilistic run-off, erosion and drainage exposure assessment method has been chosen, introduced as the GERDA ([Geobased (German) Run-off, erosion, and Drainage risk Assessment] approach into the ongoing discussion. As in FOCUS, the PRZM and MACRO models have been used to assess edge-of-field pesticide losses of active substances and metabolites into surface waters from run-off and erosion as well as from drainage.

However, the full spatio-temporal distribution of PECs does not have to be calculated for each pesticide use to be assessed, but only once for 360 (for simulation using PRZM) and 288 (for simulation using MACRO) ‘generic’ PPPs, which cover a realistic range of combinations of the key properties soil organic carbon-water partitioning coefficient (Koc), soil half-life time (DT50), crop type and application month. From a CDF the soil–climate combination can be selected which corresponds to a spatial percentile (predefined by regulation) of the overall statistical population of the CDF. This specific soil–climate scenario for the generic PPP most similar to the PPP to be assessed is then used as the soil–climate scenario for exposure assessment in the authorisation procedure for a PPP.

The methodology to derive national specific soil–climate scenarios and their use in exposure assessment for PPPs in Germany is described briefly in section 2; for more details refer to the final report. In section 3 we summarise how exposure assessments for authorisation of PPP could be conducted using the GERDA-STEPs tool. Finally, we will present results for some example PPPs and compare the PEC derived by means of the new tool with those calculated with the models currently used for PPP authorisation in Germany and the ones predicted by the FOCUS models using the default EU scenarios.
2 DEVELOPMENT OF SOIL–CLIMATE SCENARIOS FOR RUN-OFF, EROSION AND DRAINAGE EXPOSURE ASSESSMENT IN GERMANY

Figure 1 gives an overview of the methodology to derive national specific soil–climate scenarios and their use in aquatic exposure assessment for PPPs in Germany. The pre-processing starts with the classification of the soil types in Germany, which are intersected with a map of climate zones of Germany to allocate soil–climate combinations for the entire potentially pesticide treated agricultural land in Germany. From simulations runs for a set of generic PPPs the substance input into surface waters via run-off and erosion, and drainage, respectively, is calculated by means of models PRZM and MACRO for a 30-year weather time series. Consecutively the concentration in streams is calculated by the model STEPS-3 resulting in a set of CDFs of two surface water exposure variables ‘maximum annual predicted environmental concentration’ (annPECmax,sw) and ‘maximum annual area under the curve concentration’ (annAUCsw). Each CDF represents the overall statistical population for one generic PPP with the spatial component of 130 000 km² arable land and perennial cropland, and the temporal component of 30 weather years.

For the exposure assessment for a PPP to be authorised, the generic PPP with the most similar properties identifies the two CDFs (one ranked by annPECmax,sw and one by annAUCsw) and from each two soil–climate combinations are selected, one for model PRZM and one for model MACRO simulation of substance input into surface waters. Together with the input from spray drift and atmospheric deposition, subsequently the model STEPS-3 calculates 30-year time series of PEC for water body types ‘ditch’ and ‘stream’. From these time series finally the 6th highest annual maxima (equivalent to the 80th temporal percentile) of PECmax or time weighted averaged PECs are selected as exposure endpoints. The procedure is described in detail in the following sections.

2.1 Soil classification

For exposure assessment for surface water with GERDA, the soils from the 1:1 000 000 German Soil Map (BUEK1000) were classified according to the FOOTPRINT soil type (FST) system. The FST system classifies soils by four characteristics: (1) soil hydrology (15 hydrological classes); (2) topsoil texture (six classes); (3) subsoil texture (six classes); and (4) depth profile of organic carbon (11 profile types). As such, an FST describes the relevant characteristics of a soil in terms of the transport routes of soil surface run-off, erosion, drainage and leaching. The main advantages of the FST classification system are that FSTs are already parameterised for the MACRO and PRZM models and that the concept can be applied throughout Europe.

