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Solutions for present and future emerging pollutants in land and water resources management

THEME
ENV.2013.6.2-2
Toxicants, environmental pollutants and land and water resources management

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D8.2 Final products (RiBaTox, models, knowledge base and guidelines) accessible via the SOLUTIONS website

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1.1 Summary

In order to allow users to get the maximum benefit out of the models, tools and data that have been developed, tested and compiled by SOLUTIONS, the project developed a well-designed network of information platforms that are easily accessible via the SOLUTIONS website. This will be maintained and updated beyond the project duration. The products include the web-based service RiBaTox which provides the SOLUTIONS tools in a systematic and solutions-oriented way, the SOLUTIONS Model Train which provides the models to predict exposure and risk on a European scale, a Knowledge Base that consists of a searchable database on chemicals providing access to data on monitoring findings, chemical structures and properties, eco-toxicological effects, legislation, and emission and abatement data in a structured way. Finally, the guidance for the SOLUTIONS toolbox designed to support chemical and bioanalytical monitoring, and elaborated to provide problem solving strategies and provide help in applying novel and advanced methods in water monitoring.
1.2 Graph

SOLUTIONS Knowledge Base

Toolbox

SOLUTIONS Mode Train

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4. Section(s)

4.1 Introduction

While scientific papers are well perceived in the scientific community, practitioners from chemical and water monitoring, water managers and regulators need information prepared in a different format and user-friendly way. Thus, SOLUTIONS allocated specific efforts to provide the tools, models and data produced within the project as well-structured and user-friendly products that are easily accessible from the SOLUTIONS website together with a documentation of all the information included in publications and deliverables. Major instruments for providing easy access are (i) the online web-based service RiBaTox providing the user with a structured road to access strategies, approaches and methods solving stakeholder problems, (ii) the integrated data portal IDPS which provides a well-organized entry to SOLUTIONS data, (iii) the SOLUTIONS model train as a set of integrated models for the prediction of concentrations and risks of chemicals produced and used in Europe, and (iv) the guidelines for SOLUTIONS tools which are accessible as fact sheets in RiBaTox as well as an independent deliverable and as an integrated paper. All products can be accessed via the SOLUTIONS website.

4.2 RiBaTox

The web-based service RiBaTox is designed as a four stem bush system with three levels called branch, twig and leave that lead the user to informative fact sheets in a uniform format that is easy to understand. In a concise way it presents the issues that can be addressed with a respective tool or strategy, a description of the methodology and some applications. A short but well-reasoned selection of relevant references is given together with keywords, related topics and contact information. All fact sheets are connected with direct links that allow the user to easily move between the factsheets. Depending on specific preferences a user may have different ways to find an appropriate SOLUTIONS tool or service that supports the needs are offered. These pathways include (1) the fact sheets guide that represents the SOLUTIONS conceptual framework with the entry points “Chemicals”, Environment”, “Abatement options” and “Society” (Figure 1), offering different options. These represent frequently asked user
questions (e.g. How to “Identify and prioritize hazardous chemicals at different scales’’). With few clicks step by step further specifying and refining the question, the user is guided to the fact sheet most appropriate. (2) RiBaTox also provides an overview on the order of the fact sheets according to the systematic tree thus guiding through the three systematic levels to the fact sheet that is most suitable. (3) The user has the option look up fact sheets by search terms from within the title of the fact sheet. Additional services in RiBaTox are the Abatement Module that directly links to the SOLUTIONS abatement database under the label “treatment techniques information mastersheet”, the module Diagnostic Toolbox guiding to a weight-of-evidence approach for ecological assessment, and the link to the Integrated Data Portal IDPS. A detailed description of RiBaTox including the full set of fact sheets is provided in deliverable D4.1.

Figure 1: Screenshot of the RiBaTox Guide to fact sheets

4.3 The SOLUTIONS Model Train

The SOLUTIONS project developed a collection of integrated models, to increase our understanding of issues related to emerging chemicals in Europe’s river basins, to support the prioritization of chemicals
and the abatement of the problems they cause, and to evaluate future scenarios. This collection of models is referred to as the “Model Train”. The Model Train consists of four key building blocks (see Figure 2): (a) the prediction of substance properties based on their molecular structure, (b) the simulation of emissions, (c) the simulation of fate & transport, and (d) the characterization of the risk of mixtures of chemicals for human health and aquatic ecosystems.

Figure 2: Schematic overview of the Model Train.

