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The European Collaborative Project SOLUTIONS developed models to provide diagnostic and prognostic capacity and fill data gaps for chemicals of emerging concern

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Abstract

The European Union Water Framework Directives aims at achieving good ecological status in member states' water bodies. Insufficient ecological status could be the result of different interacting stressors, among them the presence of many thousands of chemicals. The diagnosis of the likelihood that these chemicals negatively affect the ecological status of surface waters or human health, and the subsequent development of abatement measures usually relies on water quality monitoring. This gives an incomplete picture of chemicals' contamination, due to the limited number of monitoring stations, samples and substances. Information gaps thus limit the possibilities to protect against and effectively manage chemicals in aquatic ecosystems. The EU FP7 SOLUTIONS project has developed and validated a collection of integrated models ("Model Train") to increase our understanding of issues related to emerging chemicals in Europe's river basins and to complement information and knowledge derived from field data. Unlike pre-existing models, the Model Train is suitable to model mixtures of thousands of chemicals, to better approach a "real-life" mixture exposure situation. It can also be used to model new chemicals at a stage where not much is known about them. The application of these models on a European scale provides temporally and spatially variable concentration data to fill gaps in the space, time and substance domains left open by water quality monitoring, and it provides homogeneous data across Europe where water quality data from monitoring are missing. Thus, it helps to avoid overlooking candidate chemicals and possible hot spots for management intervention. The application of the SOLUTIONS Model Train on a European scale presents a relevant line of evidence for water system level prognostic and diagnostic impact assessment related to chemical pollution. The application supports the design of cost-effective programmes of measures by helping to identify the most affected sites and the responsible substances, by evaluating alternative abatement options and by exploring the consequences of future trends.

Keywords: Water quality, Modelling, Emerging contaminants, Emissions, Exposure, Mixture effects, Water Framework Directive

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Challenge

More than 147,000 chemicals are registered under European Union legislative frameworks [1]. Analysis of surface water samples reveals the presence of many thousands of these chemicals in European rivers. Water Framework Directive (WFD) [2] compliant management requires a diagnosis of the likelihood that chemicals negatively affect the ecological status of surface waters or human health. When and where necessary, effective measures should be taken to reach the goal of good ecological status. Water quality monitoring gives an incomplete picture of chemical contamination due to the limited number of monitoring stations, of samples taken and analysed and of chemicals considered. These gaps in the space, time and substance domains limit the possibilities to protect against and effectively manage chemicals in aquatic ecosystems, since relevant chemicals may be overlooked, and hotspots or concentration peaks may go undetected. As monitoring programmes are designed at a river basin or sub-basin scale, inter-comparability across regions or across the EU can be improved. The high and ever-increasing number of chemicals on the market implies that protection and assessment approaches can no longer rely on substance-specific expert investigations only.

Recommendations

The modelling studies carried out in the EU FP7 project SOLUTIONS identified several applications of exposure and risk models that may substantially support monitoring and impact assessment. Thus, we recommend using models and their outcome.

- To complement water quality protection, assessment and management under the WFD to fill knowledge gaps on mixture risks and identify priorities for monitoring and management. This provides a more complete image of the likelihood of adverse effects on aquatic ecosystems and human health, both prospectively and retrospectively [3]. The SOLUTIONS project provides a consistent and integrated set of emission, exposure and effect models to achieve this goal, tested on the European scale.
- To support the assessment of chemical pollution threats. These provide consistent, spatially and temporally variable, Europe-wide estimates of the concentration of chemicals produced and used in Europe as well as risk estimates on aquatic ecosystems and on human health.
- To identify possible hotspots that would have been overlooked by chemical-safety assessment and/or using monitoring data alone.
- To identify potentially hazardous candidate chemicals for monitoring and management intervention that are missing in the current monitoring programmes.
- To use the hydrological relationships that make up water systems to better understand how upstream sources affect downstream receptors, in support to designing cost-effective remediation solutions.
- To better understand how the interplay of socio-economic trends and policies ("Drivers") influences the emissions of a wide range of chemicals and future emerging pollutants ("Pressures"), their occurrence in aquatic ecosystems ("Status") and subsequent effects ("Impact"), substantiating the DPSIR-causal framework.
- To extend the chemical safety assessment for the authorization of chemicals [4] to provide a realistic estimate of the concentrations expected in EU River Basins, and the subsequent stress on aquatic communities and human health, and thus separate the probably harmless from the possibly harmful compounds.
- To explore the use of "big data", automatic acquisition and processing protocols to address larger groups of chemicals.