The BUEK1000 is structured as follows: (1) the polygons in the soil map define soil mapping units; and (2) a soil mapping unit contains one or more soil typological units (STUs). A total of 1936 STUs are designated in the BUEK1000. Reference profiles are described in the BUEK1000 for 432 of these 1936 STUs. These reference profiles are automatically assigned to an FST using a classification key. Based on the description of the soil type in accordance with the German soil mapping guideline, the 1504 STUs in the BUEK1000 without a reference profile were assigned to an FST using a correspondence table. Soils in Germany to which PPPs have potentially been applied, i.e. soils used as...
arable land or for perennial crops, are described by a total of 102 FSTs. According to their soil profile descriptions thereof 36 FSTs would require artificial drainage to support agriculture and were assumed as tile-drained. Although STUs are not localised within the soil mapping units, their proportion of land area within the soil mapping units is known and thus, the area of each FST as a percentage of the entire arable land and perennial crop area in Germany can be calculated.

### 2.2 Climate clustering

Climate scenarios for Germany were derived based on a method developed by Blenkinsop et al. First of all, 19 key climate variables, which most influence the transfer of pesticides from soil to surface waters, were identified (see Table S1 in the supporting information). Eight of these 19 variables, relevant for drainage input, were derived by Blenkinsop et al. Based on the results of Nolan et al., relevant for transport via surface run-off and erosion were derived by the authors. The majority of these variables (14 out of 19) describe the frequency of precipitation events above various threshold values, which trigger surface run-off and drain-flow in different seasons.

These 19 variables were then used to perform the climate zoning for Germany. The German Meteorological Service (DWD) provided grid maps of daily precipitation and of monthly temperature data. The 19 climate variables were calculated from these data (time series, 1 January 1980 to 31 December 2009) for 100 m × 100 m grids covering Germany’s arable land area. Principal component analysis (PCA) was then used to reduce the dimensionality of the data. The first three principal components (PCs) explained 87.2% of the total variance. The PC scores obtained by the first three components were then calculated for each grid cell, and a cluster analysis was performed (using the k-means method) to derive 12 climate clusters (CCs) (see Fig. S1 and Table S2 in the supporting information). This number of CCs strikes a compromise between generating high spatial resolution and ensuring that individual clusters are not too similar.

Finally, a representative weather station was selected for each CC. The 19 climate variables were calculated for all German Meteorological Service weather stations. The weather station with the smallest Euclidean distance to the respective cluster centroid was then selected for each CC. These 12 weather time series serve as input for the models PRZM and MACRO both during the generation of cumulative distribution functions for the generic PPPs (see section 2.4), and when running the GERDA-STEP S tool to assess exposure for any real PPP.

### 2.3 Intersection of soil types and climate clusters

In order to identify Germany-specific soil–climate scenarios for PRZM and MACRO simulations, it was necessary to intersect the BUEK 1000 SMU map (linked to FSTs via the previously established SMU-STU-FST relation; cf. section 2.1) with the map of CCs. This resulted in a total of 973 combinations of FOOTPRINT soil type and climate cluster (FST-CC) for run-off and erosion simulations (PRZM model), which include 311 FST-CC combinations for drainage simulation (MACRO model). In other words, not all of the 1224 (102 FST × 12 CC) theoretically possible FST-CC combinations actually occur in Germany. The 973 FST-CC combinations cover the entire 129 480 km² agricultural land area in Germany that can potentially be treated with PPPs, and each FST-CC combination covers a known percentage of the entire area.

### 2.4 Simulation runs for generic PPPs

As mentioned above, due to limited processing power it is not practicable at present to routinely simulate a large number of soil–climate combinations over a long period for a PPP to be assessed, i.e. to generate the overall statistical population of the PEC of a substance for Germany. Therefore, we defined ‘generic’ PPPs for GERDA, i.e. tiered combinations of realistic values of Koc, DT50, and application month for crop types (Table 1). For these generic PPPs, active substance losses (edge-of-field) for all FST-CC combinations were calculated for the weather time series 1 January 1982 to 31 December 2011. The total number of runs was 360 generic pesticides × 973 FST-CC combinations using PRZM for run-off and erosion and 288 generic pesticides × 311 FST-CC combinations for drainage using MACRO. As a result, 350 280 (PRZM) respectively 89 568 (MACRO) 30-year time series with daily values of the following variables were generated: substance run-off loss, run-off discharge, substance erosion loss, sediment load, substance drainage loss, and drainage discharge. These time series were then used to generate 30-year time series of PECsw active substance concentrations with hourly resolution for the ‘stream’ water body type using the STEP-3 model. The STEP-3 model delivers virtually identical values for PECsw as the TOXSWA model from the FOCUSsw approach, but computes much more quickly and is numerically stable.

