SOILveR

Soil and land research funding platform for Europe

Project PREMISS

Priorisation of emerging chemical compounds in soils

Acknowledgments

To Soilver funders

How to refer to this report

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SOILveR in brief

The SOILveR platform strongly believes in the need for integrated soil and land research and knowledge exchange in Europe. We acknowledge the added value of coordinating, co-funding and disseminating cross-border soil and land management research. SOILveR is a self-financed platform. The platform members have a common interest in sharing and implementing integrated multidisciplinary research. SOILveR builds on the experiences from other funding networks such as SNOWMAN and address knowledge needs identified by e.g. the Horizon 2020 project INSPIRATION and other initiatives as well as those proposed by the members of SOILveR.

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Abbreviations

CAS: Chemical Abstract Service
CEC: Compounds of Emerging Concern
DB: Database
EC: European Commission
FAIR: Findability, Accessibility, Interoperability, Reuse
GW: Groundwater
RA: Risk assessment
RCR: Risk Coefficient Ratio
PEC: Predicted Environmental Concentration
PFAS: PerFluorinated Alkylated Substances
PNEC: Predicted No Effect Concentration
NOAEL: No Observed Adverse Effect Level
TDI: Tolerable Daily Intake
HBGV: Health Based Guidance Value
LUCAS: Land Use/Cover Area frame statistical Survey
QL: Quantification Limit
SPR: Source-Pathway-Receptor
WFD: Water Framework Directive
WWTP: Wastewater Treatment Plant

1 Context and objectives of the project

1.1 Context

Contaminants of Emerging Concerns (CECs) are raising increasing attention for the last few decades in the water media. The Water Framework Directive 2000/60/EC (WFD, and its daughter Groundwater Directive 2006/118/EC) and its application have been an important driver for water quality since 2000. However, CECs were officially considered in the monitoring of surface water in 2015 (regard to Directive 2008/105/EC of the European Parliament). For the groundwater media, CECs watch list is currently in elaboration under voluntary action of Member States. There are some other European initiatives on CECs for the water media, such as NORMAN (first from research teams such as the NORMAN project funded by the 6th Framework Programme in 2005 and existing now as a non-profit organisation since 2009).

The PREMISS project builds on several experiences from prioritisation of CECs in water compartments. Over the past decade, an increasing number of initiatives have developed to help assess and integrate CECs in environmental risk assessment. Among all actions, two of the most highlighted conclusions are a) the need to share results and b) the inability to prioritise CECs due to a lack of data. Given the complexity of CECs characterisation and assessment, it is indeed necessary to:

- 1) Put together all available data, from all sources of information;
- 2) Find some methods to plug the gaps: the lack of data must not be a hindrance to inclusion of CECs in environmental risk assessment.

There are some European initiatives on soil quality monitoring such as the LUCAS survey, which focused mainly on biodiversity and soil productivity monitoring aspects. However, in absence of a Soil Framework Directive, attention paid to soil quality monitoring in Europe remains insufficient (especially regarding CECs). In addition, there are no soil quality guidelines defined at EU level neither for known substances nor for CECs. The new EU soil strategy has been published on October 2021 and announced several actions. By 2024, develop an **EU priority list for contaminants of major and/or emerging concern** that pose significant risks for European soil quality, and for which vigilance and priority action at European and national level is needed

As an example of the initiatives on CEC's in soils, in November 2018, the first International workshop on Emerging policy challenges on New SOil contaminants (ENSOr) was held in Brussels. It gathered regulatory bodies, R&D communities and economic actors such as service providers (consultancies) and problem owners (industries) and resulted in the EmConsoil network. The EmConsoil network organised a second workshop in May 2021, which provided up-to-date expertise and knowledge on CECs in soil and sub-soil.

A family of CECs, named the PerFluorinated Alkylated Substances (PFAS), has been of increasing concerns for the last few years. For example, CONCAWE (the association for petroleum industries) and NICOLE (Network for Industrially CO-ordinated sustainable Land Management in Europe) have been working on a PFAS review in 2014 and 2015. There are many on-going R&D and management actions, and regulations initiatives on the subject, such as:

- First Flemish (OVAM) soil guidelines PFAS June 2020, Flemish PFAS updated guideline in March 2021.
- OVAM has recently commissioned a study on a review of the currently (internationally) available cleaning options and techniques for soils (including water treatment) contaminated with PFAS.
- In July 2020 the RIVM published background values for PFOA and PFOS in Dutch natural soil, and RIVM and Deltares published a report on the difference in leaching of PFAS from soil and dredging spoil. In July 2021 the RIVM published updated risk limits for PFAS in soil and groundwater based on the EFSA advice.
- The SFSE (Société Francophone Santé Environnement) chose the PFAS as its 2021 thematic. It has started gathering information in view of preparing a practical guide on PFAS contaminated sites management.

- SOILveR webinar on PFAS in 2020
- PFAS International Berlin conference strongly supported by the German Ministry of Environment in 2020
- PFAS Memorandum by the Common Forum in 2020
- PFAS in products and waste streams (Arcadis, 2021).

1.2 Objectives

In this context, the PREMISS project proposes to tackle the issue of CECs in soils and sub-soil media **by developing a modular prototype prioritisation tool for CECs** which would allow the estimation of CECs occurrence and their associated risks in the soil and the subsoil for various levels of data availability and, in fine, to select which CECs require the most attention and additional understanding from management, policy and R&D perspectives.

Detailed objectives are :

1) develop a modular prototype prioritisation tool for CECs enabling the estimation of their occurrence and the associated risks in the soil and the sub-soil for various levels of data availability (including missing or partial information),

2) Test the robustness of this prioritisation tool for a selection of CECs and make recommendations for future development

3) Based on the prioritisation approach and its results, propose opportunities for CECs management and policies (if possible) and recommendations for future R&D work.

To carry out theses actions, stakeholders have been involved all along the project.

2 PREMISS methodology

The work plan consisted of six work packages. WP connections are highlighted in Figure 1. WP3 provided knowledge on the occurrence of CECs in soil and sub-soil for Belgium, France and the Netherlands. Occurrence data were also used for comparison with soil concentration estimated in WP4 and might be used as input data in the prioritisation tool (WP5). WP4 enabled to estimate the potential for not yet monitored CECs to contaminate soils. WP5 generated toxicological information and combined it with both these pieces of information (known/measured and estimated/modelled data) to assess potential accumulation of CECs in soils. In combination with toxicological information, WP5 provided a prioritisation for CECs in soils based on a Source-Pathway-Receptor conceptual model. WP6 defined, based on researchers' and stakeholders' inputs, main expectations on CECs prioritisation and recommendations concerning CECs management in soils. WP1 ensured a smooth running of the project and WP2 organised the dissemination of the project outputs.

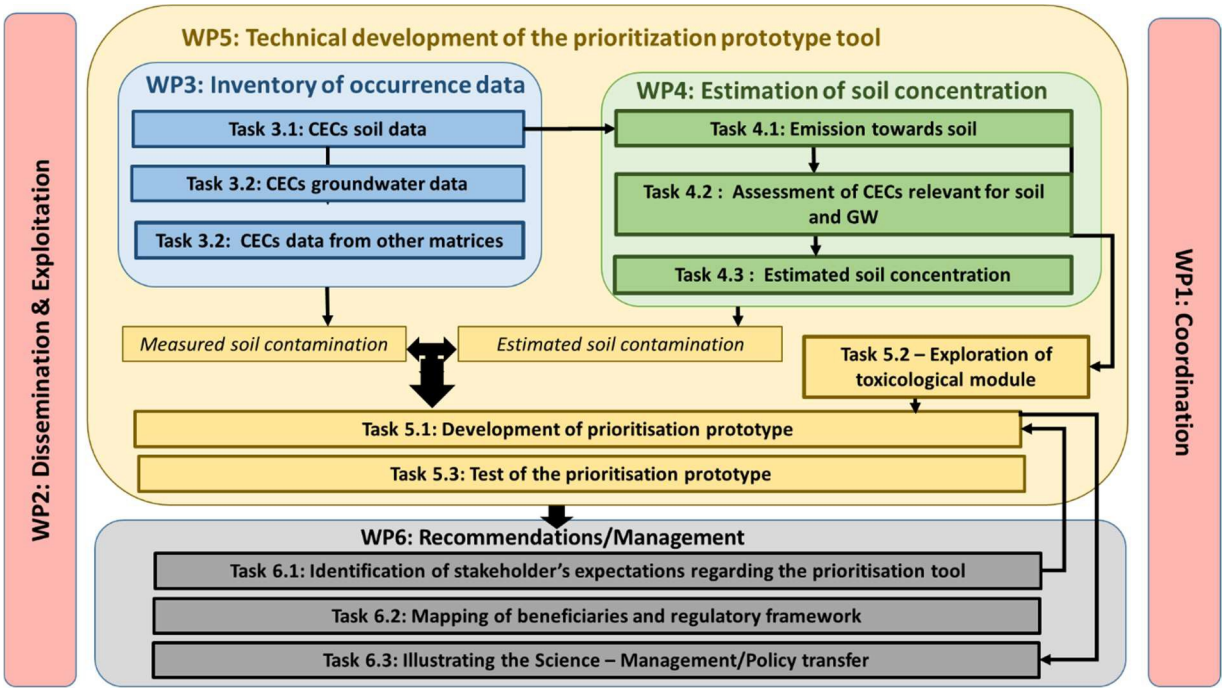


Figure 1 : PREMISS workplan

The inventory of occurrence data, the estimation of soil concentration, the toxicological risk assessment and the whole prototype tool were tested for various spectra of compounds, which were specified for each WP. In any case, PREMISS aimed at illustrating as much variety of situations as possible in testing chemicals having contrasted set of data (in terms of data availability or chemical properties).

In the frame of the PREMISS project, CECs are defined as contaminants of emerging concern in the soil or the subsoil, i.e. not regulated nor regularly monitored in the soil or the sub-soil in partners' countries (France, Belgium, The Netherlands).

3 Inventory of existing data on CECs occurrence in soils, groundwater and sources to soils (sludge, manure)

3.1 Objective

The primary aim of WP3 is to collect existing data on CECs (concentration, analytical thresholds) in soils (including agricultural soils, contaminated industrial land, …), sources to soils (e.g. sludge applied on agricultural lands) and in groundwater in participating countries (Belgium, France, The Netherlands).

The main challenge of this inventory is to identify CECs for which data are available in soils, groundwater, and sources to soils so that the prioritisation tool can be tested. Measured concentrations in soils, when available, will serve for comparison with estimated soil concentration in the transfer module (WP4) or as direct input for the prioritisation tool (WP5). Another challenge is the very large number of chemical substances to consider together with the lack of existing data related to those.

3.2 Methodology

3.2.1 The perimeter of the inventory

Occurrence data of CECs in soils, sediments, wastewater treatment plant (WWTP) sludge, and groundwater in national reports and databases (DB) were inventoried. As CECs data in soil are scarce, occurrence data from national reports or scientific literature were also included.

The inventory was in principle limited to occurrence data measured from 2010 until the end of 2020, in France, The Netherlands, the Flemish or the Walloon regions in Belgium. However, some exceptions were made when occurrence data were already aggregated for a larger geographic zone (e.g. JRC, 2012) or a larger time scale (e.g. TNO published Dutch soil background concentrations in 2004).

3.2.2 Compounds selection

Step 1

First, all chemical substances regulated in environmental matrices in the participating countries or at the European level were inventoried (see table 1 below). This step allowed to exclude a list of already regulated chemicals from the scope of the project.

Table 1: Regulated substances in soils in partners' countries

Substances excluded from the perimeter	Reason for exclusion
benzene, toluene, ethylbenzene and xylene (BTEX)	Regulated in Walloon Soil Decree of 13th of December 2018; Benzene and BTEX Regulated in French Guidelines for Excavated Soils (BRGM, 2020); Benzene regulated in Dutch Soil Decree of the 22nd of November 2007; Regulated in the VLAREBO 2008[1]
Polycyclic Aromatic Hydrocarbons (PAHs)	Regulated in Walloon Soil Decree of the 13th of December 2018; regulated in Dutch Soil Decree of the 22nd of November 2007; Naphtalene Regulated in French Guidelines for Excavated Soils (BRGM, 2020); Regulated in the VLAREBO 2008
Polychlorinated biphenyls (PCBs)	Regulated in Dutch Soil Decree of the 22nd of November 2007; Regulated in French Guidelines for Excavated Soils (BRGM, 2020); Regulated in VLAREBO 2008.
Polychlorinated dibenzo-p-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs)	Regulated in Dutch Soil Decree of the 22nd of November 2007; Regulated in French Guidelines for Excavated Soils (BRGM, 2020)
Solvents and THMS: - Methyl-tert-butylether (MTBE) - Di, tri, tetrachloromethane/ethane/ethylene - Extractable organic halides (EOX) - Vinyl chloride (VC)	MTBE, di/tri/tetrachloromethane/ethane regulated in Walloon Soil Decree of 13th of December 2018 MTBE, di/tri/tetrachloromethane/ethane/ethene regulated in Dutch Soil Decree of the 22nd of November 2007 MTBE, VC, EOX and di, trichloromethane/ethane/ethene regulated in the VLAREBO 2008 MTBE, VC and di/tri/tetrachloroethylene regulated in French Guidelines for Excavated Soils (BRGM, 2020)

Step 2

Inorganic substances were also excluded from the scope of the project, for two reasons:

1. Most of them are regulated and regularly monitored;
2. Fate of these compounds is less easy to estimate based on general formulas.

[1] 14th of December 2007 - Decree of the Flemish Government establishing the Flemish regulations regarding soil remediation and soil protection.

Step 3

As proposed by Bunting *et al*. (2021)[2], CECs were categorized into 11 categories (Table 2) in order to structure the research.

Table 2: CECs categories defined to undertake the inventory (according to Bunting et al., 2021)

N°	Substance category	Sub-categories included
1	Chemical intermediates	Chemical intermediates, dye intermediates
2	Flame retardants	
3	Lifestyle	Illicit drugs and stimulants, food additives, fragrances, sweeteners and caffeine
4	Personal care products (PCPs)	UV filters, insect repellents, fragrance
5	Pesticides (including biocides)	Pesticides and their metabolites
6	PFAS	
7	Pharmaceuticals (for humans and animals)	Hormones, psychiatric drugs, antihypertensive, cardiovascular, anti-epileptic drugs, antibiotics, antidepressants, lipid regulator, synthetic hormones, contrast agent, tranquilizers, anti-inflammatory
8	Phenols & Alkylphenols	
9	Plasticisers	Plasticisers, plasticiser metabolites, including phtalates and bisphenols
10	Solvents and trihalomethanes (THMs)	Chlorinated and non-chlorinated solvents, petroleum products, halogenated and non-halogenated solvents, chlorofluorocarbons (CFCs), THMs
11	Other CECs	Sterols, natural compounds (including natural hormones)

Step 4

As mentioned above, the high number and diversity of chemical substances is a challenge for such an inventory. Therefore, we selected substance categories based on a prioritisation of the Source-Pathway-Receptor (SPR) conceptual schemes for risk assessment. Identified priority SPR for soil contamination are:

i) WWTP sludge/pesticides application on agricultural soil

Pesticides application remains an acknowledged source of soil contamination. Some organic fertilizers, such as sewage sludge, manure and compost, can also introduce a broad mix of heavy metals and organic pollutants in soils. In France and Wallonia sludge can be spread on soils according to certain criteria (in Wallonia, decree of January 12, 1995; in France, decree of January 18, 1998; see References section).

Due to a lack of data in DB and the heterogeneity of the studies dealing with manure, compost and digestate, we decided to exclude these matrices from the PREMISS inventory.

ii) Sediment application on soil

[2] S.Y. Bunting, D.J. Lapworth, E.J. Crane, J. Grima-Olmedo, A. Koroša, A. Kuczyńska, N. Mali, L. Rosenqvist, M.E. van Vliet, A. Togola, B. Lopez, Emerging organic compounds in European groundwater, Environmental Pollution, Volume 269, 2021, 115945, ISSN 0269-7491, https://doi.org/10.1016/j.envpol.2020.115945

In the Netherlands and in the Flemish region, dredged sediments can be applied on soil if the quality meets the criteria of the Dutch Soil Regulation or Flemish regulation respectively. In the Flemish region, they can also be recycled in the construction sector ("Bouwstof") with specific quality thresholds. In France and Wallonia, they can be recycled in coverage of landfill sites, limited by the concentration of metallic trace elements, PAHs and PCBs.

Marine sediments are excluded from the scope of the project. Exceptional events such as flooding events are also excluded.

iii) Industrial emissions (i.e. releases during production)

Accidental releases and chronic leaks are out of the scope of the project.

Step 5

Relevant chemical substance categories related to the identified SPR are presented in Figure 2. These categories still involve a very large number of chemical substances (Table 3). Consequently, it has been necessary to further limit the inventory to a list of chemicals within these categories. Substances were selected in order to get a panel of substances with varied physicochemical properties. The complete list of substances included in the inventory is presented in Annex B.