Requirements

- Modelling-based assessment and management relies on access to data on chemical production, emissions, fate and (eco-)toxicity and thus on maximum transparency.
- The use volume of a chemical is the key to reliably estimate in-stream concentrations (unless the chemical is only used in ways that do not lead to environmental losses). Especially for pharmaceuticals and pesticides, there are strong differences between (sub-)basins in the use volumes of individual chemicals. River basin managers, therefore, need access to information about the actual use volume of chemicals in the basin under their jurisdiction, regardless of commercial interests to keep such information confidential.
- Similarly, toxicity data for as many chemicals as possible are required. This asks for accessibility and transparency of data from chemical authorization and REACH dossiers, including the methodology through which they were established.
- Developments in society (e.g. changes in technologies and demographic change) affect pressures exerted by the presence of chemicals. For several developments and important groups of chemicals quantitative trend

indications can be used in modelling to get a robust indication for future patterns of pollutants.

- An essential element of any spatially and temporally resolved model exercise is a good hydrology model, that provides reliable estimates of runoff and shallow groundwater flows. In SOLUTIONS we used the E-Hype hydrological model (by SMHI, Sweden). This model proved to be adequate for EU-wide assessments. For individual European river basins, the suitability needs to be confirmed.
- For further refinement of modelling more research is needed to predict the partitioning and degradability of "difficult" organic substances including volatiles, cations and zwitterions, to bridge toxicity data gaps and to model the interaction of chemicals with non-chemical stressors in ecosystems.

Achievements

Development of the Model Train

The SOLUTIONS Model Train (SMT) consists of four building blocks: (a) simulation of emissions [5], (b) simulation of fate and transport [6] (c) characterisation of the mixtures' risk for aquatic ecosystems [7], and (d) the prediction of substance properties based on their molecular structure [8]. SMT simulates the emissions, fate and transport, and mixture toxic pressure as a function of space and time, related to the variability of weather, hydrology, wastewater management infrastructure, etc. The model provides fully quantitative outputs, i.e. spatio-temporal data on exposure and on the magnitude of risk (mixture toxic pressure). SMT operates on the scale of Europe or for individual European river basins. The spatial schematisation as well as the hydrology, temperature, soil type, land use and crop cover are derived from the pre-existing Europe-wide hydrology model E-Hype [9]. The model domain for Europe-wide simulations includes 22,728 sub-catchments, with an average size of 252 km^2 (Fig. 1).

Concentrations of chemicals and stress on aquatic systems on EU scale

After a smaller scale exercise for pharmaceuticals in Sweden [10], we calculated the emissions and concentrations