### 2.5 Ranking of the time variable exposure patterns based on ecotoxicological potential

In order to identify a soil–climate combination with a specific protection level, the many 30-year time series of PECs had to be ranked for each of the generic pesticides. However, these time series can be highly dynamic including multiple exposure events within a year with different magnitude and duration and different intervals between the events. For risk assessment in most cases the maximum concentration or a time weighted average (TWA) concentration for specific time periods (e.g. 7 days) is used as the ecotoxicologically relevant concentration (ERC) to compare the Regulatory Acceptable Concentration (RAC) derived from an experiment with the predicted exposure concentration. Maximum or TWA PECs can easily be used to rank exposure profiles but these descriptors do not consider for example the number of peaks nor intervals between peaks; descriptors, which can be

| Table 1. Factor values of generic plant protection products (PPPs) for modelling edge-of-field losses from run-off and erosion (PRZM model) and drainage (MACRO model) |
| --- |
| **Generic PPP defined by factors** | **Run-off and erosion** | **Drainage** |
| **Crop type** | PRZM model | MACRO model |
| Application month | 2 (winter wheat, fodder maize) | 2 (winter wheat, fodder maize) |
| DT50 | 3 (3, 30, 300 days) | 3 (3, 30, 300 days) |
| Koc | 5 (10, 100, 1000) | 4 (10, 100, 1000) |
| Total number | 360 | 288 |

8 Winter wheat: representative for all winter cereals and rape seed; fodder maize: representative for all other crops (including perennial crops).
ecotoxicologically relevant but in isolation are not meaningful for ranking exposure time series. The full dynamics of a large number of exposure profiles can best be addressed at this stage by the use of toxicokinetic–toxicodynamic (TK-TD) models, which relate the effects on an organism to the hazard caused by the internal concentration resulting from uptake, metabolism and elimination kinetics.21,22

To address which descriptors of a PEC time series should be used for an ecotoxicologically relevant ranking, we compared a ranking based on the effect predicted by a TK-TD model with rankings based on the following descriptors of the exposure time series: PECmax, No. of days with exposure, No. of days with exposure > 0.75*PECmax, 3d-TWAC, 7d-TWAC, and AUC (area under the concentration curve over 1 year). An evaluation based on maximum concentration is useful for chemicals that have a mode of action based on a reversible interaction. For substances that interact via an irreversible mode of action, however, TWA and TK-TD models respectively parameter combinations. The rank

As the TK-TD model we used an implementation of the GUTS model26 (General Unified Threshold Model of Survival) by Ashauer et al.27 for most of the simulations. GUTS covers only lethal effects and, in practice, its substance and species specific parameters are calibrated and verified on the basis of data from toxicity tests. Here we used (1) 400 randomly generated and 26 predefined exposure patterns (see Figs S2 and S3); and (2) 400 randomly generated and 13 real TK-TD parameter combinations taken from the open literature to cover the variability of organisms and substance properties. This was considered as sufficient and relevant for the purpose of comparing several exposure descriptors.

For each of the tested exposure profiles the values of the six descriptors were rank-correlated with effect predicted by the TK-TD models respectively parameter combinations. The rank minimum from the two values of PECmax and AUC has been found to be the descriptor that correlates best with the rank of effect size (for example results see Figs S4 to S6). Therefore, we propose that for the authorisation procedure, the exposure assessment of a PPP should always be carried out using two FST-CC combinations: one FST-CC combination selected from the PECmax distribution, and one FST-CC combination selected from the distribution of the AUC over 1 year. These two FST-CC combinations focussing on short-term and long-term exposure, respectively, are considered to capture, at least in part, the temporal variability of exposure patterns that may occur in reality. For risk assessment of a specific compound it can still be decided based on the available ecotoxicological profile, if the maximum concentrations or a TWA for a specific time window should be used or if the full PEC time series should be considered via the use of effect models (e.g. TK-TD models).