Table 3 : Selected CECs categories for the inventory in PREMISS

	Category	SPR	Number of researched compounds
1	PFAS	i, ii and iii	31
2	Phenols & alkylphenols	i and ii	23
3	Pesticides	i and iii	11
4	Pharmaceuticals & veterinary drugs	i	12
		Total :	**77**

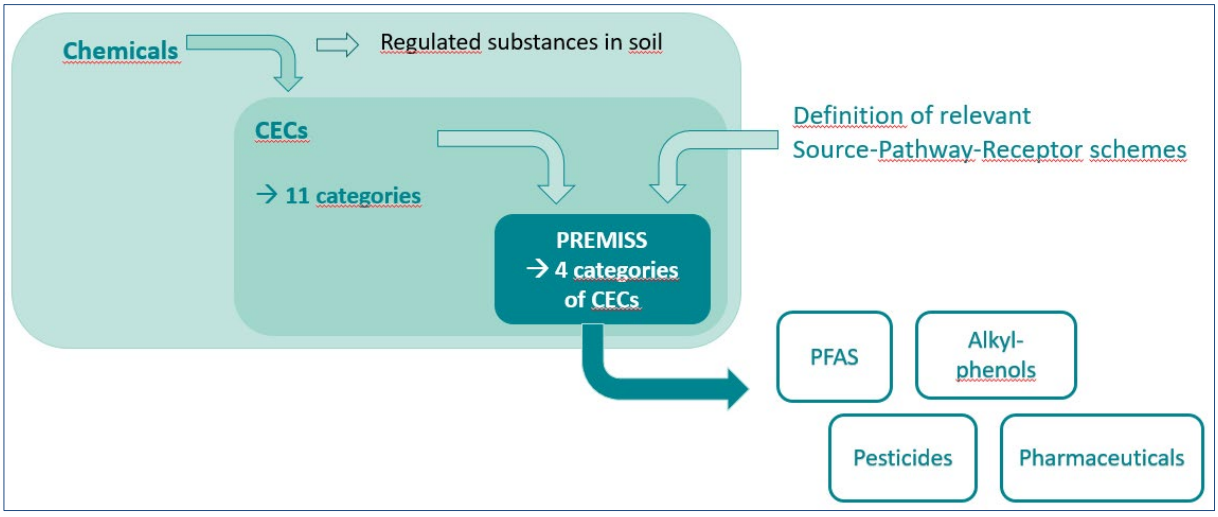


Figure 2 : Methodology used to make the PREMISS inventory of CECs occurrence data in soils and relevant matrices – Part I

3.2.3 Sources

Available concentration data in existing national/regional DB and reports for the four selected categories and corresponding 77 CECs were listed in selected environmental matrices for the 2010-2020 period. A short description of these DB and reports is given in Annex A.

3.3 Discussion on sources and collected occurrence data

A distinction was made between data reflecting background concentrations, referred to as "Global monitoring", and concentrations measured near risk activities or potentially contaminated sites referred to as "Point sources". Table 4 and Table 5 below summarize the DB and reports included in the inventory, respectively for global monitoring and point sources data.

20 DB and reports were found with global monitoring data and 12 with point sources data, for a total of 32 DB including CECs occurrence data. Data in soils are scarce. Only 6 of the 20 global monitoring sources are related to the soil matrix. On the contrary, most of the point sources DB and reports (9 out of 12) refer to the soil matrix.

3.3.1 Soil data

Twelve reports or DB include PFAS occurrence data in soils (global and point source combined). They are all from The Netherlands and Flanders. PFOA is the most analysed PFAS (in all DB and reports), followed by PFOS (analysed in 83% sources), then PFHpA and PFHxS (75%). PFBA, PFPeA, PFHxA, PFNA, PFDA, PFUnDA, PFDoA, PFTrDA, PFTeDA, PFBS and PFDS are analysed in 67% of listed DB and reports, 6:2 FTS, 8:2 FTS and GenX in 58% whereas N-MeFOSAA, N-EtFOSAA, 8:2diPAP and branched PFOA and PFOS are investigated only in 2 DB or reports (17%) in soils.

Flanders and The Netherlands have PFAS chemical industries and conducted monitoring campaigns or investigations around those facilities. Moreover, Dutch law recently introduced PFAS soil guideline values, and the Flemish Government validated PFAS soil guidelines values (in October 2019 and March 2021 respectively). This may explain the availability of PFAS occurrence data in soils. On the other hand, France and Wallonia have no data on PFAS in their DB for soil background nor point sources concentrations.

In France, the RMQS DB considers mainly pesticides and does not include PFAS. Soil analyses made in the frame of contaminated sites in Wallonia are not centralized in a DB. Besides, as they are related to environmental permits for risk industries, they are not public. Collecting these data and anonymising them would have required examining all environmental studies reports one by one. This task was too time-consuming to be completed in the frame of the PREMISS project.

Regarding other CECs categories, only 4 reports and DB include occurrence data in soils for phenols & alkylphenols and 4 for pesticides. No data for the selected pharmaceuticals were available in national reports and DB. Data may exist but they could not be identified for this project.

Several existing and upcoming policy initiatives under the European Green Deal (the Chemical Strategy, the new EU Soil Strategy for 2030, the Zero Pollution Action Plan) provide a European framework to protect land and soils from pollution. However, a more coherent EU policy framework on soil would further reinforce efforts towards sustainable soils management.

3.3.2 Groundwater

There are more occurrence data for CECs in groundwater: 11 national DB and reports were listed. 9 include PFAS occurrence data, 5 relate to phenols & alkylphenols, 6 include pesticides, and 5

pharmaceuticals occurrence data (global and point source combined). Regulations and monitoring activities are more advanced in the aquatic environment compared to soils, in relation *inter alia* with the European obligations of the WFD (2000/60/CE) and related directives (2013/39/UE, 2008/105/CE).

3.3.3 Sediment

In the implementation of the WFD, priority substances are also to be monitored in sediments, which explains the availability of some CECs occurrence data in this compartment (9 national DB or reports found). 5 national sources report occurrence data for PFAS, 5 for phenols and alkylphenols, 6 for pesticides, and 3 for pharmaceuticals.

3.3.4 Other matrices

Some organic fertilizers, such as sewage sludge, manure, and compost, can also introduce a broad mix of heavy metals and organic pollutants. Few national (or regional) studies on CECs characterisation in WWTP sludge were found: 5 national DB or reports were listed. Pharmaceuticals are the most characterized substances in sludge (100% of the 5 sources), followed by phenols and alkylphenols (4 sources out of 5), and then PFAS and pesticides (both 3 sources). No CECs occurrence data in compost, manure, or digestate have been identified in national DB or reports. Selected CECs are not regulated in organic fertilizers at the moment in Europe nor in participating countries.

Some scientific publications including measurements campaigns of CECs in participating countries (regions) were added to the inventory and are presented in Table 6.

The complete reference of the reports and scientific publications can be found in the Reference section (Chapter 9.1.1).

Table 4 : Inventoried national databases and reports and included substances categories – Global monitoring

Country/ Region	Database/Report	Monitoring type	Monitored media	PFAS	Phenols & alkylphenols	Pesticides	Pharmaceuticals Veterinary drugs	Total number of inventoried substances
BE-Vl	OVAM, 2021 - Deel 1 & Deel 2	Global	Soil	**29**	**4**	**3**	0	**36**
	VMM Sludge	Global	Sediment	0	0	**2**	0	**2**
BE-Wal	SPW Sediment DB	Global	Sediment	**1**	**4**	**4**	0	**9**
	CARIBOUH project	Global	Sludge	**5**	**10***	**1**	**6**	**22**
	BIODIEN report 2018	Global	GW	**5**	**7**	**8**	**1**	**22**
	IMHOTEP report 2017	Global	GW	0	0	0	**4**	**4**
	SPW ESO DB	Global	GW	0	0	**5**	0	**5**
FR	RMQS DB	Global	Soil	0	0	**4**	0	**4**
	INERIS, 2014	Global	Sludge	**2**	**4**	0	**5**	**11**
	NAÏADES DB	Global	Sediment	**5**	**12**	**7**	**2**	**26**
	ADES DB	Global	GW	**17**	**14**	**10**	**12**	**54**
NL	Achtergrondwaarden 2000	Global	Soil	0	**5**	**3**	0	**8**
	PFAS achtergrondwaarden DB	Global	Soil	**28**	0	0	0	**28**
	RIVM, 2020	Global	Soil	**29**	0	0	0	**29**
	Expertisecentrum PFAS, 2018c	Global	Soil	**20**	0	0	0	**20**
	Expertisecentrum PFAS, 2018d	Global	Soil	**2**	0	0	0	**2**
	FARO Advies 2020	Global	Sludge	0	**4**	**6**	**7**	**17**
	Dutch Water Authorities	Global	Sediment	**27**	**5**	0	0	**33**
	Waterbodem landelijke DB (CSO Adviesbureau 2010)	Global	Sediment	0	**5**	**3**	0	**8**
	KWR monitoring network	Global	GW	**1**	**2**	**2**	**3**	**8**
	Expertisecentrum PFAS, 2018c	Global	GW	**15**	0	0	0	**15**
EUR	JRC 2012	Global	Sludge	**17**	0	**1 (2)**	**3 (7)**	**21**

* Analytical problems with triclosan and 4-t-butylphenol; results to come later.

Table 5 : Inventoried national databases and reports and included substances categories – Point sources

Country/ Region	Database/Report	Monitoring type	Monitored media	PFAS	Phenols & alkylphenols	Pesticides	Pharmaceuticals Veterinary drugs	Total number of inventoried substances
BE-Vl	OVAM Mistral DB	Point source[3]	Soil	**4**	**5**	**4**	0	**14**
	OVAM Mistral DB	Point source[3]	Sediment	0	0	**2**	0	**2**
	OVAM Mistral DB	Point source[3]	GW	**4**	**5**	**4**	0	**14**
	Sullied Sediment DB	Point source	Sediment	**15**	0	**3**	**1**	**19**
	OVAM, 2018	Point source	Soil	**21**	0	0	0	**21**
	OVAM, 2018	Point source	Sediment	**21**	0	0	0	**21**
	OVAM, 2018	Point source	GW	**21**	0	0	0	**21**
	OVAM hotspot verkenner	Point source	Soil	0	**4**	0	0	**4**
FR	GIDAF DB	Point source	GW	**25**	**6**	**9**	**1**	**42**
	SUPREMA DB	Point source	Sediment	0	**2**	0	**1**	**3**
	SUPREMA DB	Point source	Sludge	0	**2**	0	**1**	**3**
NL	RIVM, 2020	Point source	Soil	**29**	0	0	0	**29**
	RIVM, 2018	Point source	Soil	**2**	0	0	0	**2**
	Expertisecentrum PFAS, 2017	Point source	Soil	**21**	0	0	0	**21**
	Expertisecentrum PFAS, 2018a	Point source	Soil	**21**	0	0	0	**21**
	Expertisecentrum PFAS, 2018a	Point source	GW	**21**	0	0	0	**21**
	Expertisecentrum PFAS, 2018b	Point source	Soil	**2**	0	0	0	**2**
	Expertisecentrum PFAS, 2018b	Point source	GW	**2**	0	0	0	**2**
	Expertisecentrum PFAS, 2018c	Point source	GW	**19**	0	0	0	**19**
	Expertisecentrum PFAS, 2018d	Point source	Soil	**2**	0	0	0	**2**

[3] OVAM mistral is a collection of global and point source monitoring results (mostly point contamination). However, we cannot distinguish between the two.

Table 6 : Inventoried scientific publications with CEC occurrence data in environmental matrices and included substances categories – Global and point sources

Country/ Region	Scientific publication	Monitoring type	Matrix	PFAS	Phenols & alkylphenols	Pesticides	Pharmaceuticals Veterinary drugs	Total number of inventoried substances
FR	Net et al., 2015*	Global	Sediment	0	0	**1**	**2**	**3**
FR	Mailler et al., 2018*	Global	Sludge	**2**	**1**	0	**4**	**7**
FR	Mailler et al., 2014*	Global	Sludge	**2**	**1**	0	**4**	**7**
BE-Vl	Groffen et al., 2019*	Point source	Soil	**15**	0	0	0	**15**
BE-Vl	Groffen et al., 2019*	Point source	Soil	**15**	0	0	0	**15**
FR	Mourier et al. 2019*	Point source	Sediment	**8**	0	0	0	**8**

3.3.5 Global inventory of selected substances categories in relevant matrices

For all the reports and DB including occurrence data for the 77 selected CECs[4] in soils, GW, sediments, and/or sludge, the number of samples and the quantification frequencies[5] were listed (see Annex A). This allowed a first overview of the available data for CECs in Belgium, France and The Netherlands.

However, the quantification limit (QL) for some CECs is sometimes very high. Therefore, the measured concentrations (absolute values) are more valuable information (see *Pilot CECs and data collection*).

A set of substances, referred to as "pilot CECs", is intended to serve as a showcase for a demonstration of the prioritisation tool at the end of the project (see chapter 5). Data availability was one of the considered criteria to propose these "Pilot CECs"

Measured concentrations collected through the inventory were compared to predicted concentrations in soils in the transfer module (WP4) in the section 6.2.

3.3.6 Limitations in data collection

Several difficulties were encountered when collecting available occurrence data for CECs. This led us to the conclusion that the collection of a complete set of data for 77 CECs was not realistic in the frame of PREMISS. The main difficulties encountered are described here:

- Referencing of chemical substances (name and/or acronym) across the reports and DB are not always consistent. CAS numbers are not always indicated in the reports. This resulted in additional work to check the correspondence between names and CAS numbers across different sources.
- Some occurrence data were measured at contaminated sites. In the inventory, we therefore made a distinction between "Global monitoring" reflecting background concentrations and "Point sources" concentrations measured near risk activities or potentially contaminated sites.
- Data in soils are scarce in national DB and reports, except for PFAS in Flanders and the Netherlands. CECs occurrence data from scientific literature articles were thus added to the inventory. These scientific publications are mentioned in a specific section in the References (9.1.1).
- The comparability of data was the major difficulty. Indeed, some of the DB/reports consider detection limit (DL) while others take into account quantification limit (QL). Furthermore, DL/QL values are not always stated. Subsequently, quantification frequencies cannot be calculated. Concentrations lower than DL/QL are not evenly managed across DB and reports. Some exclude concentrations lower than the QL in the statistical treatment, others consider the value of the QL itself, others consider half the value of the QL, while others set it equal to 0. In addition, the treatment of values lower than the QL is not always stated.
- Finally, some studies involved poorly sampled matrices (one or two sample(s)). Representativeness of those can therefore be questioned.
- Statistical treatment of individual data sets or harmonisation of different data sets is too time consuming and unrealistic in the scope of the PREMISS project. Therefore, quantification frequencies[6] were used in the first step. The complete set of available data was collected only for a subset of compounds, the "Pilot CECs" (Figure 3).

[4] 31 PFAS, 23 phenols/alkylphenols, 11 pesticides and 12 pharmaceuticals.

[5] The quantification frequency in a matrix is defined as the percentage of samples where the substance was quantified divided by the total number of measures in that matrix.

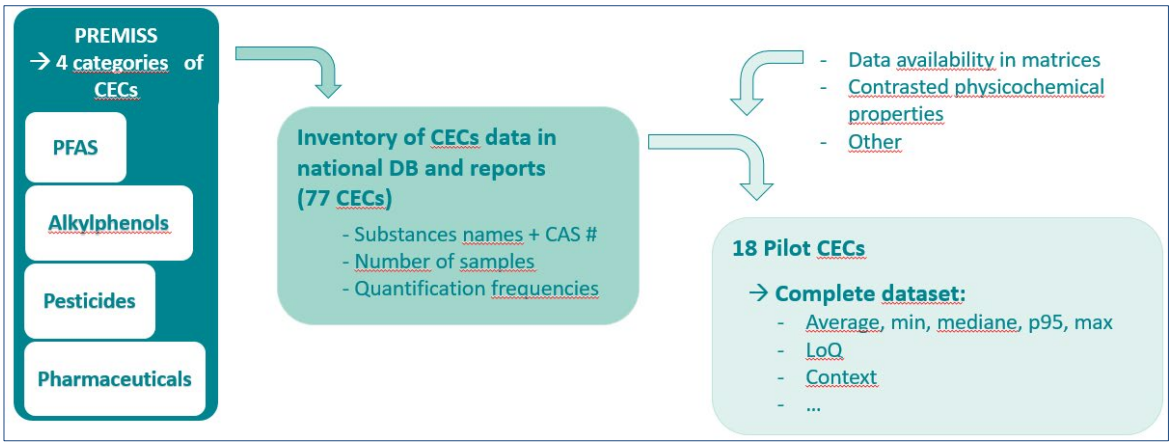


Figure 3 : Methodology used to make the PREMISS inventory of CECs occurrence data in soils and relevant matrices – Part II

3.3.7 Pilot CECs and data collection

A selection of 18 "Pilot CECs" was made (Table 7). A complete inventory of existing data was undertaken for these pilot CECs. This complete inventory includes the following information:

- environmental matrix (soils, WWTP sludge, sediment, groundwater)
- average concentration;
- minimum concentration;
- maximum concentration;
- median concentration;
- 95th percentile;
- quantification limit (QL);
- quantification frequency;
- number of samples;
- number of sites;
- data property (published data/report, public database, …);
- comments, when relevant (e.g. statistical treatment hypotheses);
- context, when relevant (e.g. WWTP sludge treatment, distance from fluorochemical production plan (FPP)).

The complete set of data for pilot CECs is presented in Annex B.

The rationales for the selection of these Pilot CECs followed several criteria:

- Data availability
- Spreading over the four selected chemical groups
- Contrasted physico-chemical properties (eg. different chain length PFAS, different persistence)
- Contrasted contexts (eg. banned versus still used CECs, parent molecule vs transformation product or precursor)
- Interest: widespread use, antibiotics, neonicotinoid.

Initially, 10 pilot CECs were to be selected. But it was extended to 18 pilot CECs to fulfil as much as possible the above mentioned criteria.

At least a few substances with data available in the four relevant environmental matrices (soils, GW,

sediments, and WWTP) were needed to investigate the transfer module in WP4. In addition to those, CECs with different physico-chemical properties were selected in order to develop, test and validate the transfer and risk modules developed in WP4 and 5. CECs with different characteristics were also chosen for developing the prioritisation tool in WP5, in order to picture different scenarios as well as respond to the stakeholders (SKH) interest expressed at the 1st SKH meeting held in January 2021.