The Model Train operates on the scale of Europe or for one or more individual river basins. The spatial schematization as well as the hydrology, soil type, land use and crop cover are derived from the Europe-wide hydrology model E-Hype, developed by SMHI (http://hypeweb.smhi.se/). Figure 3 shows the model domain and river network for Europe-wide simulations (EU28P), as well as the case study areas for model demonstration. The Model Train considers the day-to-day variations of the emissions and hydrology and can therefore discriminate between extreme conditions and normal conditions. The substances properties models used are all pre-existing models. An overview of these models and the results they produce is available in SOLUTIONS Deliverable 17.2 (Kutsarova et al. 2017). The fate and transport model is called STREAM-EU (Spatially and Temporally Resolved Exposure Assessment Model for European basins). Its description and some relevant applications have been published (Lindim et al., 2016; 2016a; 2017). A tiered assessment framework for human and environmental risk assessment has been designed, implemented and applied (Kortenkamp et al., 2018), encompassing single and multi-species environmental mixture risk assessment and human health risk assessment via the exposure pathways drinking water and fish consumption.
Figure 3: Europe-wide model domain (EU28 Plus) and case study basins in SOLUTIONS: Rhine, Danube and Spanish Basins (Ebro, Guadalquivir, Júcar and Llobregat)

The SOLUTIONS Model Train is publicly available insofar as software development and application has been financed from within the project or is based on pre-existing open source software, and insofar as data sources are public. This implies that the Emissions, Fate & Transport and Risk Characterization sub-models are available, while the substances properties models are not. The latter is accommodated by providing the substance properties input data for the 1,835 chemicals that have been included in the Europe-wide SOLUTIONS modelling (van Gils et al., 2018).

The publicly available version of the Model Train can be accessed via the SOLUTIONS website, consisting of software, a fully functional set of input files for the Scarce Case Study (see Figure 3), aggregated output from the three sub-models for the EU28P domain and documentation.

4.4 The SOLUTIONS Knowledge Base

The Integrated Data Portal for SOLUTIONS (IDPS) was designed for providing solutions for monitoring, assessment, prioritisation, abatement and regulatory problems in water resources management. Its main
goals are to exchange compound- and structure associated data within the consortium, hold and link to additional survey data, provided also by external databases and providers, and present SOLUTIONS products to stakeholders. It has been described in detail in deliverable D5.1.

The portal provides a coherent and combined data management integrating all information in one knowledge base as interlinked database architecture in order to enable information flow from multiple data sources to each member of the project, thus facilitating a multidisciplinary. IDPS pools data in a searchable format through provision of one end-user friendly portal, which also allows an optimal interfacing with the models. The SOLUTIONS Knowledge Base is directly accessible via the SOLUTIONS website “Results and Products” and can be found under https://www.normandata.eu/solutions/. The Knowledge Base is a modular system that can be searched for chemicals according to different classifiers in the modules shown in Figure 4.

4.5 The SOLUTIONS Toolbox

SOLUTIONS put major efforts into the development and validation of innovative monitoring techniques that also have been demonstrated in the case studies. Recommendations for the application of these tools are elaborated in the context of specific monitoring questions and targeted strategies, which are provided by RiBaTox in a highly systematic and user-friendly way leading to fact sheets as detailed in deliverable D4.1. A more detailed guidance on SOLUTIONS monitoring toolbox, including access to technical standard operating procedures can be found in deliverable D9.1 accessible via the SOLUTIONS website “Results and Products”. It addresses three major topics relevant for the users of the SOLUTIONS toolbox. Moreover, it provides (1) guidance on methods for advanced diagnosis of the status of chemical contamination of freshwaters including sampling, chemical analytical and bioanalytical methods, (2) problem solving strategies for the identification of River Basin Specific Pollutants, impact assessment and the establishment of cause-effect relationships, and (3) the use of novel and advanced methods in water monitoring.
5. Conclusions

In order to allow users to get the maximum benefit out of the models, tools and data that have been developed, tested and compiled by SOLUTIONS, the project developed a well-designed network of information platforms that are easily accessible via the SOLUTIONS website. These will be maintained and updated beyond the project duration. In addition, the persisting European network NORMAN, which has been strongly collaborating with SOLUTIONS and where many SOLUTIONS partners are active members of, will take care of the maintenance and further development of the SOLUTIONS products.

6. References


Kutsarova S., I. Dermen, C. Kuseva, P. Petkov, R. Kuehne and O. Mekenyan (2017): SOLUTIONS D17.2 Predictions of transformation products, physico-chemical properties, fate and toxicity of candidate compounds from chemical screening, EDA and emission modelling. Laboratory of mathematical chemistry (LMC), Prof. Assen Zlatarov University, Bourgas, Bulgaria.