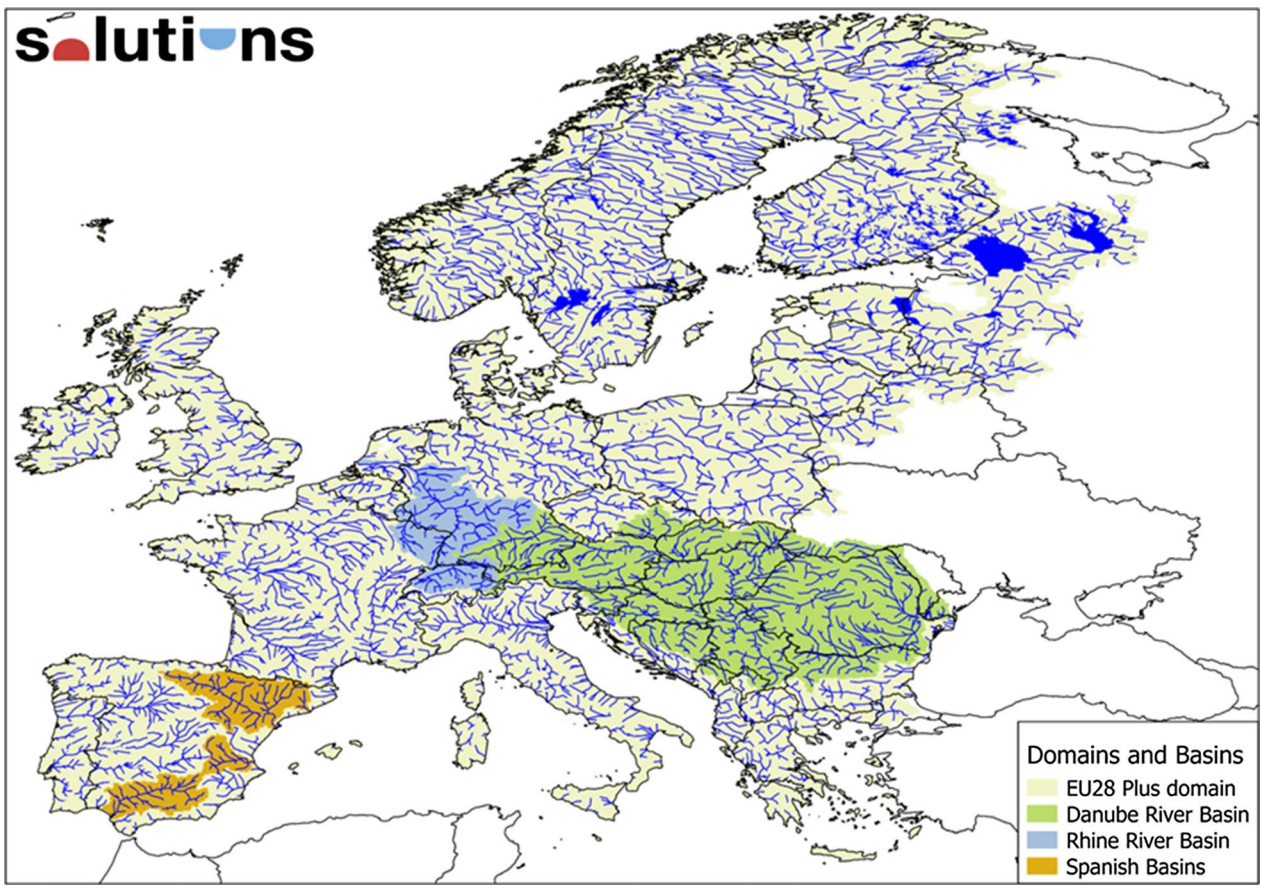

Fig. 1 SOLUTIONS modelling domain and case study areas for validation and demonstration

of 1785 chemicals on the scale of the EU. Figure 1 shows the computational domain, consisting of all river basins covering parts of the 28 EU countries, Norway and Switzerland. Figure 2 shows an example of the simulated emissions to surface waters of the pharmaceutical Fluconazole (CAS 86386-73-4; one of the 1785 chemicals). Figure 3 shows an example of the simulated concentrations in surface waters of the same chemical. The 1785 simulated chemicals include 1348 chemicals of various uses, extracted from REACH registration dossiers, 105 pharmaceuticals and 332 pesticides. They are a subset of 5100 chemicals with quantified emissions, for which sufficient degradability [11] and toxicity data [7] are already available. In addition, the mixture toxic pressure of these 1785 chemicals on aquatic communities was derived from simulated time-variable bioavailable concentrations. The result was converted to one overall map showing a classification of the mixture toxic pressure to diagnose sites with probably insufficient protection in line with Water Framework Directive guiding principles (Fig. 4). Note that for the remaining 3315 chemicals, current Predicted Environmental Concentrations may serve to identify chemicals that possibly occur in high concentrations and need to be prioritised for toxicity assessment. This study only considered direct effects of chemical exposure to effect endpoints such as growth and reproduction. Specific effects, such as endocrine disruption, were not addressed.

The validation of simulated concentrations [5] showed that their accuracy is not perfect, often associated to the limited availability of key input data (see "Requirements"). For 226 validation cases, the simulated concentrations were correct on average, with possible significant under- or overprediction for individual substances: for 65% of cases the error was within one order of magnitude, while for 90% of cases the error was within two orders of magnitude. This should be seen in a context of concentrations of chemicals spanning up to 16 orders of magnitude, and toxicity data spanning up to 9 orders of magnitude. Thus, the models can still provide a meaningful image of the expected impact, variable in space and time. The models can also cover a large number of substances. For these reasons, the models can supplement monitoring data for