2.6 Percentile-based selection of soil–climate scenarios

The 90th percentile is often used as exposure endpoint for exposure assessment at present.2 In a spatio-temporal CDF (or in a spatio-temporal contour diagram, cf. Bach et al.2 and Tiktak et al.23), the overall 90th percentile of a target variable represents a combination of the spatial component and the temporal component of the overall distribution. The values of the spatial and the temporal percentiles that meet at the 90th overall percentile of a PECmax distribution can vary considerably between CDFs and can also differ substantially from each other (e.g. the 90th overall percentile for a certain PPP may result from the combination of the 73.4th spatial and the 86.6th temporal percentile, for another PPP it may be the 92.1th spatial and the 63.5th temporal percentile). If the 90th percentile value is always stringently singled out in all CDFs, the result will be very different combinations of spatial and temporal percentiles, meaning that disparities between the level of the protectivity in space and the level of protectivity in time might occur.

To overcome this problem, a different approach was chosen for GERDA. The risk of exceedance of a given threshold concentration in time and space was considered to be of equal importance and was set to 20% for both dimensions. From each of the simulated PECsw time series (cf. section 2.4) the 6th highest of the annual maximum PECsw (annPECmax) and the annual AUCsw (annAUC) were extracted representing the 80th temporal percentile of the annPECmax and annAUC over the 30-year simulation period. Subsequently, for each generic substance four spatial CDFs were created by ranking the 973 FST-CC combinations for run-off/erosion and the 311 combinations for drainage according to the values of these 6th highest annPECmax and annAUC (see Fig. 2). To consider the different percentages of the FST-CC combinations over the agricultural land area in Germany, each FST-CC combination was weighted accordingly for the calculation of the spatial CDF. In the end, four sets of spatial CDFs were at hand for Germany: 360 CDFs of the annPECmax,sw respectively annAUCsw for run-off/erosion, and 288 CDFs of annPECmax,sw respectively annAUCsw for drainage. From these spatial CDFs finally the 80th percentile is used to identify the FST-CC combination which represents the 80th spatial/80th temporal percentile soil–climate combination of the overall population (cf. section 3).

The percentile of the overall statistical population that corresponds to the 80th spatial/80th temporal percentile annPECmax value has been evaluated for the generic PPPs (cf. Table 2). The median of the 360 overall percentiles of annual PECmax caused by run-off/erosion fits the aimed 90th overall percentile almost exactly, but the range spreads relatively wide from the 83.2nd to the 93.2nd overall percentile. The median of the 288 overall percentiles of annual PECmax caused by drainage corresponds to the 82.6th percentile, and hence diverges more strongly from the 90th percentile target; values range from the 80.0th to the 89.1st percentile. In order to ensure uniform procedures, however, we refrained from determining any other combinations of spatial and temporal percentiles for the selection of soil–climate scenarios for drainage simulation (MACRO model), whose resulting overall percentiles would then be closer on average to the aimed 90th percentile. Another possibility to shift the range of the overall annPECmax percentiles of the drainage simulation more towards the 90th percentile might be another delineation of the spatial population. For both, exposure from run-off and erosion as well as drainage, the results presented here are based on CDFs for the entire area of 130 000 km² potentially pesticide treated agricultural land in Germany. However, just ca 30% of this land is assumed as tile drained and consequently the CDF curve starts only at a cumulative density of 70%. If one restricts the spatial population for drainage simulation only to the ca 39 000 km² drained area, the 80th spatial percentile position of the CDFs is shifted to a higher PECmax concentration range, corresponding to a FST-CC combination with a higher exposure risk to be selected as national-specific soil–climate scenario.

Finally it should be noted that in the assessment procedure for a real PPP the CDFs for generic substances are not directly used for the exposure assessment for the PPP to be authorised but only
Figure 2. Spatio-temporal distribution of maximum annual predicted environmental concentrations in surface waters (annPECmax,sw) using the example of a given generic plant protection product (PPP, defined by Koc, DT50, crop type and application month). The 973 soil–climate combinations for model PRZM simulation (or 311 combinations in case of model MACRO simulation) are ranked by the 6th highest of 30 annPECmax,sw (i.e. the 80th temporal percentile). From the ranked soil–climate combinations, the 80th spatial percentile was selected, defining the soil–climate scenario for exposure assessment of a PPP with similar properties to be assessed. In total, this procedure reveals approximately the 90th percentile of the overall cumulative distribution of the 30 × 973 (or 30 × 311) annPECmax,sw values.