Table 7 : Selected Pilot CECs for the complete inventory

Substance category	#	CAS	Substance name	Substance acronym
PFAS	1	335-67-1	perfluoro-n-octanoic acid	PFOA
	2	1763-23-1	perfluoro-1-octane sulfonic acid (PFOS)	PFOS
	3	307-24-4	perfluorohexanoic acid	PFHxA
	4	355-46-4	perfluoro-1-hexane sulfonic acid (PFHxS)	PFHxS
	5	13252-13-6	hexafluoropropyleneoxide dimer acid	GenX
	6	375-22-4	perfluoro-n-butanoic acid (PFBA)	PFBA
	7	2991-50-6 & 1336-61-4	N-ethylperfluorooctane sulfonamidoacetic acid	N-EtFOSAA
Phenols & Alkylphenols	8	84852-15-3	4-nonylphénol (branched) mixture	-
	9	80-05-7	bisphenol A	BPA
Pesticides	10	51218-45-2	metolachlore	-
	11	171118-09-5	metolachlore ESA	-
	12	152019-73-3	metolachlore OXA	-
	13	1071-83-6	glyphosate	-
	14	138261-41-3	imidacloprid	-
Pharmaceuticals	15	15307-86-5	diclofenac	-
	16	3380-34-5	triclosan	-
	17	81103-11-9	clarithromycin	-
	18	83905-01-5	azithromycin	-

3.4 Results: collected measured concentrations in the environment

In this section, collected occurrence data are presented and discussed for some pilots CECs. However, one should be cautious when comparing the data for the reasons explained in the "Limitations in data collection" section: QL are different, not always specified and treatment of values lower than the QL vary from one source (report or DB) to another. See section "Limitations in data collection" for more details.

For some CECs categories, discussion is focused on a specific environmental compartment, where enough occurrence data were found in national reports and DB. However, the complete set of collected occurrence data is presented in Appendix B.

3.4.1 PFAS

PFAS concentrations in soils were collected in Dutch and Flemish reports (Table 8). No occurrence data in soils are available in French or Walloon reports.

PFOA is the most studied PFAS, followed by PFOS. The highest maximum concentrations values in soils are observed for PFOS (36.100 µg/kg dw). GenX seem to be present in lower concentrations compared to other selected PFAS, with maximum reported concentration of 1 µg/kg dw in contaminated sites,

whereas it was not detected in reported soil background concentrations (global monitoring). GenX has been introduced to the market as a replacement of PFOA. Investigations on GenX therefore started later leading to fewer occurrence data on GenX. Lower observed concentrations in soils could be due to its higher mobility (BRGM, 2020). N-EtFOSAA is almost undetected in available occurrence data in national reports and DB. It was only detected at a frequency of 3% of the samples taken in the RIVM study from 2020.

Table 8 : Concentration range in µg/kg dry weight (number of samples analysed) of selected PFAS reported in soils in Belgium (Flanders) and The Netherlands. Where minimum and maximum concentrations were not available, average concentration is given.

PFOA	PFOS	PFHxA	PFHxS	PFBA	GenX	N-EtFOSAA	Source	Country
Global								
0,19-2,2 (50)	< QL - 2,1 (50)	0,2 - 0,39 (50)	< QL (50)	0,35 - 2,6 (50)	< QL (50)	< QL (50)	OVAM, 2021	BE-VL
0,62 (100)	0,42 (100)	-	-	0,14 (100)	< QL (37)	0,07 (100)	RIVM, 2020	NL
Point source								
0,97 (100)	0,7 (100)	-	-	0,23 (100)	0,08 (38)	0,08 (100)	RIVM, 2020	NL
0,3 - 7,7 (11)	-	-	-	-	0,1 - 1 (11)	-	RIVM, 2018	NL
<QL - 48 (40)	< QL - 36100 (61)	< QL - 160 (40)	< QL - 280 (40)	< QL - 12 (40)	-	-	OVAM, 2018	BE-VL
<QL - 112 (79)	0 - 89 (114)	-	< QL - 5,6 (55)	-	-	-	Mistral DB	BE-VL
Global + Point source								
0,1 - 380 (6279)	31 (6361)	0,9 (2625)	0,2 (2287)	2,3 (2792)	0,1 (139)	< QL (1724)	PFAS Back-ground DB	NL

PFAS concentrations in groundwater were available in the three partners' countries (Table 9). Indeed, PFOA and PFOS are regulated in the WFD (Directive 2013/39/EU). PFOA, again, is the most studied substance. The highest maximum concentration in groundwater is observed for PFOA (10.200 µg/l, ADES, FR). However, PFOA is actually detected only in 9% of samples, meaning this very high concentration is probably the exception and does not reflect a frequent situation. ADES contain some point source measurements, not clearly identified in the DB. The second highest maximum concentration is measured for PFOS (990 µg/l). No data on GenX nor N-EtFOSAA in groundwater was found in national reports and DB. In France, N-EtFOSAA was detected in three samples but not quantified (NQ).

Table 9: Concentration range in µg/l (number of samples analysed) of selected PFAS reported in groundwater in Belgium, France and The Netherlands. Where minimum and maximum concentrations were not available, average concentration is given.

PFOA	PFOS	PFHxA	PFHxS	PFBA	GenX	N-EtFOSAA	Source	Country
Global								
<QL - 0,34 (488)	-	-	-	-	-	-	KWR	NL
0,0005 (122)	0,0006 (122)	0,0007 (122)	0,0005 (122)	-	-	-	BIODIEN	BE-WAL
Point source								
<QL - 140 (48)	<QL - 990 (48)	<QL - 210 (48)	<QL - 480 (48)	<QL - 34 (48)	-	-	OVAM, 2018	BE-VL
1,7 (90)	<QL - 470 (104)	-	-	-	-	-	Mistral DB	BE-VL
<QL - 377 (47)	-	-	0,02 - 3,1 (22)	<QL - 0,6 (43)	-	NQ	GIDAF	FR
Global + Point source								

<QL - 10200 (15586)	<QL - 5,01 (9757)	<QL - 2,85 (15336)	<QL - 0,859 (14992)	<QL - 0,02 (3296)	-	-	ADES	FR

PFAS concentrations in sediment were also available in the three partners' countries (Table 10). Highest maximum concentration is observed for PFOA (94 µg/kg dw), which is much lower than the highest concentration measured in soils. The second highest maximum concentration is measured for PFHxA (59 µg/kg dw) which is also lower than the highest concentration of PFHxA in soils. PFHxS and PFBA were never detected in sediments. No data on GenX in sediment was collected in the inventory. N-EtFOSAA concentrations in sediment were reported only from the Dutch water authorities network, where it was detected in 35% of samples, with a median concentration of 0,28 µg/kg_{dw}.

*Table 10: Concentration range in µg/kg dw (number of samples analysed) of selected PFAS reported in sediments in Belgium, France and The Netherlands. *Where minimum and maximum concentrations were not available, median concentration is given.*

PFOA	PFOS	PFHxA	PFHxS	PFBA	GenX	N-EtFOSAA	Source	Country
Global								
0,09* (6500)	0,37* (6300)	< QL* (4800)	< QL* (4800)	< QL* (4800)	-	0,28 * (4800)	Dutch water	NL
<QL - 94 (4034)	-	< QL - 59 (3413)	-	-	-	-	Naïades	FR
-	<QL - 12 (176)	-	-	-	-	-	SPW ESO DB	BE-WAL
Point source								
<QL (1)	14 (1)	< QL (1)	< QL (1)	< QL (1)	-	-	OVAM, 2018	BE-VL
0,15 - 2,9 (18)	< QL - 4,6 (18)	< QL (18)	< QL (18)	< QL (18)	-	-	Sullied Sediment	BE-VL

PFAS occurrence data in sewage sludge are scarce (Table 11). Only one study and its screening phase (CARIBOUH), in Wallonia reported PFAS concentrations in sewage sludge. Highest maximum concentrations are observed for PFOS (up to 246 µg/kg dw). No data on PFBA, GenX nor N-EtFOSAA in WWTP sewage sludge was collected in the inventory. A JRC report from 2012 records PFOA occurrence data in European sewage sludge. Measured maximum concentrations in this study are higher than those measured in Wallonia.

Table 11: Concentration range in µg/kg dw (number of samples analysed) of selected PFAS reported in sewage sludge in Belgium and in Europe.

PFOA	PFOS	PFHxA	PFHxS	PFBA	GenX	N-EtFOSAA	Source	Country
Global								
0,27 - 5,95 (147)	0,22 - 13,9 (147)	0,23 - 4,97 (147)	< QL - 0,59 (147)	-	-	-	CARIBOUH	BE-WAL
3,3 - 11,5 (31)	1,16 - 246 (31)	0,17 -2 (31)	-	-	-	-	CARIBOUH (screening)	BE-WAL
1,2 - 47,5 (61)	-	-	-	-	-	-	JRC, 2012	EUR
0,2 -24,6 (58)	-	-	-	-	-	-	JRC, 2012	EUR

PFBA and PFOA were chosen to further discuss collected occurrence data on PFAS in soils. Table 12 and Figure 4 present PFOA minimum, maximum and median concentration values listed in the inventory for background monitoring as well as point sources data.

Collected data confirms PFOA is found ubiquitously [6,7,8] with quantification frequencies ranging from 56% to 89% even in "natural" or "undisturbed" places (global monitoring data).

QL are similar (ranging from 0.05 to 1 µg/kg dw). Median values are low (lower than 0.5 µg/kg dw), except in the RIVM 2018 study where the median concentration value reaches 3.7 µg/kg dw (point source). Maximum values can reach high concentrations, not only in contaminated locations, as in the PFAS background levels study in The Netherlands (380 µg/kg dw) but P95 concentrations do not exceed 10 µg/kg dw. PFOA P95 concentrations in uncontaminated soils are between 1.2 and 2.3 µg/kg dw.

Table 12 : Measured PFOA concentrations in soils (µg/kg) in Flanders (Belgium) and The Netherlands

Source	OVAM, 2021 (BE-VL)	OVAM, 2018 (BE-VL)	Mistral DB (BE-VL)	PFAS backgr. DB (NL)	RIVM, 2020 natural (NL)	RIVM, 2020 contam (NL)	RIVM, 2018 (NL)
Type of monitoring	**Global**	**Point source**	**Point source**	**Global**	**Global**	**Point source**	**Point source**
n	50	40	79	6279	100	100	11
QL	*0,2*	*1*	-	*0,1*	*0,1*	*0,1*	*0,05*
Min	0,19	< QL	< QL	0,1	-	-	0,3
Max	2,2	48	112	380	-	-	7,7
P95	1,15	< QL	9,07	2,3	1,81	3,21	-
Median	0,35	< QL	< QL	0,2	0,4	0,4	3,7
Quant. freq (%)	56 %	38 %	-	62 %	89 %	91 %	100 %

[6] Brusseau, M. L., Anderson, R. H., & Guo, B. (2020). PFAS concentrations in soils: Background levels versus contaminated sites. Science of the Total Environment, 740, 140017. https://doi.org/10.1016/j.scitotenv.2020.140017

[7] Bräunig, J., Baduel, C., Barnes, C. M., & Mueller, J. F. (2019). Leaching and bioavailability of selected perfluoroalkyl acids (PFAAs) from soil contaminated by firefighting activities. Science of the Total Environment, 646, 471–479. https://doi.org/10.1016/j.scitotenv.2018.07.231

[8] Wang, W., Rhodes, G., Ge, J., Yu, X., & Li, H. (2020). Uptake and accumulation of per- and polyfluoroalkyl substances in plants. Chemosphere, 261. https://doi.org/10.1016/j.chemosphere.2020.127584

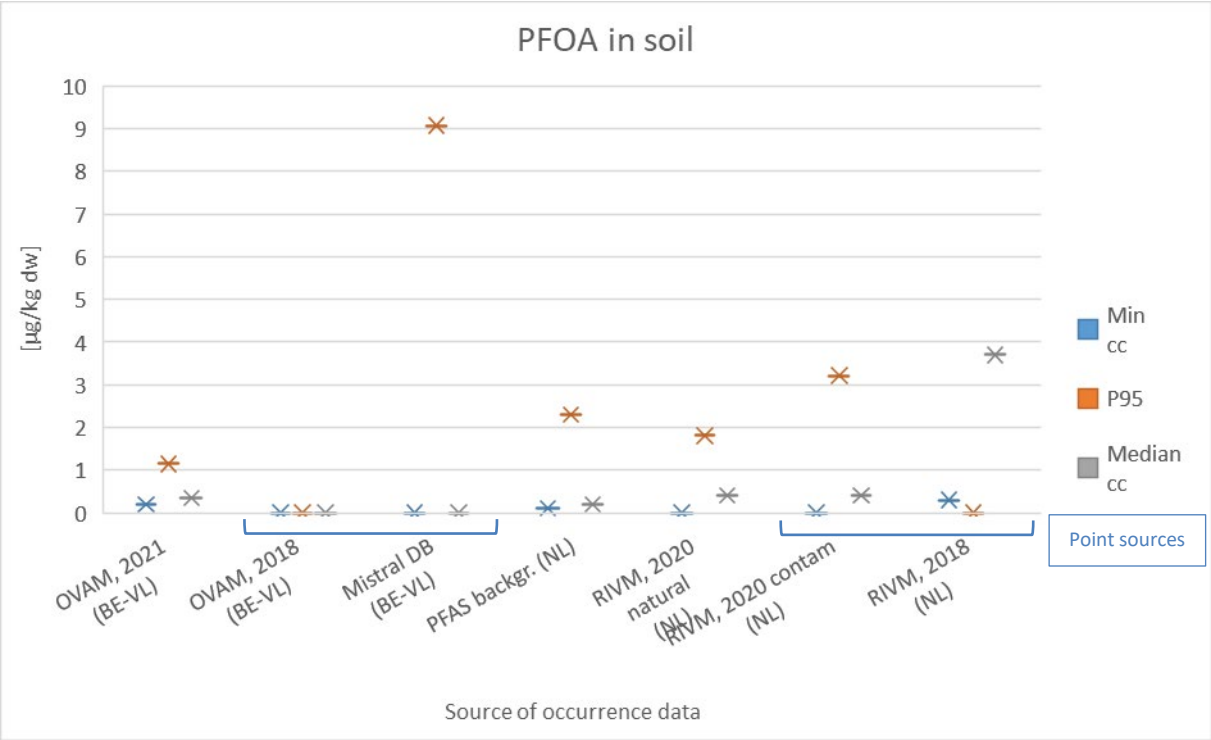


Figure 4 : Minimum, maximum and median concentration values (µg/kg) of PFOA in soils in Belgium (Flanders) and The Netherlands

PFBA minimum, maximum and median concentration values listed in PREMISS inventory for background monitoring and point sources data are presented in Table 13 and Figure 5. QL range from 0.1 to 1 µg/kg dw. Quantification frequencies are generally lower than PFOA, unless in the OVAM study from 2021 where it was detected in 100% samples. The lower quantification frequency in the OVAM study from 2018 is probably to be related to the higher QL. Median concentrations values are low (lower than 1 µg/kg dw), sometimes even lower than the QL. The highest observed maximum concentration is significantly lower than for PFOA (12 µg/kg dw compared to 48 µg/kg dw) but the highest P95 value is similar to PFOA (6 compared to 9 µg/kg dw). PFBA P95 concentrations in uncontaminated soils range between 0.3 and 1.5 µg/kg dw.

Table 13: Measured PFBA concentrations in soils (µg/kg) in Flanders (Belgium) and The Netherlands

Type of monitoring	**Global**	**Point source**	**Global**	**Global**	**Point source**
Source	**OVAM, 2021 (BE-VL)**	**OVAM, 2018 (BE-VL)**	**PFAS backgr. DB (NL)**	**RIVM, 2020 natural (NL)**	**RIVM, 2020 contam (NL)**
n	50	40	2792	100	100
QL	*0,2*	*1*	*0,1*	*0,1*	*0,1*
Min	0,35	< QL	-	-	-
Max	2,6	12	-	-	-
P95	1,5	6,52	0,4	0,3	0,9
Median	0,62	< QL	< QL	0,07	0,14
Quant. freq (%)	100%	33%*	17%	18%	25%

* The lower quantification frequency in this point source study is probably related to its higher QL.

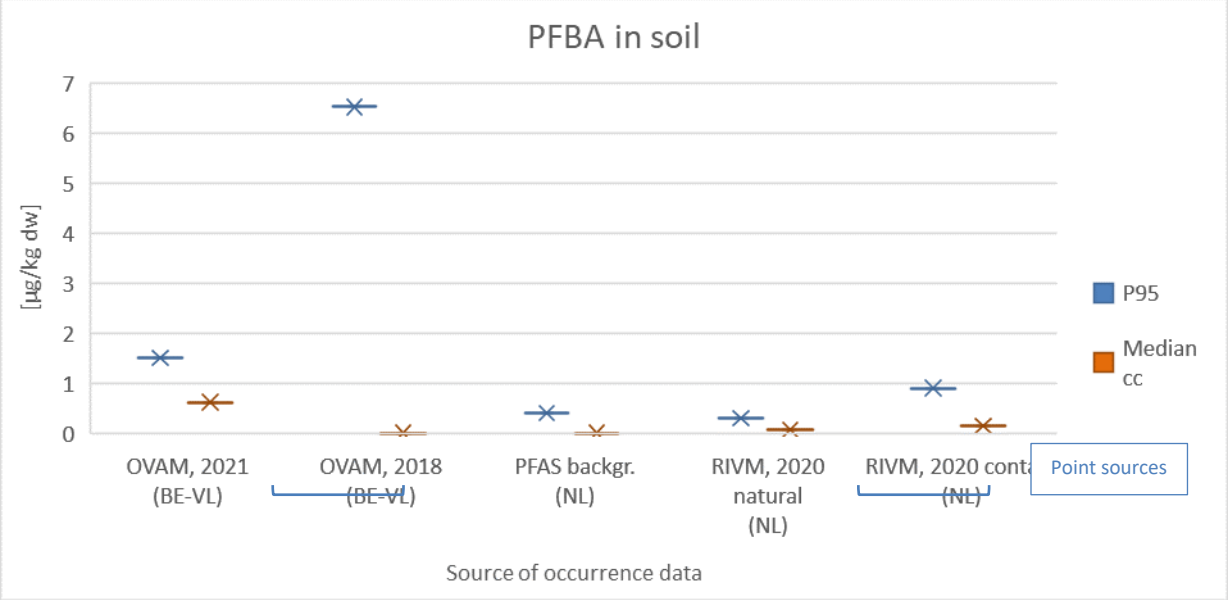


Figure 5 : Minimum, maximum and median PFBA concentration values (µg/kg) in soils in Belgium (Flanders) and The Netherlands

The complete set of data for PFOA and PFBA can be found in Annex B .