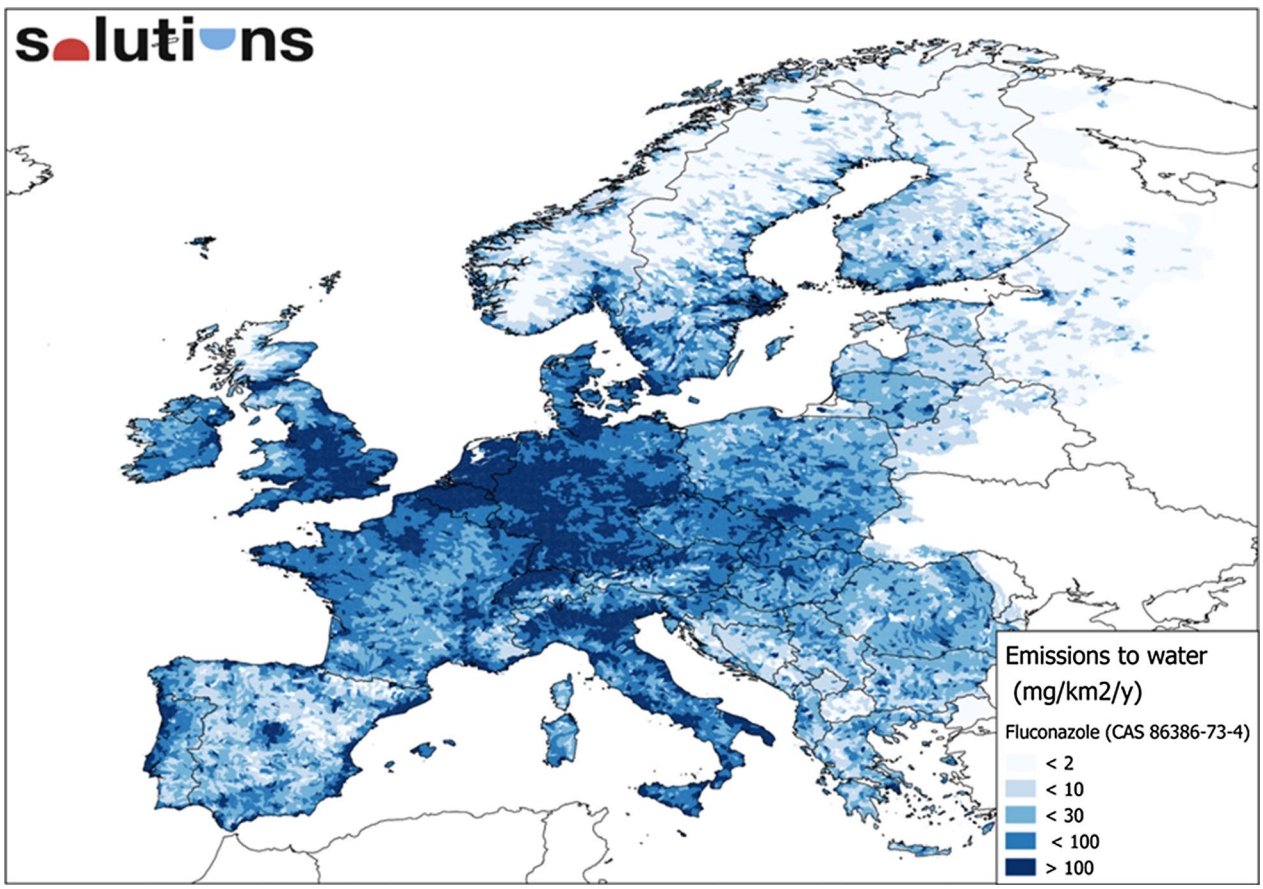

Fig. 2 Example of simulated emissions to surface waters of the pharmaceutical fluconazole (CAS 86386-73-4; one out of 1785 chemicals)