Table 2. Descriptive measurements of the overall population percentiles of the target values annPECmax,sw and annAUCsw for run-off and erosion input (PRZM model) of 360 generic PPPs and drainage input (MACRO model) of 288 generic PPPs, both for the water body type ‘stream’

| Entry route (model) | Target variable | Minimum | Median | Maximum | Standard deviation |
|--------------------|-----------------|---------|--------|---------|-------------------|
| Run-off & erosion (PRZM) | annPECmax,sw | 83.2 | 90.1 | 93.2 | 2.40 |
| Drainage (MACRO) | annPECmax,sw | 80.0 | 82.5 | 93.2 | 3.28 |
| Drainage (MACRO) | annAUCsw | 83.2 | 88.8 | 92.7 | 1.78 |
| Drainage (MACRO) | annAUCsw | 80.0 | 82.6 | 89.1 | 3.38 |

Target values are extracted as a combination of the 80th spatial percentile (from 973 or 311 soil–climate combinations) and the 80th temporal percentile (from 30 annual maximum values).

To select the national specific FST-CC scenarios for subsequent 30-year simulations for the PPP (cf. next section).

3 Exposure Assessment

The procedure described above was carried out only once for pre-processing purposes. Any PPP to be assessed is characterised by its individual properties (Koc, DT50, application month and crop type), which will usually differ to a smaller or greater extent from the graded values for generic PPPs. For exposure assessment of PPP with the GERDA approach, the generic PPP whose properties come closest (measured as Euclidean distance) to the relevant values of the specific PPP is identified. It is assumed that the CDFs calculated for this generic pesticide reflect the (unknown) overall statistical population of the PPP to be assessed with sufficient accuracy. The soil–climate combination that corresponds to the 80th spatial percentile is selected from each of the four CDFs attributed to the identified generic PPP (note that this soil–climate combination...
The GERDA project developed an approach to define and use soil–climate scenarios for assessing the exposure of aquatic organisms to PPPs within the national authorisation procedure. The approach involves defining and using specific soil–climate combinations for exposure assessment. The GERDA approach is compared to the FOCUS approach, and the results indicate that the GERDA approach provides a more consistent and practical approach for PPP exposure assessment.

The approach involves defining exposure scenarios based on soil–climate combinations and using these combinations to simulate exposure endpoints. The exposure scenarios are determined based on the FOCUS approach and the national procedure for PPP authorisation. The approach includes the following steps:

1. Defining exposure scenarios based on soil–climate combinations
2. Simulating exposure endpoints based on the defined exposure scenarios
3. Comparing the results of the exposure assessment to determine the risk mitigation measures required

The approach is compared to the FOCUS approach, and the results indicate that the GERDA approach provides a more consistent and practical approach for PPP exposure assessment. The approach is currently being implemented in Germany and is expected to be adopted by other countries in the future.
in Germany. However, the approach per se is not restricted to Germany. CDFs of soil–climate combinations in relation to the population of all potential applications within a territory over a given period can be developed for each EU Member State with a manageable amount of effort. The necessary soil and climate data is already available for (nearly) all EU Member States. In our opinion, the methodology of geo-data-based run-off, erosion and drainage risk assessment presented here would constitute a practicable basis for harmonising the method of exposure assessment among Member States. For one, it has been made possible to meet the original call by the FOCUSsw workgroup to implement ‘realistic worst-case’ scenarios for the risk assessment of PPPs at the national level for all Member States. In addition, the GERDA approach could also be applied for the entire territory of the EU or for the three regulatory zones (North, Central, South). As a result, the general approach allows (for the first time) to predict pesticide exposure in surface waters due to inputs via run-off, erosion and drainage with a statistically comprehensible spatio-temporal exceedance probability at the EU level. This procedure represents an compromise between what was necessary from a scientific point of view and what would be cost-effective and user-friendly. It is important to briefly address a few of these aspects.