3.4.2 Phenols – 4-nonylphenol (branched, mixture) in sewage sludge

4-NP (branched mixture, #CAS 84852-15-3) is found in most sewage sludge samples listed in Belgium, France and The Netherlands with quantification frequencies between 57% (FR) and 98% (BE-WAL), as presented in Table 14. 4-NP is not quantified in the FARO study (NL) but the QL is high (810 µg/kg dry weight).

In the two Walloon campaigns, median concentration values in sewage sludge are similar, but maximum measured values are much higher (factor 3) in the final CARIBOUH study compared to the screening phase. Measured concentrations in the French campaign from INERIS seem higher (median and maximum values) but QL is also higher. These occurrence data are representative of the background concentrations (global monitoring). It is important to remark that the range of QL values varies considerably (from 15 to 810 µg/kg dry weight). It is not possible to compare concentrations found in The Netherlands because of the unique sample in the FARO study, which cannot be considered representative of a whole country.

Table 14: 4-NP (branched, mixture) concentrations in sewage sludge (µg/kg dry weight) listed in Wallonia, France and The Netherlands.

[µg/kg]	CARIBOUH (BE-WAL)	CARIBOUH screening (BE-WAL)	FARO Advies, 2020 (NL)	INERIS, 2014 (FR)
n	132	31	1	44
QL	*50*	*15*	*810*	*212*
Min	59	135	< QL	160
Max	20.790	6.268	< QL	31.000
Median	562	454	< QL	1.680
Quantification frequency	98%	97%	0%	57%

To make the graph (Figure 6), values lower than the QL value were set to the value of the QL itself. The log10 of the concentration values were calculated in order to be able to represent all measured values in the same graph.

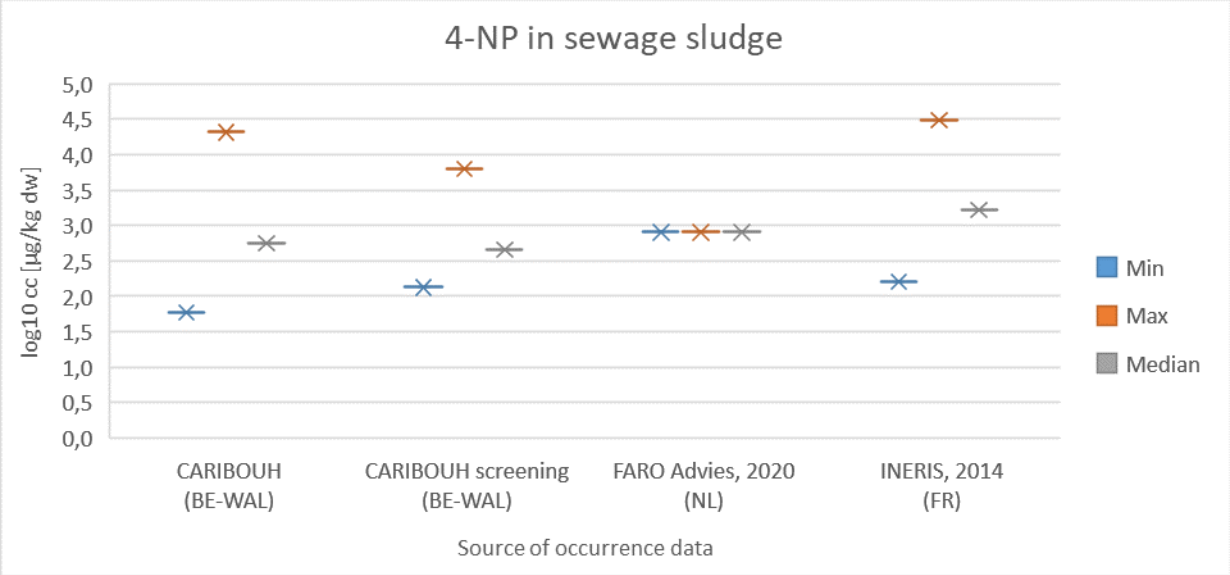


Figure 6 : Minimum, maximum and median concentration values (µg/kg) of 4-NP (branched, mixture) in sewage sludge in Belgium, France and The Netherlands

3.4.3 Pesticides - Glyphosate in groundwater

Glyphosate is the only pesticide amongst the pilot CECs with occurrence data in the three participating countries. Glyphosate is rarely found in groundwater, with quantification frequencies between 0.8% to 11% for background monitoring. The Table 15 below presents minimum, maximum and median concentration values listed in PREMISS inventory for background monitoring and point sources data (Table 15). To calculate these, values lower than the QL value were set to the value of the QL itself.

Table 15: Glyphosate concentrations listed in groundwater in France, Belgium and The Netherlands

	Global monitoring				Point source	
[µg/l]	**ADES (FR)**	**SPW ESO (BE-WAL)**	**BIODIEN (BE-WAL)**	**KWR (NL)**	**GIDAF (FR)**	**MISTRAL (BE-VL)**
n	77.499	64	122	876	31	27
QL	*0,01-2*	*0,05*	*0,05*	*0,01*	*0,01-2*	-
Min	< QL	< QL	< QL	< QL	< QL	0,05
Max	312	2,62	0,097	5,49	< QL	963
Median	0,058	< QL	< QL	< QL	< QL	20
Quantification frequency	1,8 %	11 %	0,8 %	3,9 %	0 %	-

The Figure 7 presents minimum, maximum and median concentration values listed in the project. The log10 of the concentration values were calculated in order to be able to represent all measured values in the same graph. Median values are generally close are equal to the QL value. Maximum values however very from one to three orders of magnitude. Respect to point sources, no glyphosate was detected in GIDAF analysis (31 samples) whereas higher median and maximum glyphosate concentrations are listed in Mistral DB.

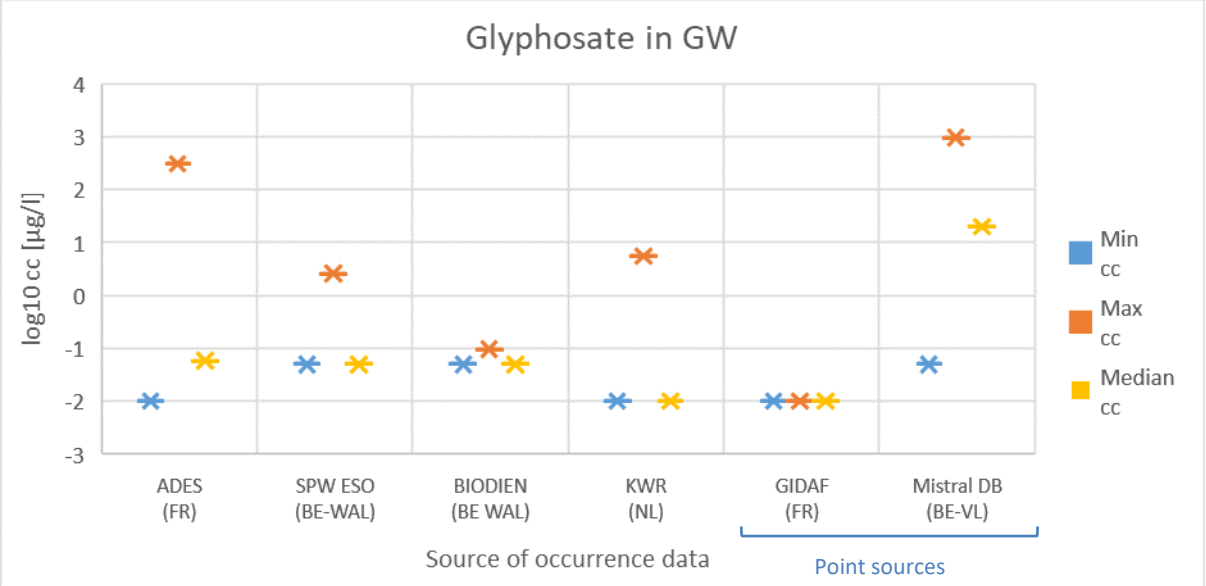


Figure 7 : Minimum, maximum and median concentration values of glyphosate in groundwater in Belgium, France and The Netherlands

3.4.4 Pharmaceuticals – Diclofenac in sewage sludge

Diclofenac occurrence data in sewage sludge are available from 3 different DB or reports for comparison (Table 16). Diclofenac is found most sewage sludge with quantification frequencies ranging from 71% to 100% in global monitoring data (assumed to represent background concentrations).

The Figure 8 presents minimum, maximum and median concentration values listed in the PREMISS project's inventory for background monitoring. Minimum concentration values range from 0 to 22 µg/kg dw whereas maximum concentration values range from 6.8 to 217 µg/kg dw. However median values are restricted to a short range of concentration values: 0.2-22 µg/kg dw. It is not reasonable to conclude about differences or similarities in diclofenac concentrations in sewage sludge based on these numbers because of the unique sample in the study in The Netherlands, which cannot be considered representative of a whole country.

Table 16: Diclofenac concentrations (µg/kg dry weight) in sewage sludge in Wallonia, The Netherlands and Europe

[µg/kg dw]	CARIBOUH (BE-WAL)	FARO advies, 2020 (NL)	JRC, 2012 (EU)
n	147	1	58
QL	*0,2-12,5*	*5*	-
Min	0,8	22	0
Max	217	22	6,8
Median	18,4	22	0,2
Quantification frequency	71 %	100 %	81 %

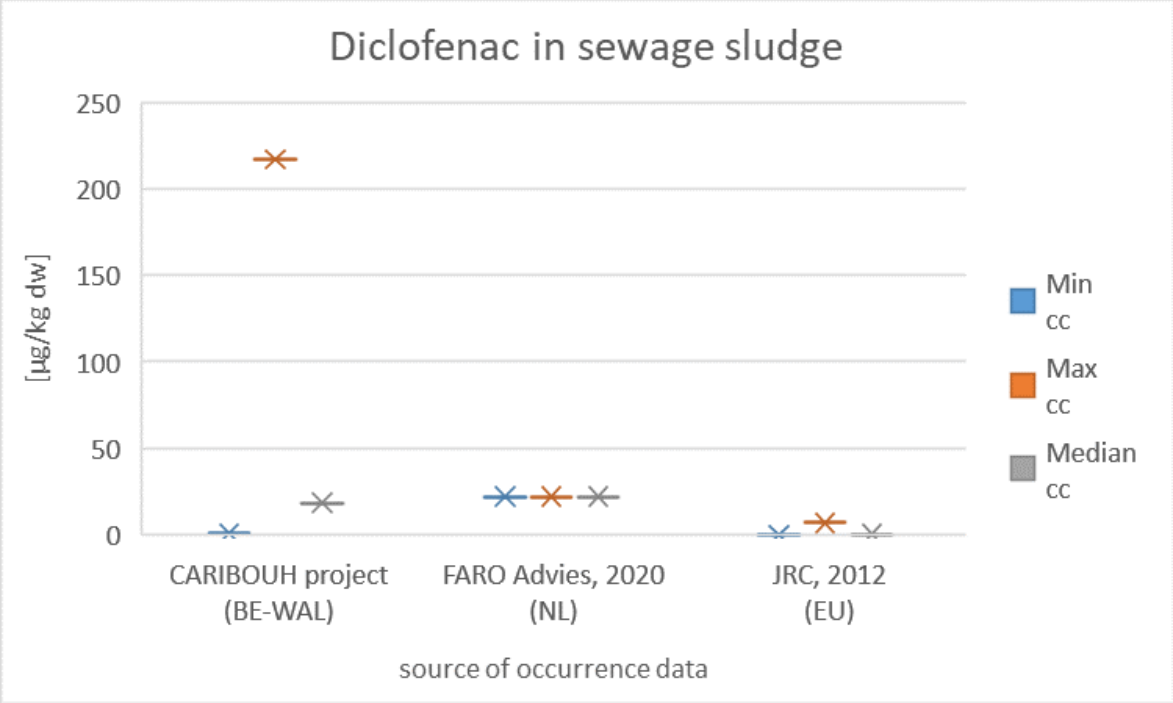


Figure 8 : Minimum, maximum and median concentration values (µg/kg dry weight) of diclofenac in WWTP sludge in Belgium, France and The Netherlands

3.5 Discussion and conclusion

Listing the number of samples and the quantification frequencies[9] in national (regional) DB and reports allowed a first overview of the available data for CECs. However, quantification limit (QL) for some CECs are sometimes very high. Therefore, measured concentrations (absolute values) provide more valuable information than quantification frequencies. The complete set of available measured data were collected for 18 Pilot CECs.

From this inventory, several observations can be taken up as recommendations at national levels and EU level.

Improvements need to be done on the one hand on **referencing** substances for international signalling. CAS numbers were not always referenced, and used acronyms were sometimes different (in relation with the language).

On the other hand, data treatment needs to be harmonised, in particular for the concentrations lower than the QL value. There is also a need of **harmonisation** of the associated **metadata**. Using the same references (CAS number), using the same units for a given environmental matrix, adding metadata (QL, context), etc. would make easier the (re-)use of existing data. Achieving **FAIR[10] data treatment** is indeed one of the EC goals for Europe.

Available data in soils for the selected CECs are scarce, except for PFAS near contaminated sites in Flanders and the Netherlands, who have PFAS production plants on their territory and recently introduced soil guidelines values for PFAS. In France and Wallonia, existing DB do not currently cover emerging contaminants selected in PREMISS. This tends to confirm the effectiveness of regulatory guidelines to protect the soil resources. Several existing and upcoming policy initiatives under the European Green Deal (the Chemical Strategy, the new Soil Strategy, the Zero Pollution Action Plan) provide a European framework to protect land and soil from pollution. However, a more **coherent EU policy framework on soil** would further reinforce efforts towards a sustainable soils management.

Furthermore, there is no **centralized storage of WWTP solid effluents data** nor for manure, compost or digestate data. In The Netherlands, the 'Watson DB' collects wastewater concentration data (emissieregistratie.nl).

Little attention has so far been given to soils in terms of CECs data collection and research. We recommend a **European DB** and national DB, **for soils**. LUCAS (Land Use/Cover Area frame statistical Survey) topsoil survey is the first attempt to build a consistent spatial DB of the soil cover across the EU based on standard sampling and analytical procedures, with the analysis of all soil samples being carried out in a single laboratory[11]. The 2009 survey focused on soil physico-chemical properties (particles size distribution, pH, organic content…). Approximately 20.000 points of the main LUCAS grid were sampled. The last LUCAS survey (2021-2022: still ongoing) will cover some CECs: 90 pesticides will be analysed, amongst which neonicotinoids, as well as antibiotics. In parallel and pending the latest LUCAS survey, Member states should centralise their soil data in **harmonised DB** in order to make the best use of it for future research and/or policies.

[9] The quantification frequency in a matrix is defined as the percentage of samples where the substance was quantified divided by the total number of measures in that matrix.

[10] In 2016, the 'FAIR Guiding Principles for scientific data management and stewardship' were published. They intend to provide guidelines to improve the **F**indability, **A**ccessibility, **I**nteroperability, and **R**euse of digital assets by both humans and machines.

[11] https://esdac.jrc.ec.europa.eu/projects/lucas, consulted on the 9th of November 2021.

4 Fate module, toxicological modules and prioritisation: Methodology

4.1 Prioritisation

4.1.1 Aim of the tool and tiered approach

This chapter describes the design of a robust and flexible prototype to prioritise CECs in soil and sub-surface, to which updates and improvements could be made in the future, such as substance and data addition.

The prioritisation tool has the following aims:

- Assessing which CECs are likely to be present in soils and subsoils,
- Evaluating which of these CECs may pose higher risks for human health and/or the environment.

4.1.2 Risk assessment and prioritisation

The prioritisation module uses practices from risk assessment (RA) to prioritise a large number of substances. In RA, the risk is determined by combining the substance concentration actually present in the environment (estimated or measured) with the effects of the substance on a receptor (human, ecosystem) at certain concentrations (F.A. Swartjes, 2011). In other words, the risk is a combination of the fate of the substance in the environment and the toxicity of the substance. This risk can be expressed as a Risk Characterisation Ratio (RCR), as the quotient of the fate and toxicity (see equation 1, and equations 2 and 3 in section 4.3.4.3). Risks for the chosen receptor are deemed to be present when the RCR exceeds 1. However, when a substance has a high RCR for one receptor, for example, human health, it does not automatically have a high RCR for another receptor. Each receptor must be assessed separately.

Equation 1. Calculation of the Risk Characterisation Ratio (RCR). For human health the PNEC is substituted by the Health Based Guidance Value (HBGV)

$$RCR = \frac{[Predicted\ environment\ concentration\ (PEC)]}{[Predicted\ no\ effect\ concentration\ (PNEC)]}$$

It follows that when comparing the RCR of multiple substances, the substance with the highest RCR poses the highest risk for the assessed receptor. This is in essence a prioritisation. When extending this principle to a large number of substances, for example, to all substances produced and imported in the EU under REACH, a more comprehensive prioritisation can be made. However, the quality of a prioritisation depends on the quality of the RCR. A lower quality RCR based on more uncertain data will result in a prioritisation with high uncertainty.

4.1.3 A tiered approach to prioritisation

The demands on data quality in RA are high as the results may lead to regulatory measures. Due to extensive quality evaluation, the RA process can be laborious and time-consuming, limiting the assessment to merely a handful of substances. Therefore, it is important to prioritise those substances for which elaborate RA is of added value. This can be done by splitting the prioritisation into three tiers. This implies that first a large number of substances can be assessed and that further analysis of

compounds can be performed for substances with higher priority. The following tiers are proposed.