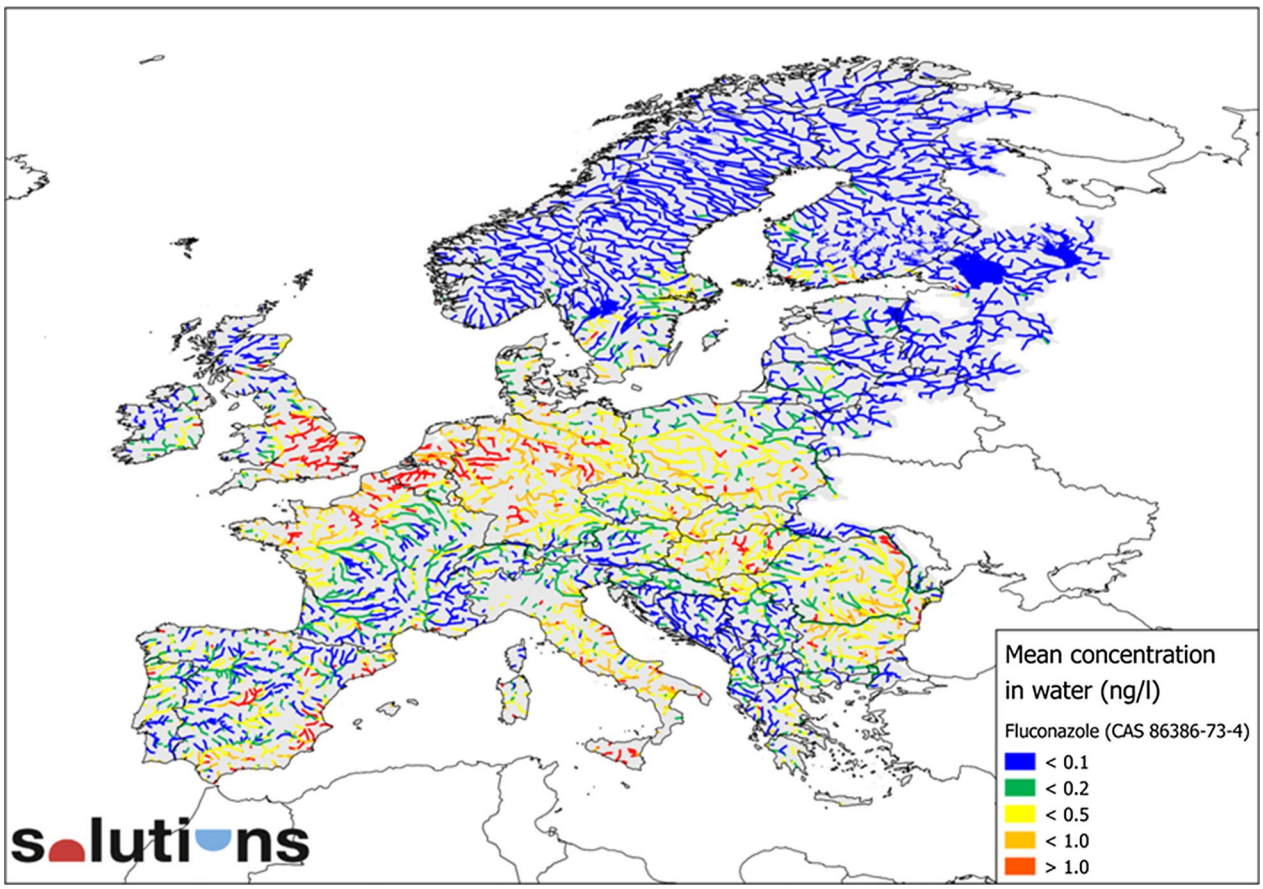

Fig. 3 Example of simulated concentrations in surface waters of the pharmaceutical fluconazole (CAS 86386-73-4; one out of 1785 chemicals)

the diagnosis of current occurrence of and effects from chemicals and can provide a prognosis of the changes thereof as a result of socio-economic changes or the implementation of abatement measures. The below results illustrate this.

Differences between river basins

The assessment of the model-derived data, both input and output, allowed for an analysis of differences between European river basins [12]. Which basins are the most affected? What factors are responsible? In a broad sense, the simulated chemicals' pressure in different river basins is determined by the pressure from population centres and economic activities (including agriculture and industry), relative to the dilution capacity of the surface water system. The highest effects are therefore encountered in relatively small river basins, if they happen to be highly developed and densely populated. An example of the latter is the Llobregat basin in Spain ($\approx$5000 km^2, including the city of Barcelona).

Analysis of hotspots

The assessment of model-derived data also allows for an analysis of hotspots of high mixture toxic pressures—likely associated with high impacts on ecological status [see Policy Brief MARS-SOLUTIONS]—within river basins [12]. These hotspots are found in water systems of densely populated areas throughout Europe, such as Lisbon, Madrid, Valencia, Barcelona, Athens, the western part of the Netherlands, Essen-Dortmund, Brussels, Paris, St Petersburg and Belgrade.