The total area for arable land is always used as the statistical spatial population for Germany. In principle, however, other more differentiated spatial populations could be defined. For example, the cultivated areas of permanent crops (vineyards, hops, orchards) are not distributed evenly, but are concentrated in locations with a favourable climate, and hence on certain soils. Likewise, some field crops such as potato and sugar beet are also only grown on soils that have certain properties. In all cases where it cannot be assumed that the land area potentially treated with pesticides is distributed evenly across all soil types in Germany, a sub-set of the

While developing the GERDA approach, every attempt was made to design the approach as closely to the FOCUSsw method as possible. On the other hand, the main goal was to address some of the flaws in the FOCUSsw methodology mentioned by Bach et al.2 Table S3 provides a detailed overview of the changes introduced in GERDA compared to the FOCUSsw approach. One difference is the model used to simulate substance transport and fate in the water-sediment system. In the FOCUSsw approach, this is done using the TOXSWA model; in GERDA, the STEP-3 model is used, which requires considerably less computing time and runs stably, in contrast to previous TOXSWA versions (older than FOCUS_TOXSWA 4.4.x). A comparative simulation study of STEP-3 and TOXSWA demonstrated that STEP-3 delivers virtually identical values to TOXSWA (model executable from FOCUS_TOXSWA 3.3.1) for the solute phase (PECsw, TWACsw), with the exception of a few cases of extreme parameter combinations. In the case of sediment concentrations (PECsed, TWACsed), there are some larger differences between the two models with respect to ranges used for several parameters. However, there is no reason to assume a priori that the results of PECsed generated by TOXSWA are more accurate than those generated using STEP-3.

In the course of developing the GERDA methodology, a number of simplifying assumptions had to be set that represented a compromise between what was necessary from a scientific point of view and what would be cost-effective and user-friendly. It is important to briefly address a few of these aspects.

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In the course of developing the GERDA methodology, a number of simplifying assumptions had to be set that represented a compromise between what was necessary from a scientific point of view and what would be cost-effective and user-friendly. It is important to briefly address a few of these aspects.

The total area for arable land is always used as the statistical spatial population for Germany. In principle, however, other more differentiated spatial populations could be defined. For example, the cultivated areas of permanent crops (vineyards, hops, orchards) are not distributed evenly, but are concentrated in locations with a favourable climate, and hence on certain soils. Likewise, some field crops such as potato and sugar beet are also only grown on soils that have certain properties. In all cases where it cannot be assumed that the land area potentially treated with pesticides is distributed evenly across all soil types in Germany, a sub-set of the
species and the other factors such as the Kom- and DT50-value of the protonated ionising compounds depends not only on soil pH but on various CDFs for pH-dependent sorption; however, the behaviour of neutral species, DT50 of neutral species and pK_a, CDFs for such substances can only be calculated on demand for a restricted number of dummy compounds, and by no means for the whole parameter space of substance properties.

For climate clustering, a principal component analysis was conducted jointly for all 19 climate variables; in the subsequent cluster analysis, the 12 climate clusters were identified without differentiating between the routes of entry run-off/erosion and drainage. It would also be conceivable to analyse the 12 climate variables that are relevant for run-off/erosion and the nine variables that are relevant for drainage separately, and then to undertake two separate climate zonation for arable land in Germany. However, this would double the complexity of the procedure.

Another limitation concerns the distribution of flowing bodies of water in Germany. The target of surface water exposure assessment is to protect water bodies. For this reason, under close scrutiny, the statistical population of CDFs should not be the application area, but water body reaches. According to our evaluation, the median river water network density in Germany is 1.3 km km\(^{-2}\) with a range of 0.8 to 1.8 km km\(^{-2}\) for the 25th to the 75th percentile (detailed findings will be published elsewhere). In order to achieve a more precise determination of soil–climate scenarios, the FST-CC combination would actually have to be weighted with the mean river water network density in the FST-CC area concerned. If mean river water network densities vary among the 973 FST-CCs, possibly a different FST-CC scenario would represent the 80th spatial percentile than in the current approach. If this approach is taken further, however, the routing of substances (and hence also exposure) in the water system would also have to be taken into account. The majority of the surface water network is made up of flowing water bodies. This means that substance entries (regardless of their route) along a stretch of water could also send waves downstream and impact those stretches as well. The basic spatial population would then be estimated as approximately 450 000 km of watercourse in Germany, for which the concentration profile over time C(x,t) across the watercourse and the time after entry would have to be modelled probabilistically as a function of dilution and degradation. In view of these extensive problems, weighting by river water network density in the GERDA approach was ruled out.