- Tier 1: Basic prioritisation with generic emission, fate modelling, and toxicity data;
- Tier 2: Prioritisation with additional national or regional data on emissions, fate (PEC) and/or experimental toxicity;
- Tier 3: Risk assessment based on measurements in exposure media and/or appraised toxicity data.

For comparing substances, data uncertainty should be on a comparable level for all substances within a tier. Nonetheless, the increased uncertainty resulting from lower data quality must be addressed. Going from tier 1 to tier 3, the uncertainty of the data used in the calculations ranges from generic data (lowest detail) to measured data (highest detail). Figure 9 characterises the three tiers of the prioritisation approach. In the following sections, these tiers are described in more detail.

In PREMISS, we focus mainly on tier 1, for which a prototype was developed, and provide general suggestions for tier 2 and 3 for future development.

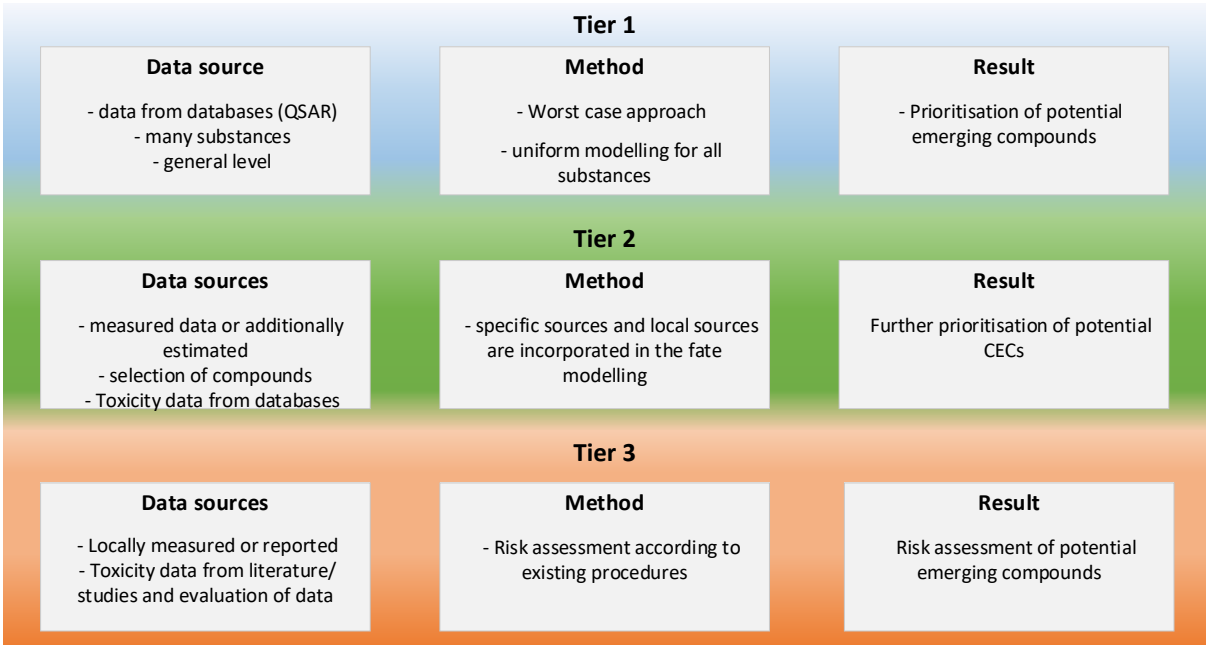


Figure 9 : Characteristics of the tiers in the Prioritisation prototype. The data source, method and results are described for each tier.

Moreover, for each tier the prioritisation approach is split into a Fate module in which the environmental concentration is calculated, and a Toxicity module in which a toxicological endpoint relevant to the receptor is derived. Detailed descriptions of these modules are provided in Section 4.2 (Fate) and section 4.3 (Toxicity). The following paragraph provides a concise overview of the first-tier prioritisation.

4.1.4 Tier 1 - Generic prioritisation

For tier 1 a prototype was built which prioritises a large number of substances based on publicly available data. The prototype calculates an environmental concentration (or exposure) in the Fate module, and a toxicity value relevant to the receptor (an effect concentration) in the Toxicity module.

Finally, the Fate and Toxicity are combined in order to predict an RCR.

The Fate module calculates the estimated environmental concentrations based on publicly available emission data and the environmental fate model SimpleBox 4.0[12]. The data sources are chosen so that emissions and substance properties can be gathered for a large number of substances. This module provides a list of concentrations in environmental compartments relevant to the RA of soil, i.e. concentrations in porewater and air. The toxicological module uses QSAR calculations to derive the threshold value (i.e. PNEC) for the receptor assessed in the prioritisation. Four relevant receptors are assessed in tier 1:

- human toxicity (drinking water);
- human toxicity (ingestion);
- direct ecotoxicity;
- secondary poisoning (indirect ecotoxicity).

Since the source-receptor pathways are receptor-specific, a distinct method was developed to derive a PNEC for each receptor (see section 4.2). The methods make use of existing assessment tools which allow for a large number of substances to be assessed.

After performing the fate and toxicity calculations, the prioritisation of the substances is carried out by calculating and sorting the Risk Characterisation Scores (RCR) for multiple substances from high to low. A prioritisation list can be generated for each of the four receptors. Figure 10 shows the Fate and Toxicity calculation steps and how these are used for prioritisation.

The main purpose of tier 1 is to prioritise substances based on information that is available for many substances, because it is collected in large databases or it can be calculated. The absolute value of the RCR is uncertain and not relevant at this tier. The uncertainty of using the RCR to prioritise will be discussed in paragraph 5.4.3.

[12] SimpleBox4.0, see rivm.nl/en/soil-and-water/simplebox

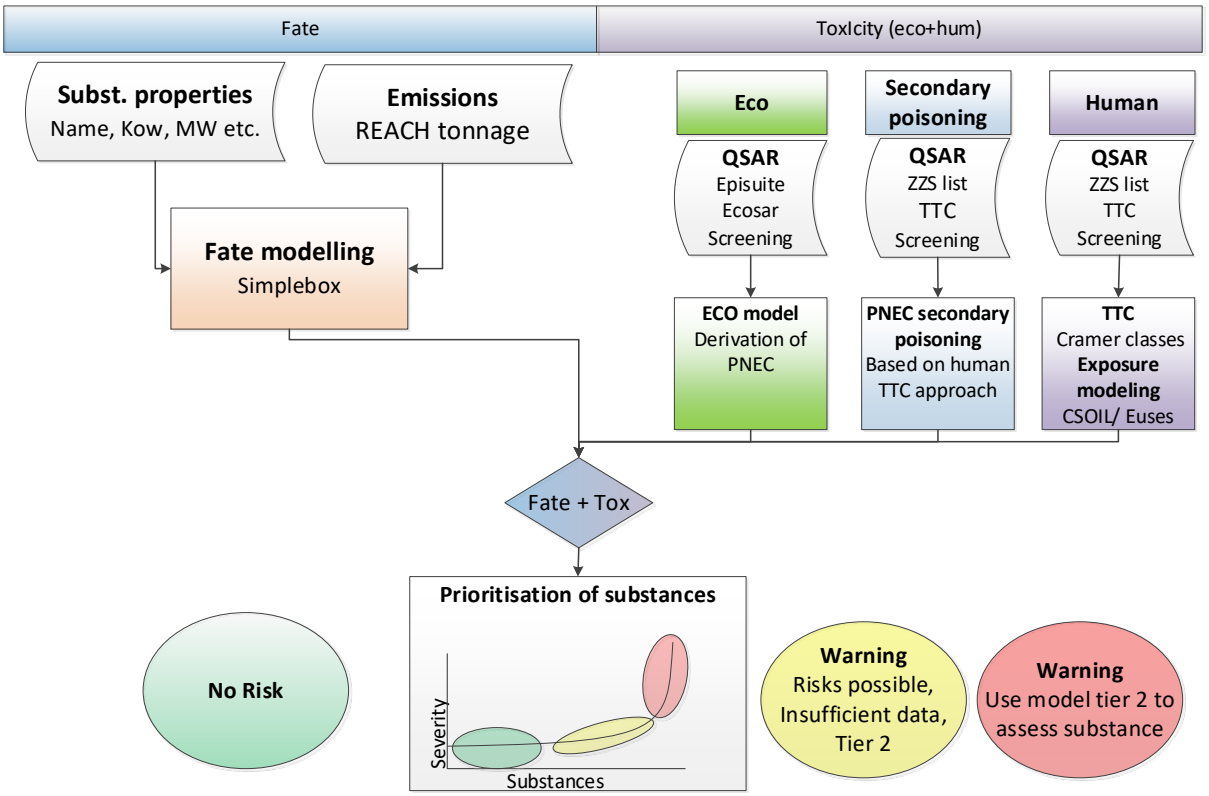


Figure 10 : Illustration of the Tier 1 Fate and Toxicity modules and the resulting prioritisation. The Fate module provides the environmental concentrations whereas the Toxicity module provides the receptor specific effect concentrations. In this figure, the human toxicity for drinking water and ingestion are combined.

4.1.5 Tier 2 and 3

Both tier 2 and tier 3 follow the same general structure as tier 1, where an environmental concentration and receptor-specific effect concentrations are determined and then combined into an RCR.

In tier 2 the fate modelling can be carried out with emission data for specific sources and customized fate modelling. In section 4.3 this is done for the application of pesticides and PFOS. For toxicity, PNEC values reported in literature can be used. When available, experimental toxicity data can also be used. Additionally, in section 4.3.4.2 a method based on chemical similarity is proposed as a less time-consuming alternative. **The prioritisation resulting from tier 2 can be used to decide on what specific compounds should be monitored in soil or groundwater.**

In tier 3, measurements in soil or groundwater are used as the source of environmental concentrations. For toxicity, extensively evaluated literature data can be used (when available). This will be done for a limited number of compounds. **With these data on fate and toxicity, the potential risk of a substance can be assessed**. It differs from tier 2 as a more extensive evaluation is performed on the data. However, data sources and procedures are to be further identified and developed in future research. Figure 11 shows an overview of the prioritisation approach including the tier 2 and tier 3 Fate and Toxicity assessments.

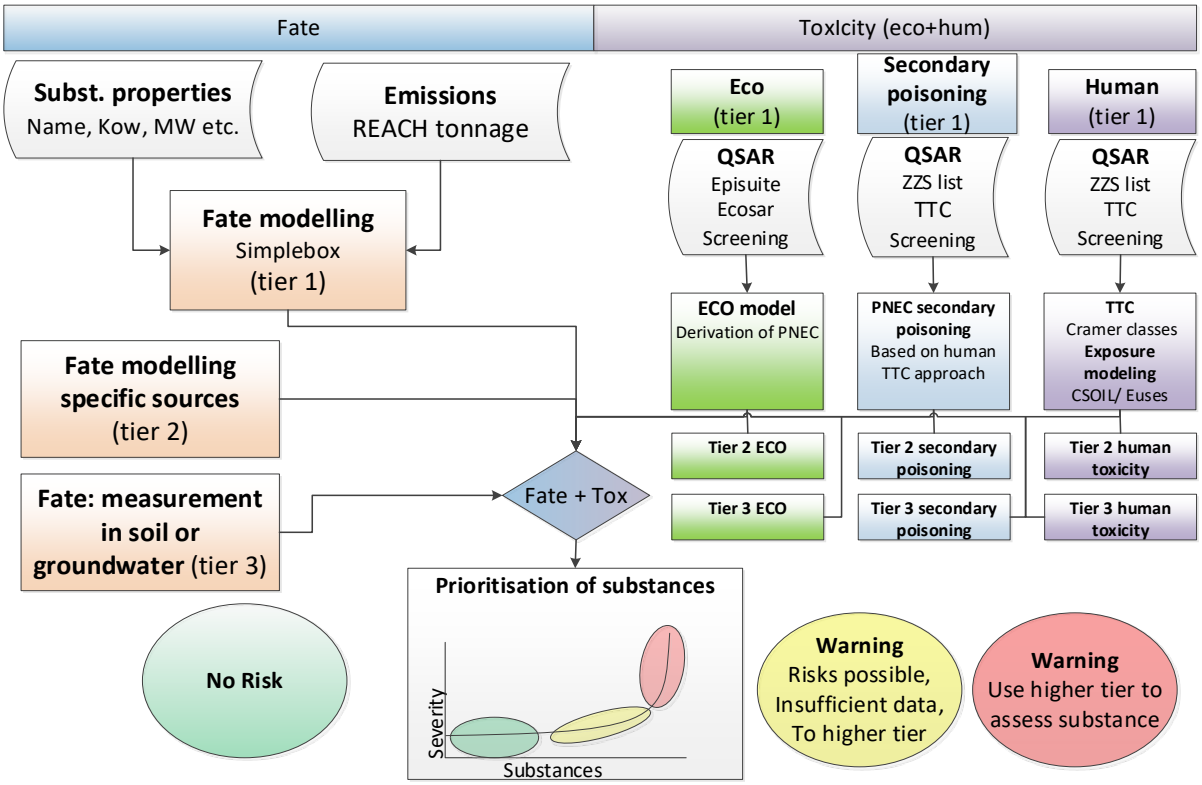


Figure 11 : Illustration of the prioritisation approach including second and third tier prioritisation steps. The overall approach of deriving an RCR remains similar throughout the different tiers.

4.2 Module on fate

In this chapter the module on fate is described in more detail. The chapter is split into three sections. Section 4.2.1 describes the tiered approach within the fate module. In section 4.2.2 the set-up of tier 1 is explained and in section 4.2.3 the set-up of tier 2 is described. Tier 3 was not performed within the scope of PREMISS.

4.2.1 Tiered approach

In PREMISS, the prioritisation of CECs was done using a tiered approach (see 4.1.3). In Tier 1 general data was collected and assumptions on emissions, expressed as use/production volume were made. Fixed emission pathways regarding the distribution over the compartments air, soil and water were determined. In reality, the emissions to the three different compartments are of course not fixed percentages. In Tier 2, we aim to quantify CECs specific source and input to soil. This replaces the direct load to soils used in Tier 1 (the generic percentage of the use/production volume).

4.2.2 Tier 1

The fate of selected soil CECs was determined using the SimpleBox 4.0[13] tool. SimpleBox is a steady state model which is run for one substance at a time. It requires chemical properties and emission data of the selected substance and landscape data for the chosen region, all of which will be explained in more detail in the following paragraphs.

SimpleBox 4.0 includes a regional and a continental scale, each containing nine compartments, and a global scale containing five compartments, see Figure 12. In this project three different regional scales were modelled after Belgium, France and The Netherlands. Therefore, fate estimation was done for these three countries separately.

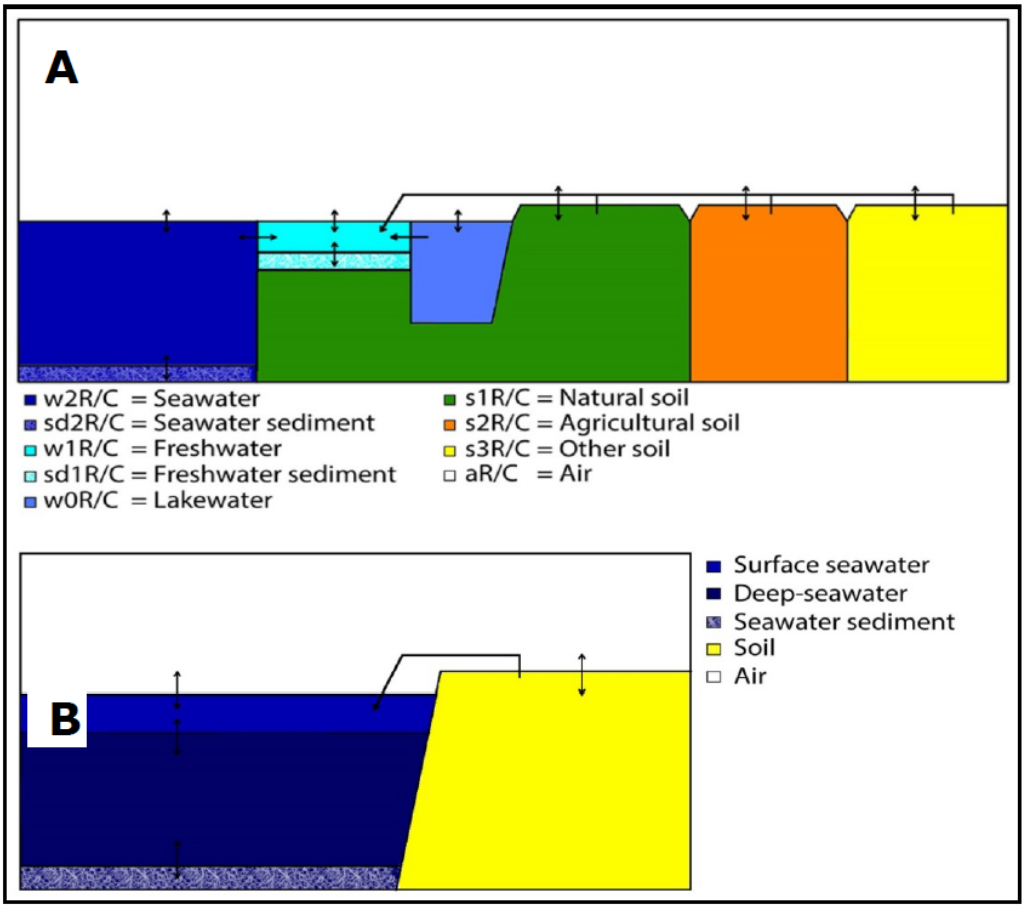


Figure 12 : Overview of the regional and continental scales (A) and global scale (B) (Hollander et al., 2007).