Ranking of substances

After model applications for individual substances (PFOS, PFOA, [13, 14]), toxic risks to aquatic ecosystems of 1785 chemicals produced in Europe have been simulated and potential drivers of mixture toxicity have been identified [12]. This exercise provided a spatially variable picture, especially for pharmaceuticals and pesticides, due to differences in the use intensity between EU countries. On a European scale, the substances expected to be the most relevant regarding ecological impacts via direct

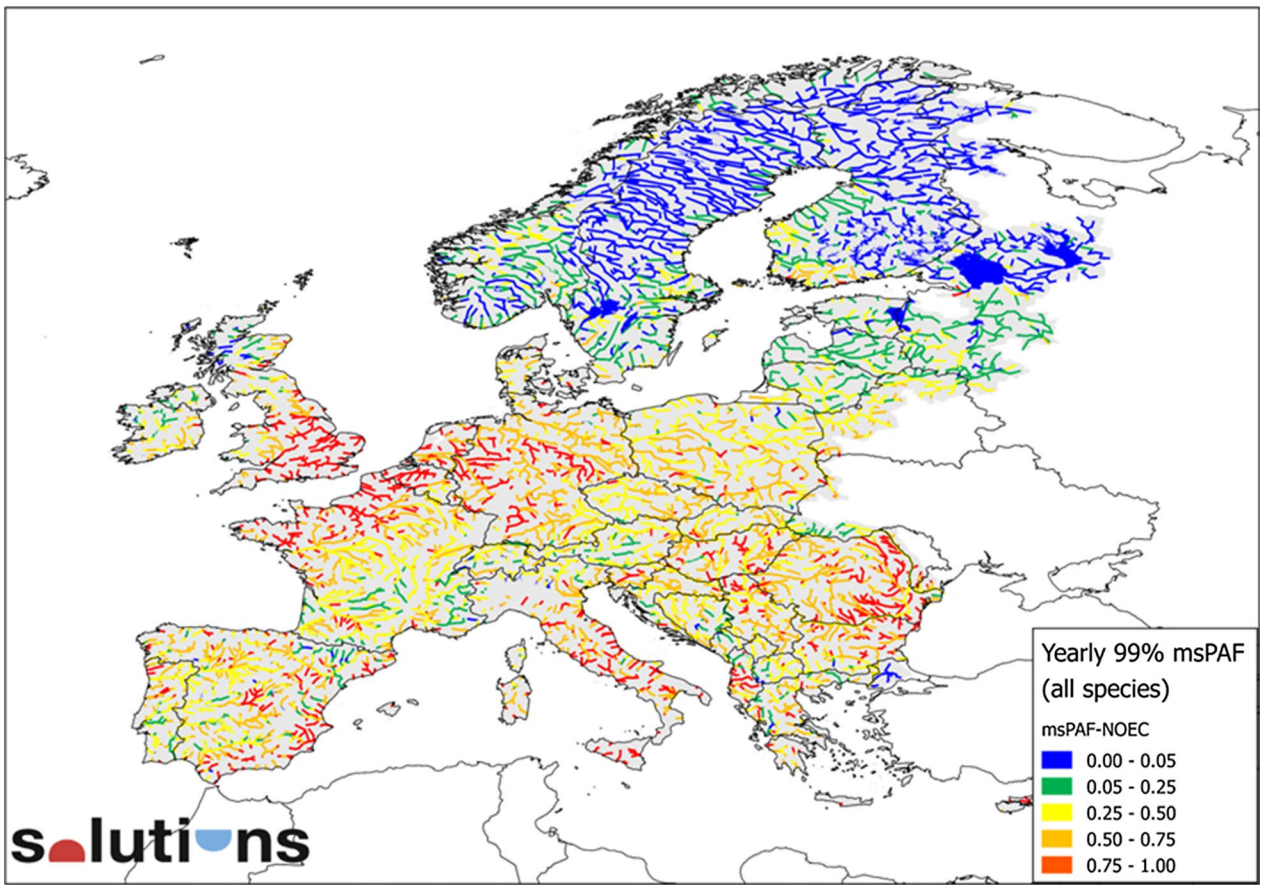

Fig. 4 Classification of level of protection against mixture effects derived from simulated time-variable, bioavailable concentrations of 1785 chemicals. Expected effects are quantified using the multi-substance potentially affected fraction of species (msPAF) derived from species sensitivity distribution effect model, based on no-observed effect concentration endpoint (SSD-NOECs)