As in FOCUSsw, no specific soil–climate scenarios were identified for the simulation of concentrations of the active substance in the water sediment system (PECsed). The same scenarios (or more precisely their time series of active substance discharges) were used for PECsed as those selected for simulation of the PECsw values. One reason was that doubling the computing time in GERDA-STEPs would have been counter-productive. Furthermore, the run-off and erosion processes are closely coupled with each other, such that it can be assumed that the order of soil–climate combinations on a CDF for erosion entries would be similar to the order on the CDF for run-off.

It is noted that the selection of soil–climate scenario for substances with soil organic matter-water partitioning coefficient (Kom) values that depend on pH is not addressed straightforward by the 360 (288) generic PPPs. In principle one could create CDFs for pH-dependent sorption; however, the behaviour of ionising compounds depends not only on soil pH but on various other factors such as the Kom- and DT50-value of the protonated species and the pK_a, Kom- and DT50-values of the deprotonated species. Thus, in practice it would be hard to create generic CDFs for pH-dependent sorption. If Kom and DT50 of the basic species would be set to default values and only the acid species are treated, at least a three-dimensional grid is needed for each substance with Kom of neutral species, DT50 of neutral species and pK_a. CDFs for such substances can only be calculated on demand for a restricted number of dummy compounds, and by no means for the whole parameter space of substance properties.

The determination of statistically based national surface water exposure scenarios for Germany was not extended to spray drift deposition but was limited to run-off and erosion and drainage for several reasons. The dimensioning of the FOCUSsw water body types ‘ditch’ and ‘stream’ with respect to their width/depth (w/d) ratio of 3.33 probably does not reflect the real situation for most of the streams and ditches in the EU. For example, from a country-wide channel geometry analysis for the Netherlands, a trapezoidal ditch with a surface width of 2.62 m and a depth of 0.23 m, i.e. a w/d ratio of 11.4, was stipulated as a reference water body for a national specific spray drift scenario. A comparable national database on water body geometry does not exist for Germany; a review on a number of local studies revealed a median w/d ratio of approximately 10 for smaller, freely flowing water bodies in Germany (cf. Kubiak et al. and Table S7). Furthermore, a full probabilistic approach of spray drift calculation has to take into account the frequency distributions of wind speed, wind direction, and distance between treated fields and water stretches as main factors. Tiktok et al. developed such surface water exposure scenarios for the Netherlands combining spray drift together with drainage input, but to our knowledge up today this approach is not adopted as standard exposure model for pesticide risk assessment in the Netherlands.

In general there is no apparent reason why the run-off and erosion and drainage scenarios used by FOCUSsw (Step 3) approach should present a ‘realistic worst-case’ situation, while the initial dilution of spray drift deposition is systematically over-estimated by a factor of approximately 3 with respect to the water body geometry introduced to the drift calculation scheme. This objection holds also for GERDA which is not satisfying from a scientific point of view. However, on the EU level as well as to our knowledge in all Member States it is common practice to combine the simple FOCUSsw spray drift approach together with more refined approaches to calculate substance input via run-off and erosion and/or drainage, as is realised by FOCUS-SWASH.

6 CONCLUSIONS

The kernel idea of the GERDA approach – calculation of CDFs for a set of generic PPP and thereof selection of the soil–climate scenario which corresponds to the 80th spatial percentile for the PEC simulation of a PPP to be assessed – represents a compromise between the call for statistically reliable percentile-based exposure endpoints on the one hand and contemporary computational limitations on the other. In the long term, the GERDA methodology presented here may possibly only represent a temporary solution. In the future, higher computation power can be expected in combination with a faster version of the MACRO model. It would then no longer be necessary to use predefined CDFs for selecting 90th percentile soil–climate combinations. Instead, one could then calculate the entire spectrum of 973 or 311 soil–climate combinations over 30 weather years for every PPP to be assessed using PRZM and MACRO. In other words, the individual overall PEC distribution could be determined for every substance for Germany,
enabling an exact exposure endpoint to be determined for a selected percentile.

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SUPPORTING INFORMATION
Supporting information may be found in the online version of this article.

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