Environmental compartments are represented by boxes. The mass of a chemical in these boxes is the result of various mass flow processes to and from the boxes. Entry mechanisms of chemicals into a box are: (a) emission (EMIS), (b) import flows of air or water (IMP) from boxes outside the spatial scale to which the box belongs, and (c) intermedia transport (IMT) from another box inside the spatial scale. Loss mechanisms are: (d) degradation (DEG), (e) export (EXP) to outside the spatial scale, and (f) intermedia transport (IMT) to other boxes in the same spatial system. A mass balance equation can be written for each of the boxes. The mass balance equations have the following format (Equation 2):

[13] SimpleBox4.0, see rivm.nl/en/soil-and-water/simplebox

$$\frac{d\vec{m}_x(t)}{dt} = EMIS_x + IMP_{y\to x} \cdot m_y - EXP_{x\to y} \cdot m_x + IMT_{z\to x} \cdot m_z - IMT_{x\to z} \cdot m_x - DEG_x \cdot m_x$$

[Equation 2]

with

m_x: mass of the chemical in box x [mol]

t: time [s]

$EMIS_x$: emission rate of the chemical into box x [mol·s^{-1}]

$IMP_{y\to x}$: import rate of the chemical from box y into box x [s^{-1}]

$EXP_{x\to y}$: export rate of the chemical from box x into box y [s^{-1}]

$IMT_{z\to x}$: intermedia transfer rate of the chemical from box z into box x [s^{-1}]

$IMT_{x\to z}$: intermedia transfer rate of the chemical from box x into box z [s^{-1}]

DEG_x: loss rate of the chemical from box z [s^{-1}]

For more information on SimpleBox, please check RIVM Report 2015-0161[14].

4.2.2.1 Chemical properties

Chemical properties are required in order to estimate the fate of a specific compound in SimpleBox. The tool includes an integrated database with chemical substance properties. If a substance misses from the database, chemical properties can be added manually as well. In the Annex A the list of substances in the current SimpleBox database is presented.

In this project, CECs are targeted. In the SimpleBox database emerging compounds are often not yet included, therefore chemical property data was collected from the EPA dashboard[15]. In the first tier, fate calculation predicted averages were used as input for the SimpleBox model. If necessary certain parameter units were transformed into the required SimpleBox parameter input units. Chemical property data was collected for the following parameters, including the units of the parameter output in between brackets:

1. Octanol/water partition coefficient, $LogK_{OW}$
2. Vapour pressure (Pa)
3. Melting point (K)
4. Molecular weight (g/mol)
5. Solubility (mol/m^3)

As no predicted values for ready to use degradation rates are available on the EPA dashboard, default values were used for degradation in sediment, water and air. As soil is the compartment of interest in this project, the calculations should be based on a worst-case scenario for soil degradation, assuming there is no degradation at all, and a substance slowly accumulates. The default value for soil degradation was thus set to zero. Accumulation will become steady over time, a situation which is modelled in SimpleBox, as SimpleBox is a steady state model. If based on the worst-case calculations a substance is not identified as posing a risk, no further action is required. If, however, a substance is identified as posing a risk, then specific degradation rates should be acquired. This task is not included in PREMISS.

4.2.2.2 Emission and emission pathways

Substance emission data is required to determine the fate of a certain quantity of a substance, divided over the various environmental compartments. Emission data are split into emissions to soil, water and

[14] Schoorl et al., 2014. Available via rivm.nl/bibliotheek/rapporten/2015-0161

[15] See https://comptox.epa.gov/dashboard

air.

In this project, four different substance groups were assessed: pesticides, pharmaceuticals, alkylphenols and PFAS. For each substance group, emission data was collected using a slightly different approach.

4.2.2.2.1 Alkylphenols and PFAS

In this project, emission data of alkylphenols and PFAS was collected by consulting the REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) database. Most businesses located in Europe are required to register their chemical use and, based on these registrations, a Europe scale emission range in tons/year is determined and presented in the REACH database. To calculate the national emissions, we considered that 13% of total emissions are from France, 2.5% are from Belgium and 4% are from the Netherlands. These EU wide estimates of emissions were spatially distributed using an approach outlined by van Gils *et al.* (2020) based on, amongst others, gross domestic product and population. Calculations are based on assumptions made in the SOLUTIONS project[16]. If REACH data were not available, a default emission range was used to determine the fate of industrial chemicals. The default range was set to 0.1-1 tons/year. It should be noted that calculations based on a default emission range may be erroneous and total emission numbers may in reality be much higher or lower.

If a substance is no longer in use, REACH data and national data are no longer available. In this case, we propose to use the default emission range of 0.1-1 tons/year as input for emission data. However, estimating the emissions of a banned substance based on a default emission range may underestimate the total emissions, especially if the substance tends to accumulate in the environment overtime.

Once the national emission is derived, the release to the environment was estimated by assuming losses to air (8.5%), water (12%) and soil (3.0%), see Figure 13 . This distribution was determined for REACH chemicals by Van Gils *et al*. (2020). In this paper a lot of efforts had been put in the estimation of emissions, but the group of industrial chemicals includes a broad range of chemicals with various uses. A fixed percentage appeared to be the only option.

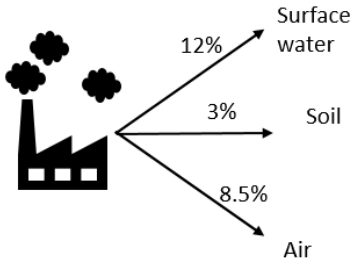


Figure 13 : Losses of chemicals to the environment for industrial (REACH) chemicals

This assumed distribution does not hold for pharmaceuticals and pesticides as these substances enter the environment differently (as specified below) than REACH chemicals.

4.2.2.2.2 Pharmaceuticals

In this project, the emission data of pharmaceuticals was collected by gathering national emission data. Pharmaceuticals generally enter the human body after ingestion, after which they are partly taken up by the human body and partly excreted. According to Lindim et al. (2016), who studied the release from over 50 pharmaceuticals in Sweden, the average excretion from the human body is 12%, all of which is assumed to be released to waste water treatment plants (WWTP). The release from WWTP is calculated

[16] https://www.solutions-project.eu/

with the removal efficiency, see Figure 14.

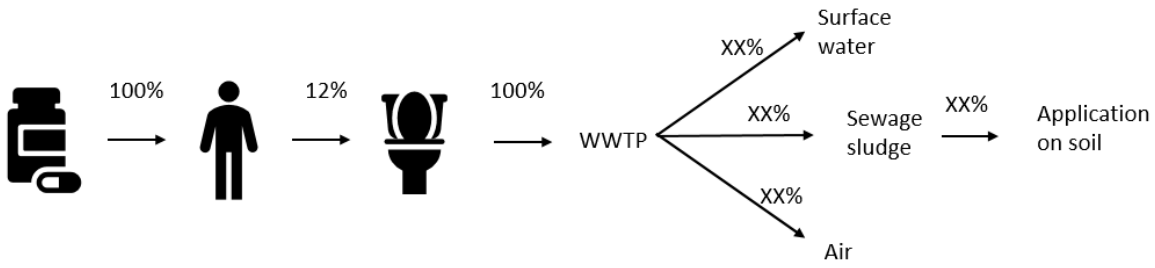


Figure 14 : Pathways of pharmaceuticals as a percentage of the total use or total sales.

The XX-values in Figure 14 vary for different substances or different countries. The pathways within the WWTP for each individual compound (to surface water, sewage sludge and air) were retrieved from the database from the SOLUTIONS project and originate from the SimpleTreat tool[17]. Removal efficiencies (the XX-values) for the selected substances in PREMISS are included in Annex E. The application of sewage sludge to soil is specified for each country.

4.2.2.2.3 Pesticides

In this project, emission data of pesticides was collected by gathering national emission data. Pesticides behave differently than industrial chemicals and pharmaceuticals as pesticides are directly applied on land. Van de Meent et al. (2020) estimated the overall release of pesticides to the environment in Europe to be 100%, of which 15% is emitted to air, 84% to soil and 1% to surface water, see Figure 15.

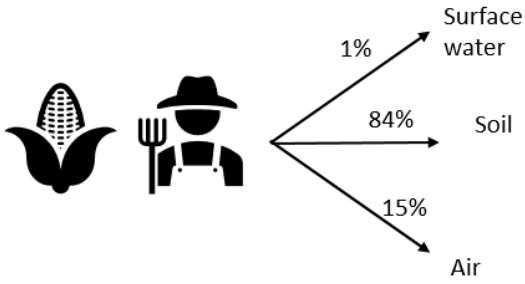


Figure 15 : Pathways of pesticides based on de the total use per surface unit.

4.2.2.3 Landscape settings

The so-called 'landscape' has two scales: regional and continental. Landscape data consists of the following:

- Area land
- Area sea
- Fraction lake water
- Fraction fresh water
- Fraction natural soil
- Fraction agricultural soil

[17] https://www.rivm.nl/en/soil-and-water/simpletreat

- Fraction urban/industrial soil

Emissions to surface water are assumed to be emissions to the fraction freshwater, as this fraction represents rivers and streams; emissions to these compartments are expected to be higher than emissions to lakes and ponds due to run-off and leaching. It is considered that rivers and streams are more subject to leaching because they have more contact with surfaces from which leaching can happen.

4.2.3 Tier 2

Soil may be contaminated by the application of (permitted) materials on the soil. We distinguished direct sources (pesticides application) and indirect sources (manure, organic fertilizer / compost, digestate, sewage sludge, and dredged material application) in rural areas[18]. The latter refers to applying materials for soil fertility improvement, which may contain small amounts of contaminants.

Tier 2 is not fully elaborated, but the principle is explained, and some examples are included in the results (section 5.1.2).

4.2.3.1 Direct sources

National information is available in all countries regarding the use or sales of pesticides. Because most pesticides are limited to a number of crops, the treated surface can be estimated. The contaminant load is then:

Direct Load = use (or sales) x surface x fraction to soil [Equation 3]

In which:
Load: the contaminant load (active ingredient) on the soil (mg/m²)
Use/sales: Mass that is used/sold (kg/year)
Surface: Area treated with the specific pesticide based on land use (m²)
Fraction to soil: fraction of the chemical being discharged to the soil (the rest goes to air and water).

4.2.3.2 Indirect sources

For indirect sources the approach is slightly different. The general approach is represented by equation 4:

Indirect Load = Activity level x Emission factor [Equation 4]

In which:
Load: the contaminant load on the soil (mg/m²/year)
Activity level: Mass of the additive applied to the soil (kg/m²/year)
Emission factor: Contaminant concentration in the additive (mg/kg)

We collected the available information on sewage sludge, manure, organic fertiliser/compost, digestate, and dredged material for each country/region represented in PREMISS consortium (BE-Fl, BE-Wal, FR and NL).

[18] Urban areas are not included/studied in PREMISS, but you might think of deposition of road material, traffic outlet, public waste, biocides, etc.

4.3 Modules on toxicity

4.3.1 General

The first tier prioritisation is based on (theoretical) models predicting physicochemical properties, hazards, and exposure. These models are more specifically introduced in the respective sections, but some general characteristics will be discussed here. The models require a chemical structure representation in order to estimate the required substance properties for the first tier prioritisation (see Figure 10). The (software) models used in the PREMISS tier 1 prioritisation are all limited to predictions for organic chemical substances. **Metals, metal-containing substances, proteins, nanomaterials, or radioactive materials are outside the scope of these models**, and can therefore not be prioritised in the PREMISS project. When encountered, these substances receive a flag suggesting to include them into a tier 2 prioritisation. Further (model-specific) limitations will be mentioned in the respective sections.

This chapter is split into five sections. Section 4.3.2 describes the chemical structure input for the various toxicity modules, and section 4.3.3 describes the use of the ZZS (Zeer Zorgwekkende Stoffen, Substances of Very High Concern, SVHC) similarity tool to assign hazard labels to substances. In the following sections, the modules for human toxicity (section 4.3.4), ecological toxicity (section 4.3.5), and secondary poisoning (section 4.3.6) are described.

4.3.2 Chemical Structure representation as input for Tier 1

A chemical structure in the form of a representative Simplified Molecular Input Line Entry Specification (SMILES), (DAYLIGHT, 2019) is used as input for all models in tier 1. SMILES is a specification in the form of a line notation for describing the structure of chemical species. SMILES were used instead of chemical names or CAS numbers, as they are more consistently interpreted by the various models[19].

Although SMILES provide a more consistent input for models, often multiple SMILES exist for a single substance. For example, separate SMILES are generated for a substance in its neutral form and its ionic form, or for substances with the same chemical structure but with different counterions. The US-EPA QSAR-ready chemical structure standardisation workflow provides a systematic approach to creating a normalized list of SMILES for a large number of substances (KNIME, 2020). A list of 750.000 SMILES – CAS number combinations generated using this workflow is available for download from the US-EPA website.

Although the QSAR-ready workflow provides a structured method, the resulting SMILES may not always be best suited for the models used to assess the toxicity for the various receptors. Fortunately, for the majority of SMILES generated in this way, this is not the case. Nonetheless, when required, SMILES can also be found on the PubChem online webservice (NIH, 2021). A procedure to arrive at SMILES using the PubChem online webservice is described in Annex F.

[19] For Ecotoxicity a combination of SMILES and CAS numbers is used.

4.3.3 Hazard labels and the ZZS similarity tool

Whether a substance may be a (potential) Substance of Very High Concern (SVHC) can be relevant information to take into account during prioritisation. In the tier 1 prioritisation approach, indications that a substance might be an SVHC are generated as an additional flag for each substance. These 'flags' do not influence the position of a substance in the prioritisation, but function as an extra point of information.

Under the European chemicals regulation REACH, the status SVHC is used for substances that are considered to have such a hazard that any (consumer) exposure is considered unwanted. SVHC are CMR substances (i.e. cat.1a or 1b Carcinogens or Mutagens or cat. 1a, cat. 1b, or cat. 2 Reprotoxic), PBT/vPvB substances (i.e. Persistent Bioaccumulating and Toxic or very Persistent and very Bioaccumulating), and substances of equivalent concern (e.g., endocrine disruptors). Since the current project focuses on CECs, an alert for potential SVHC properties is considered as an additional reason for prioritisation.

In order to generate a flag for (potential) SVHC substances, the ZZS-similarity tool was used (Wassenaar et al., 2019, Wassenaar et al., 2021). The ZZS substance list is a Dutch list of substances comparable to the SVHC-list used internationally. The ZZS similarity tool compares the chemical structure of a substance to a database containing chemical structures of known substances of high concern and provides information on why the substance was added to the ZZS list. Based on this information the labels for the prioritisation can be assigned. A workflow for the use of the ZZS similarity tool is described in Annex H. The list of possible labels that can be assigned through the ZZS similarity tool is given below:

- Persistent, Bioaccumulative, Toxic (PBT)
- Very persistent, very Bioaccumulative (vPvB)
- Carcinogenic, Mutagenic, Reprotoxic (CMR)
- Endocrine Disruptive (ED)

4.3.4 Human toxicity and exposure module

The section describes the calculation of the Risk Coefficient Ratio for human health (RCR_{human}) for human toxicity prioritisations (see also section 4.1.4). Assessment of human toxicity of substance requires information about both the toxicity of the substance inside the human body, as well as the concentrations to which humans are exposed (see equation 1). In the assessment of human toxicity, the effect concentration in the human body is called a health-based guidance value (HBGV)[20]. This HBGV however relates to a concentration inside the human body (an internal concentration), and not a concentration in soil. A substance in the soil can take various pathways, like for example the consumption of vegetables, to reach the human body. In order to calculate an RCR for humans, an internal exposure must first be calculated from the concentrations in the environmental media from the Fate module (soil, air, water) (see section Fate). Section 4.3.4.1 describes human exposure and section 4.3.4.2 describes the determination of a human HBGV.

[20] A Health-Based Guidance Value (HBGV) is a scientific-based recommendation for the maximum exposure to a substance that is not expected to result in an appreciable health risk.

4.3.4.1 Human exposure

4.3.4.1.1 Introduction.

Human exposure models use exposure pathways to calculate the (indirect) human exposure to contaminants in soil. Many of the available exposure models (like S-RISK, EUSES, and CSOIL) have a fate part and an exposure part. For the PREMISS prioritisation tool the exposure part uses the calculated concentrations of the fate of the contaminants, as modeled with SimpleBox in WP4. The exposure pathways combined with the environmental concentration in various compartments result in a human exposure expressed in an intake (µg/kg body weight per day). This daily intake is then compared to a human HBGV (see section 4.3.4.2) to derive an RCR to be used for prioritisation.

4.3.4.1.2 Choice of model and exposure pathways

Several exposure models were developed by institutes in EU member states, as well as by European institutions, like the European Chemicals Agency (ECHA). For example, the European Union System for the Evaluation of Substances (EUSES), developed by ECHA and RIVM, has a broad aim to assess the risks of chemicals in the environment as a whole (Lijzen and Rikken, 2004). Furthermore, in Belgium, the model 'S-RISK' was developed by VITO as a web application for assessing risks at contaminated sites (Cornelis et al., 2019). In the Netherlands, the model CSOIL was developed by RIVM for a similar purpose (Van Breemen et al., 2020). Both Dutch and Belgian models aim at assessing risks associated with contaminated soil and make use of a Mackay-type fate modelling (Parnis and Mackay, 2020) before deriving human exposure through various exposure routes.

Due to its wide scope, and use throughout Europe, as well as the integration with Simplebox, the EUSES model has been selected as a starting point for human exposure in the PREMISS prioritisation. In future research, usability of model concepts from S-RISK and CSOIL can be explored. For the purpose of PREMISS, only the pathways for direct consumption of groundwater (EUSES), and vegetable consumption (EUSES) combined with soil ingestion (CSOIL, not included in EUSES) will be taken into account (see section 3.4.1.3). The consumption of filtered or treated drinking water is not included, as the direct consumption of groundwater generally leads to higher exposure and therefore can be considered as a worst-case assumption for the exposure to contaminants in drinking water. The treatment of groundwater to drinking water may also vary between countries (and even locations within countries). Therefore, only the direct consumption of groundwater is included in the prototype as a proxy of drinking water (worst case). It is, however, possible to include a treated drinking water pathway in the prioritisation during future research. Additional pathways could also be added in future research.