effects on vital traits such as growth and reproduction (out of the 1785 we analysed) were identified. Among these were the commercial chemicals octamethylcyclotetra-siloxane (CAS 556-67-2), dodecan-1-ol (CAS 112-53-8) and anthraquinone (CAS 84-65-1), as well as the fungicide chlorothalonil (CAS 1897-45-6). A similar assessment was done for different individual river basins. On such smaller spatial scales, however, the results get more sensitive for the availability of reliable regional information about the use intensity of chemicals.

Ranking of sites and substances in a context of uncertainty

Sites and substance ranking based on predicted environmental concentrations (PECs) is sensitive to details of the methodology applied and to the uncertainty of the PECs. Ranking based on measured environmental concentrations (MECs) is sensitive to the available sampling stations and sampling times and to the accuracy of the laboratory analytical methods. Both approaches are sensitive to the method and data used for toxicity evaluation of the studied compounds. Consequently, sites and substances cannot and should not be ranked in absolute terms but can be classified, for example in a traffic light fashion:

- Site or substance is expected to present a risk ("red")
- Site or substance is not expected to present a risk ("green")
- Site or substance cannot be classified in the above categories ("yellow").

The latter group needs more information to arrive at a conclusion, while they can still be ranked according to the likeliness to be "red" or "green".

Cost-effective abatement

The SOLUTIONS approaches and models have been used to test the efficacy of end-of-pipe measures in the wastewater chain to alleviate effects in surface waters [15, 16]. We demonstrated this in the Rhine Basin Case

Study, first by evaluating the changes brought about by extra wastewater treatment throughout the basin, to evaluate the potential effect of such measures. By limiting the end-of-pipe measures to those sources with the highest contribution to the effects, a higher return-on-investment can be expected. In one example, about 70% of the maximum reduction of mixture toxic pressure was achieved by extra treatment of only 20% of the emission sources. Such a high return-on-investment was found only if a spatially differentiated water quality improvement was pursued: for example, improvement only in areas where drinking water is abstracted, or only at the basin outlet to protect the receiving marine waters.

Future scenarios

The SOLUTIONS models have been used to investigate the effects of expected trends in the use of chemicals towards the year 2030. One of such trends is the expected increased use of pharmaceuticals because of the ageing of the population. Based on the assumptions made, the simulation results indicated that the pressure from this substance group would increase by 36% [8]. The scenario simulations also pointed out that the phasing out of substances of very high concern (SVHC), listed on the REACH Candidate List, can have a strong positive effect on water quality, whilst regrettable substitution (substitution by equally harmful substances) can be identified via modelling, and therefore, avoided. Candidate List substances include important groups of chemicals (e.g. plasticisers). The results show that regulation can have a high impact on the reduction of emissions of problematic chemicals [17] and is an important element for the transition to a more sustainable chemistry [18].

Abbreviations

CAS: Chemical Abstracts Service (system for identification of chemicals); DPSIR: drivers, pressure, status, impact and response; a causal framework for describing the interactions between society and the environment, adopted by the European Environment Agency; EC50: effect concentration causing 50% effect; MEC: measured environmental concentration; msPAF: multi-substance potentially affected fraction of species; NOEC: no effect concentration; PEC: predicted environmental concentration; PFOS: perfluorooctanesulfonate; PFOA: perfluorooctanoic acid; REACH: registration, evaluation, authorisation and restriction of chemicals; SSD: species sensitivity distribution; SVHC: substances of very high concern; WFD: Water Framework Directive.

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Authors' contributions

JvG has been responsible for the concept of the manuscript and drafted the manuscript. LP, WB, IC, DB and CL helped to further elaborate the manuscript and contributed specific aspects. All authors improved the final manuscript. All authors read and approved the final manuscript

Availability of data and materials

Not applicable; presented information is based on previously published data only.

Ethics approval and consent to participate

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Consent for publication

Not applicable.

Competing interests

The authors declare that they have no competing interests.

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