The groundwater pathway is assessed according to the WHO method, which assumes that 20% of the total intake is attributed to exposure through consumption of drinking water (WHO, 2011, Van der Aa et al., 2017). Therefore, for the groundwater pathway, the calculated exposure will be compared to 20% of the HBGV. An overview of exposure pathways used in the EUSES, S-RISK, and CSOIL models, as well as the pathways used in PREMISS is given in Table 18.

Several exposure pathways used in the PREMISS prioritisation tool are used in EUSES as well as S-RISK and CSOIL. The parameterisation of these exposure pathways may however differ as each model is developed with a specific purpose in mind. The parameterisation of the PREMISS prioritisation tool will mostly adhere to the values used in EUSES when combining exposure pathways into one intake. By having the parameterisation adhere mostly to EUSES, the relative contribution of the separate exposure pathways to the aggregated intake remains similar (i.e. weighting of the pathways). In case the exposure pathways are not present in EUSES the default parameterisation of the source model is applied (e.g. CSOIL parameters for soil ingestion). The exposure parameters used in the PREMISS model are shown in Table 19.

Table 17 : Overview of exposure pathways in the exposure models EUSES, S-RISK, and CSOIL. Highlighted in orange are the exposure pathways used in PREMISS Tier 1.

Aggregated pathway	Exposure pathway	EUSES	S-RISK	CSOIL
Oral	Soil ingestion	No	Yes	Yes
Oral	Consumption of vegetables	Yes (not local)	Yes (local, including background)	Yes (local, no background)
Oral	Consumption of food products	Vegetables, meat, dairy, fish	Vegetables, meat, milk, eggs	Vegetables (homegrown)
Oral	Drinking water	Yes	Yes	Yes
Oral	Direct consumption of groundwater (worst case)	Yes	Yes	Yes
Dermal	Absorption via particles	No	Yes	Yes
Dermal	Absorption during showering/bathing	No	Yes	Yes
Inhalation	Inhalation during showering	No	Yes	Yes
Inhalation	Inhalation indoor air	No	Volatilisation from soil	Volatilisation from soil
Inhalation	Inhalation outdoor air	From fate concentration air	Volatilisation from soil	Volatilisation from soil
Inhalation	Inhalation of particles	No	Yes	Yes

4.3.4.1.3 Exposure pathways selected for the PREMISS project

This paragraph provides the pathways used for the tier 1 prioritisation in the PREMISS prototype and the models they are based on. The pathways are listed below.

- Soil Ingestion (CSOIL 2020)
  This pathway relates to the purposeful or accidental ingestion of soil. (For example, by transfer from hand to mouth.)
- Consumption of crops (EUSES)
  This pathway relates to the exposure through ingestion of vegetables (root and leafy) grown in the country (store-bought as well as home grown).
- Direct consumption of groundwater (EUSES)
  This pathway relates to the consumption of untreated groundwater. (For example, a groundwater well at a camp site.)

The exposure pathways for soil ingestion and consumption of crops are combined into one aggregated exposure pathway. The direct consumption of groundwater is treated as a separate exposure pathway. This separation leads to two prioritisations of emerging contaminants relevant to human toxicity, based on $RCR_{Human\text{-}SoilCrops}$ and $RCR_{Human\text{-}Groundwater}$. The calculation of the two RCR for human toxicity is explained in paragraph 4.3.4.3. Annex F provides the formulas used to calculate human exposure through the various exposure pathways.

Table 18 : Overview of exposure parameters used in the PREMISS model, including the source model for the parameters.

Parameter	Abbreviation	Value	Unit	Source
Daily intake of leafy crops	Qleaf	1.2	$kg.d^{-1}$	EUSES
Daily intake of root crops	Qroot	0.384	$kg.d^{-1}$	EUSES
Daily intake of drinking water	QDW	2	$L.d^{-1}$	EUSES
Soil ingestion daily intake	AID_A	5 E-4	$kg_{dw}.d^{-1}$	CSOIL
Bodyweight	BW	70	kg	EUSES

4.3.4.2 Human Health Toxicity - Point of Departure

4.3.4.2.1 Introduction

The prioritisation based on human health risk requires – apart from a human exposure estimate (see 4.3.4.1) – a HBGV to which the exposure can be compared. These safe levels are normally derived from (chronic or sub-chronic) in-vivo repeated dose toxicity tests, giving a NOAEL (No Observed Adverse Effect Level) which can be used as a Point of Departure (PoD). This kind of toxicological information will not be available for a large number of substances. Therefore, in the first tier of the prioritisation, an estimate of a safe level of human exposure is generated based on chemical structure considerations only.

4.3.4.2.2 Tiered approach

A tiered approach was developed in which the first step is to estimate HBGVs for a large number of substances in a similar, structured and preferably automated way. In later steps a more case-by-case approach can be adopted to assess the remaining substances.

Tier 1 makes use of a human HBGV as PoD. The best option to derive a HBGV in an automated way is to use a theoretical model to predict the substance toxicity. Several models are available, however, most theoretical models for estimation of toxicity are not capable of quantitatively estimating the toxicity of a substance. Rather, these models provide an indication of the possibility a substance may cause a certain effect. This is more alike the Hazard labels described in section 4.3.3. One of the few generically applicable methods to estimate a 'safe daily intake' for chemicals is the Threshold of Toxicological Concern (TTC) approach (EFSA and WHO, 2016). A TTC is based on an estimation of the NOAEL divided by an assessment factor of 100. The ratio of the TTC (as a HBGV) to the (estimated) exposure provides a RCR_{human} (comparable to a PEC/PNEC ratio in ecotoxicology) that can be used for prioritisation purposes. Figure 16 provides a schematic depiction of the use of the TTC to derive a HBGV. The screening for ZZS depicted in this figure is described in section 4.3.3 and is only run once for all toxicity modules.

For tier 2 a possible refinement in the PREMISS prioritisation is to look up the HBGV of the SVHC or of the closest similar SVHC structure identified. The ZZS similarity tool described in section 4.3.3 could be modified and used for this step. However, future research is required for this. Development and identification of tier 3 HBGV should be performed in future research.

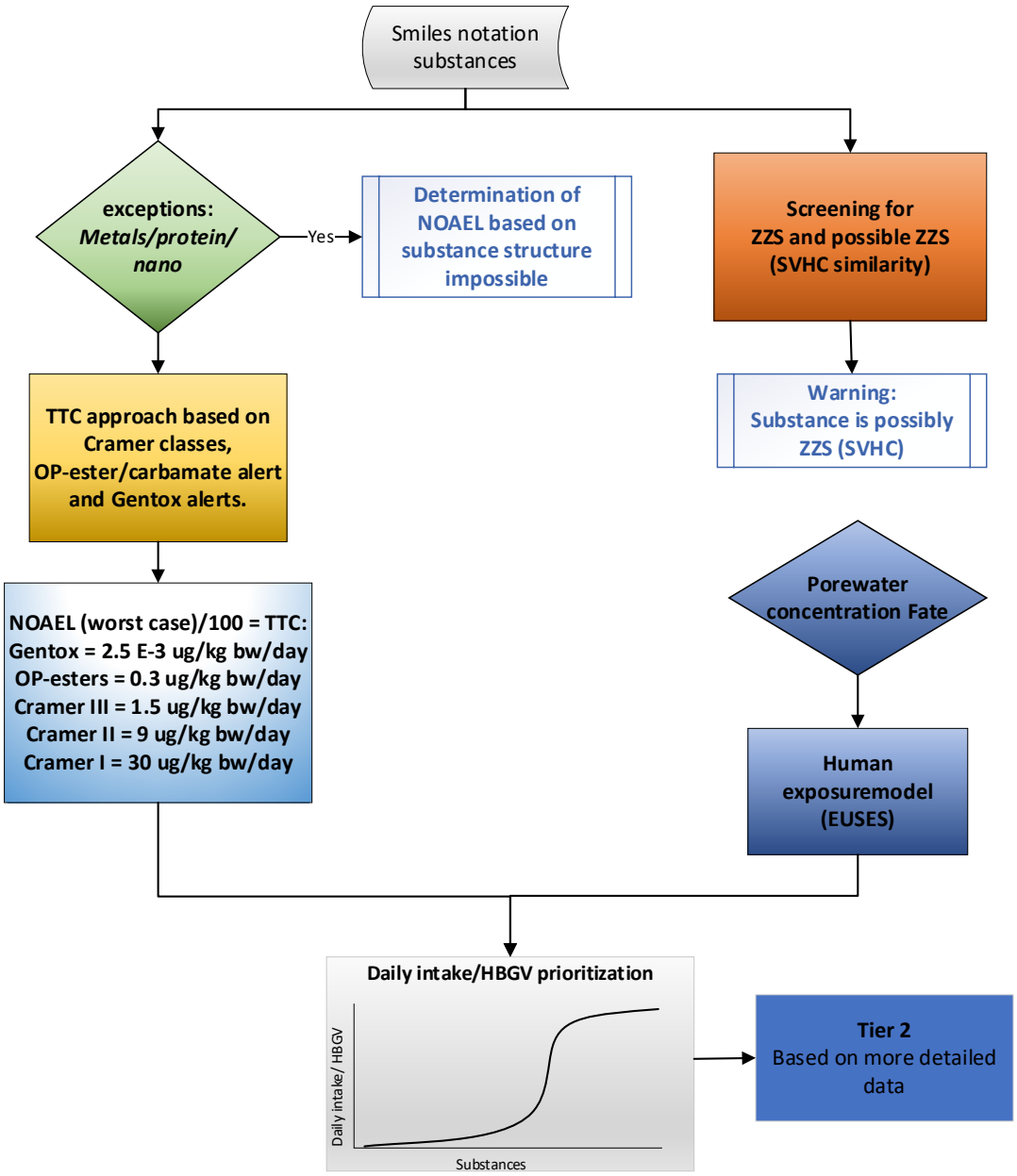


Figure 16 : Scheme depicting the module for human toxicity. ZZS is a Dutch list of substances comparable to SVHC. The screening for ZZS is described in section 4.3.3 and although depicted in this figure is only run once for all the toxicity modules.

a) Tier 1: choice of models and TTC

This section describes the use of the models to determine a HBGV for the tier 1 prioritisation. Information on the technical considerations for the use of the models is provided in Annex G.

1) To generate an estimate of the TTC of a substance the freely available OECD QSAR Toolbox software version 4.4 (OECD, 2020) and the 'profiles' provided therein were applied. The concept of TTC is described in detail in several EFSA opinions (EFSA, 2012, EFSA and WHO, 2016, EFSA, 2019).
2) To generate an indication of the SVHC - or potential SVHC - status of a substance the chemical similarity module (ZZS) developed at RIVM is applied (see section 3.3). This tool is available online for single chemical screening (RIVM, 2020). For the batch generation of Structural Similarity with the appropriate similarity measures, it is necessary to run either working R-

scripts (Wassenaar et al., 2019) or a KNIME workflow (KNIME software, KNIME | Open for Innovation) of the similarity tool. These are already available for future prototype developments and can be obtained from the authors (Pim Wassenaar or Emiel Rorije) at RIVM.

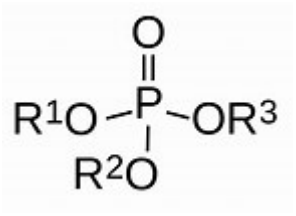
The assignment of the TTC value of an individual substance starts with the identification of the chemical structure. The identified SMILES code (see paragraph 4.3.1) is used as input for the OECD QSAR Toolbox in the 'Input' tab (the starting screen in the Classical interface of the Toolbox), by choosing the input option "Structure" (see Annex G). Once the chemical structure is recognised by the QSAR Toolbox, the following steps can be performed to generate the correct TTC value for the given substance (see Annex G):

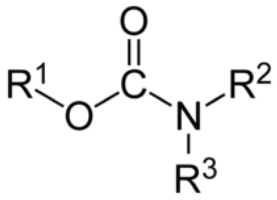
A. Step 1: Estimate potential genotoxic activity. This is achieved by selecting and applying the following Profiling methods in the Profiling tab of the OECD QSAR Toolbox (Annex K):
    a. DNA alerts for AMES, CA, and MNT by OASIS
    b. In vitro mutagenicity (Ames test) alerts by ISS
    c. In vivo mutagenicity (Micronucleus) alerts by ISS

    If any of these three mutagenicity profiles gives one or more alerts, the lowest TTC of 0.0025 µg/kg bw/day is applicable, and the evaluation stops here. If the software reports "No alerts found", we continue with step 2.

    *In the example of Aniline, both the in vitro as well as the in vivo mutagenicity alerts by ISS report an alert: "Primary aromatic amine". The lowest TTC value (*0.0025 µg/kg bw/day) *is therefore applicable to aniline, and no further TTC evaluation steps are necessary.*

B. Step 2: The chemical structure has to be checked for the presence of organophosphate or carbamate substructures:



or


    where R1, R2, and R3 can be alkyl or aromatic substituents. The user can do this manually by checking the chemical structure drawing given in the OECD QSAR Toolbox, or use the profile included in the supporting information. If these substructures are present, the OP-ester/carbamate substances TTC value of 0.3 µg/kg bw/day is applicable, and TTC evaluation can stop. If these substructures are not present, we continue with step 3.

C. Step 3: Establish the correct Cramer Class (Cramer et al., 1978) for the substance of interest, by selecting and applying the Profiling method; "Toxic hazard classification by Cramer (extended)" (See Annex G). This profile results in either High (Class III), Intermediate (Class II) or Low (Class I) toxicity with the following associated TTC values: High – 1.5 µg/kg bw/day, Intermediate – 9 µg/kg bw/day, Low - 30 µg/kg bw/day (assuming an average human body weight of 70 kg).

    Aniline as an example results in Cramer High toxicity (Class III) (Annex G). However, as aniline also has genotoxicity alerts the TTC of 0.0025 µg/kg bw/day applies, and not the Cramer Class III TTC of 1.5 µg/kg bw/day.

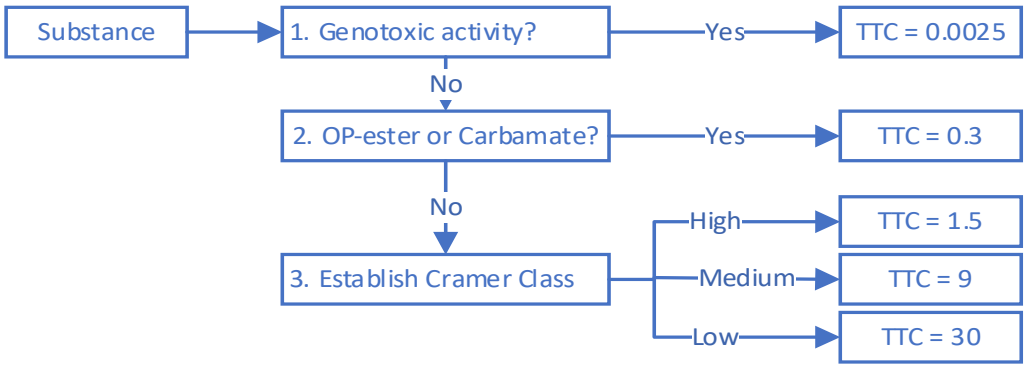


Figure 17 :Flowchart for the derivation of a TTC using the OECD QSAR Toolbox. TTC are expressed in µg/kg bw/day.

The resulting TTC values can be compared directly to the estimated exposure in the form of a (lifelong) daily intake. The ratio of the daily intake over the TTC gives the RCR_{human}, which can be used for prioritisation (explained in the next section).

4.3.4.3 Derivation of the Risk Characterisation Ratio (RCR)

The RCR is defined as the quotient of exposure divided by a human HBGV in the form of a TTC value as explained in section 4.3.4.2. The PREMISS prioritisation prototype provides two separate prioritisations for human health based on (i) exposure through ingestion of soil and vegetables, and (ii) direct consumption of groundwater. The RCR formula for each prioritisation is given in equations 5 and 6.

Equation 5. RCR for ingestion of soil and consumption of crops.

$$RCR_{Human-soilCrops} = \frac{Exposure_{vegetables} + Exposure_{soil\ ingestion}}{TTC_{human}}$$

Equation 6. RCR for direct consumption of groundwater.

$$RCR_{Human-Groundwater} = \frac{Exposure_{cons.groundwater}}{TTC_{human} * 0.2}$$

Equation 6 includes an allocation factor of 20% in line with the WHO method to assess risks of consumption of drinking water using the TTC (WHO, 2011). Although this allocation factor will have no effect on the resulting prioritisation, the factor is included in the eventuality other drinking water related exposure pathways are added in future research. In that case, the relative contribution between the different pathways and the use of the allocation factor should be re-evaluated.

4.3.5 ECOTOX module

4.3.5.1 Introduction

The ecotoxicological prioritisation is based on a comparison of predicted environmental concentrations (PEC) with an ecotoxicological predicted no effect concentration (PNEC) (see 4.1.2, equation 1). Although terrestrial ecotoxicity data have been generated for quite some chemicals, their number is still limited as compared to aquatic ecotoxicity data. As a consequence, hardly any QSARs are available to estimate ecotoxicological endpoints for soil organisms. The current version of the US EPA ECOSAR program is programmed to identify 120 chemical classes for which more than 600 aquatic QSARs are available (US EPA, 2017). However, the number of terrestrial QSARs for earthworms is very limited (US EPA, 2017). Most regulatory frameworks use the concept of equilibrium partitioning (EqP) as a screen for identifying substances requiring further testing (ECHA, 2008, ECHA, 2017). The EqP-approach is based on the assumptions that soil organisms are primarily exposed via soil pore water, and that their intrinsic sensitivity is comparable to related species in surface water. From this, it follows that a comparison of the PEC in porewater with a PNEC for aquatic species represents a reasonable way to prioritise emerging chemicals for soil.

4.3.5.2 Tiered approach

A tiered approach was developed in which the first step is to estimate PNECs for a large number of compounds in a similar, structured and preferably automated way.

Tier 1 makes use of the aforementioned ECOSAR program (US EPA, 2017a and 2017b). ECOSAR 2.0 offers well documented QSARs for different aquatic species for a wide range of substance classes. It is noted that options for running aquatic QSARs are also available in other programs. For instance the NORMAN-database also contains QSAR-based PNECs. However, it is not clear from the underlying substance datasheets how the latter are derived. Data for several organisms are provided, but the only reference is to a paper on QSARs for *Daphnia* (Aalizadeh et al., 2017) and not for other organisms . Therefore, ECOSAR 2.0 is used to estimate critical ecotoxicity endpoints in a uniform and consistent way from which the $PNEC_{tier1}$ for porewater can be derived (see Figure 18).

For future development of Tier 2, compound specific PNECs can be used that are derived using the SOLUTIONS SSD database (Posthuma et al., 2019). This database contains Species Sensitivity Distributions (SSD) that are derived from experimental aquatic ecotoxicity data. The SSD concept uses the distribution of the sensitivity of the tested species, from which the concentration can be derived at which 95% of all species in the ecosystem are protected (HC5; Hazardous Concentration for 5% of the species) could be derived. For further prioritisation or assessment of measured soil concentrations, a cross-check with established aquatic PNECs is possible, as the Quality Targets of the NORMAN database for instance (https://www.norman-network.com/nds/ecotox/). Note that the database returns all types of measured and modelled PNECs are returned, including QSAR-based PNECs and care should be taken to focus on verified quality criteria based on experimental data. NORMAN includes a reliability score for the key study underlying the PNEC. However, it appears that the highest reliability score is assigned to QSAR predictions as well, and this should be clarified. Another question to be solved is whether it is possible to automatically extract experimentally based PNECsfrom the database. Both issues should be explored in future projects.

The next section describes how to derive Tier 1 PNECs for pore water, including a basic introduction for working with the ECOSAR program.

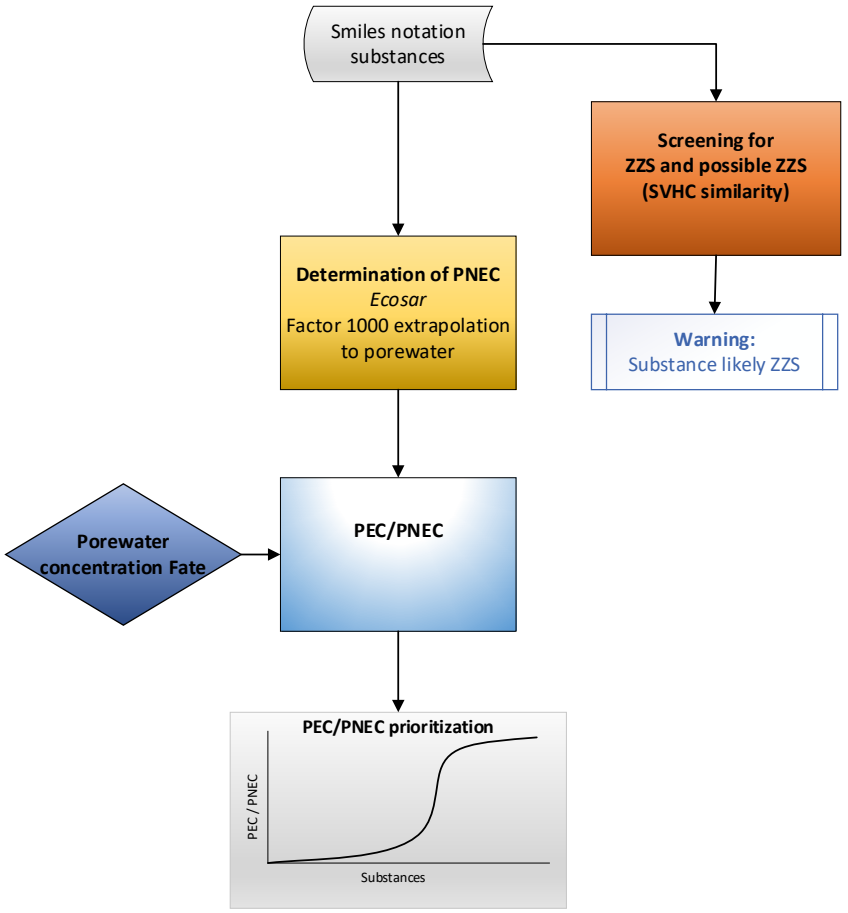


Figure 18 : Scheme for module on tier 1 direct ecotoxicity. The top-left blue box shows which data can be used in a tier 2 approach. The screening for ZZS is described in section 4.3.3 and although depicted in this figure is only run once for all the toxicity modules.

4.3.5.3 Tier 1: Derivation of PNECs for pore water based on ECOSAR results

4.3.5.3.1 General considerations on the ECOSAR program

This section describes the derivation of the $PNEC_{tier1}$ for porewater using ECOSAR version 2.0 (US EPA, 2017, US EPA, 2017). Note that this version is an update of the 1.11 version that is integrated in the EpiSuite program. ECOSAR is not applicable to inorganic and organometallic chemicals. These compounds cannot be prioritised, but compound specific data can be used in Tier 2. ECOSAR is also not recommended for compounds with a Molecular Weight (MW) >1000 (g/mol). However, the program has no restrictions on chemical input and it has to be decided beforehand whether or not running ECOSAR is appropriate. For compounds for which the uptake is related to passive absorption and have a MW > 1000 g/mol, it can be argued that no ecotoxicity is expected because absorption is considered negligible. From this it follows that neutral organics with MW >1000 g/mol are labelled as 'not ecotoxic' in the prioritisation. For surface active chemicals, however, MW is not limiting because toxicity is related to other mechanisms than passive absorption and it is suggested that the program can be run for this type of compounds (US EPA, 2017). It is also noted in ECOSAR's help function that many polymers may be made up of dimers, trimers, and oligomers that have a MW of less than 1000 Da. These smaller molecules often contain the same components as the larger polymers and, therefore, could be run through the ECOSAR model when performing an aquatic ecotoxicity assessment before extrapolating to pore water.

The chemical classes in ECOSAR 2.0 are defined on the basis of chemical structures. The program may provide results for multiple classes if the entered structure includes base structures from more than one

class. If this is the case, the user must determine the most suitable class for estimating toxicity using knowledge of environmental toxicology, organic chemistry, and statistics (US EPA, 2017). For further information, see below in the explanatory section on working with ECOSAR.

4.3.5.3.2 Derivation of the PNEC tier1

As indicated above, there is only a limited number of terrestrial QSARs for earthworms available in ECOSAR 2.0 (US EPA, 2017) and aquatic PNECs are used as a surrogate for pore water-based PNECs for terrestrial species. A PNEC represents the concentration at which no ecosystem effects are expected, and is derived by putting an assessment factor (AF) on the critical ecotoxicity value. The AF addresses the uncertainties associated with the extrapolation of single species laboratory ecotoxicity tests to multi species field ecosystems. The value of the AF depends on the number of studies, the diversity of species for which data are available, and the type and the duration of the experiments. Table 20 shows the generic AF scheme that is used to derive freshwater PNECs for long-term exposure in the context of several European legal frameworks, such as REACH, the Water Framework Directive and the Biocidal Products Regulation (ECHA, 2008, ECHA, 2017, EC, 2018).

Table 19 : Basic assessment factor scheme used for the derivation of PNECs for freshwater ecosystems used in several European regulatory frameworks. The AF is applied to the lowest ecotoxicity value.

Available data	
At least one short-term L(E)C_{50} from each of three trophic levels (fish, invertebrates (preferred *Daphnia*) and algae)	1000
One long-term EC_{10} or NOEC (either fish or *Daphnia*)	100
Two long-term results (e.g. EC_{10} or NOECs) from species representing two trophic levels (fish and/or *Daphnia* and/or algae)	50
Long-term results (e.g. EC_{10} or NOECs) from at least three species (normally fish, *Daphnia* and algae) representing three trophic levels	10

As can be seen from this table, the minimum requirement is the presence of acute ecotoxicity values for three taxonomic groups, representing different trophic levels. This is called the *acute base set*. The presence of additional long-term tests allows for a gradual decrease of the AF to a minimum of 10 in case the *chronic base set* is complete. ECOSAR 2.0 is able to produce an acute base set (i.e. acute ecotoxicity values for three taxonomic groups) for many chemical classes (EPA, 2017a, US EPA, 2017b). Additional to acute L(E)C_{50}s for freshwater fish, *Daphnia* and algae, ECOSAR also generates data for saltwater fish and mysids. Since saltwater species are less relevant for soil, only the freshwater data are used for prioritisation in the PREMISS project. A PNEC for soil traditionally does not include vertebrates and it may be argued that inclusion of fish in the dataset is not relevant. However, the acute aquatic base set should be seen as a representation of the biological diversity encountered in the field. In that context using the base set including fish is considered appropriate for deriving a PNEC that is representative for ecotoxicity of soil pore water.

The program also generates chronic toxicity values (ChV; geometric mean of LOEC and NOEC). However, these are generally less reliable than the acute $L(E)_{50}$, because they are based on fewer experimental data and/or extrapolated from acute data using acute-to-chronic ratios (US EPA, 2017). Since the purpose of Tier 1 is to process as many compounds as possible in a consistent way, ECOSAR will only be used to generate an acute base set. For the derivation of risk limits in a regulatory context, an additional AF would be applied to account for the fact that estimated rather than experimental values are used (De Poorter et al., 2015). However, for the purpose of this prioritisation, the extra AF has no added value and may suggest premature conclusions on the actual risk. Therefore, the $PNEC_{tier1}$ is derived by dividing the lowest acute freshwater value by the default AF of 1000. Compounds for which an acute base set cannot be generated, are automatically prioritised for Tier 2, except for neutral organics with MW >1000

g/mol that are already labelled as 'not ecotoxic' due to their molecular mass.

4.3.6 Secondary poisoning module

4.3.6.1 Introduction

Secondary poisoning addresses the risks for birds and mammals that are indirectly exposed to chemicals via consumption of soil inhabiting organisms and plants. The $RCR_{secpois}$ is based on a comparison of predicted environmental concentrations (PEC) with a predicted no effect concentration ($PNEC_{secpois}$) in the diet that leads to no effects for birds and mammals higher in the food chain (see section 1.2). Following the method of Verbruggen (2014), the PNEC value for secondary poisoning is expressed as the concentrations in vertebrate food. The basis for this $PNEC_{secpois}$ are NOAELs for birds and mammals. The PNEC is then compared with a PEC that is calculated using information on the uptake of chemicals from soil by earthworms or plants to calculate the $RCR_{secpois}$. Figure 19 gives an overview of the module on secondary poisoning.

Toxicity data for birds and mammals have been generated for quite a number of chemicals and many of them are included in the US EPA ECOTOX database, but QSARs to estimate toxicity for these species are sometimes not available. However, the estimation of Cramer Classes for the human toxicological assessment (see section 4.3.4.2) is based on NOAELs for rats and therefore, the Cramer Classes can be used to assign a separate NOAEL for rats for each of the classes. In the PREMISS project, we therefore used NOAELs for rats as a starting point to derive $PNEC_{secpois}$ that is expressed as a concentration in earthworms or leaves (see section 4.3.6.3, step 1).

For the route of birds and mammals consuming terrestrial plants (leaves), the PNEC derived for birds and mammals, expressed as concentration in leaves, can be compared to the PEC in leaves, which is derived during the exposure calculations in the human toxicity module (see section 4.3.4.1).

For the route of birds or mammals consuming earthworms, the $PNEC_{secpois}$ cannot be compared directly to a concentration (PEC) in pore water. However, predicted concentrations in pore water can be converted into equivalent concentration in worms on the basis of bioaccumulation data. a limited amount of experimental data is available for the bioaccumulation of substances from soil into terrestrial plants or earthworms in the US EPA ECOTOX database (US EPA). Fortunately, QSARs are available for bioaccumulation in earthworms, based on a log K_{ow} (which can be obtained from the fate module of the prioritisation tool). These QSARs express the relation between soil and earthworms as bioconcentration factors (BCF). The BCF_{worms} values resulting from these QSARS are actually based on accumulation from pore water. These relationships can thus be used to convert a PEC, expressed as a concentration in soil pore water, into an equivalent concentration in worms (see section 3.6.3, step 2). However, if in higher tiers experimentally determined Biota-Soil Accumulation Factor (BSAF) values are used, the same exercise could be performed to calculate a PEC in soil (normalised to organic carbon content).

4.3.6.2 Tiered approach

A tiered approach was developed in which the first step is to estimate PNECs for a large number of compounds in a similar, structured and preferably automated way, followed by a more case-by-case evaluation of compounds in Tier 2 that are determined in Tier 1 to be of high priority. Tier 1 makes use of the aforementioned TTC approach. In this way, it is possible to estimate critical secondary poisoning endpoints in a uniform and consistent way from which the $PNEC_{tier1}$ in porewater can be derived. In higher tiers, compound specific PNECs based on experimental mammalian and avian toxicity data, as well as experimental bioaccumulation data in e.g. earthworms, that are retrieved from US EPA ECOTOX database, can be used.

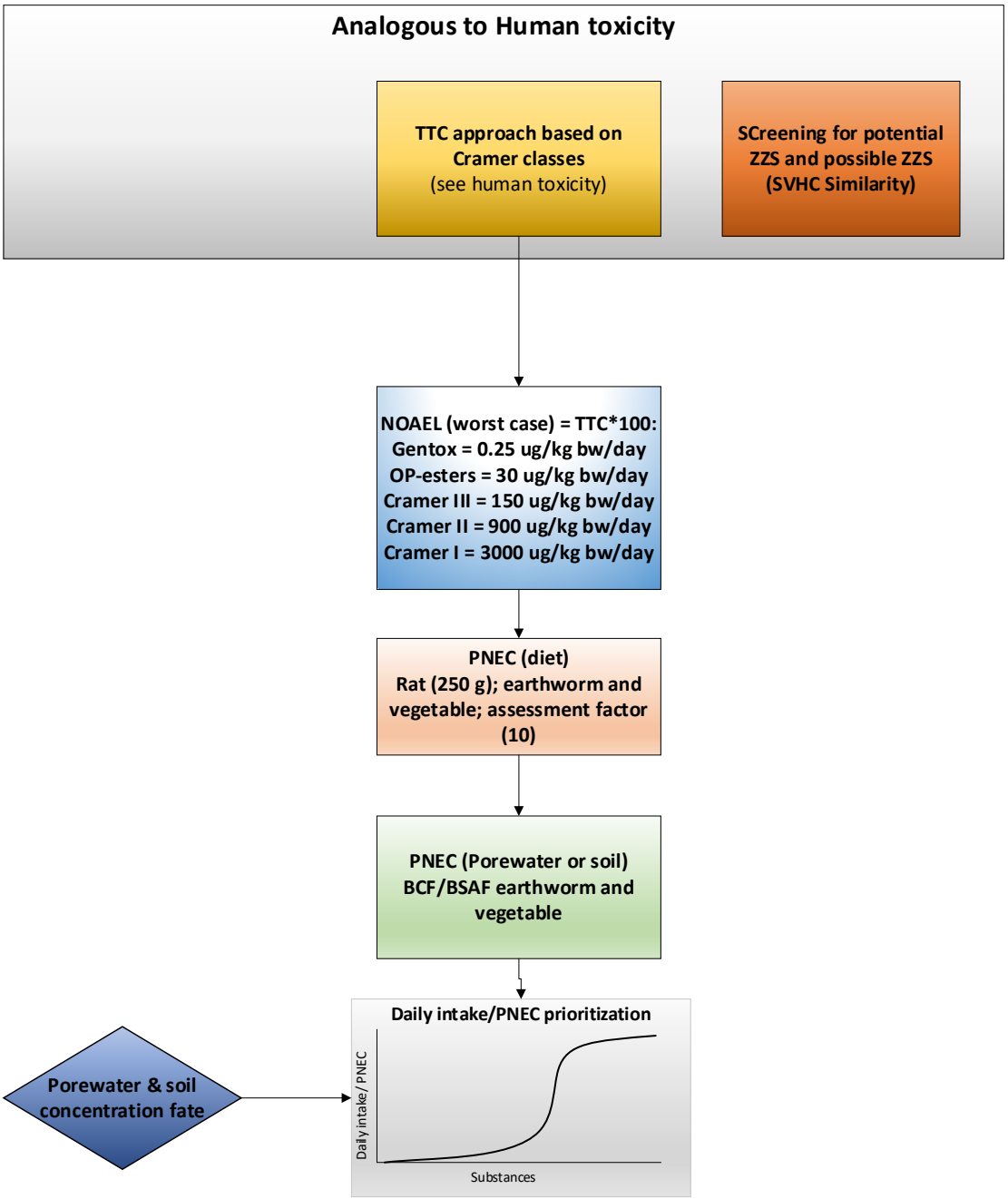


Figure 19 : Scheme for tier 1 module on secondary poisoning. Additional data for the Tier 2 are depicted in the left blue box. The screening for ZZS is described in section 4.3.3 and although depicted in this figure is only run once for all the toxicity modules.

4.3.6.3 Tier 1: Derivation of PNECs for secondary poisoning

4.3.6.3.1 Step 1 Estimation of the PNEC in earthworms and leaves

In order to derive a PNEC for birds and mammals, a NOAEL for birds and mammals must be estimated. This is done using the TTC methodology on which the assessment for human toxicology is based (see section 4.3.4.2). As a reminder, in the TTC methodology, the substances are divided based on their structure into five classes (Cramer Classes I-III, organophosphate and carbamate group and the genotoxic carcinogen group) (Cramer et al., 1978). The associated TTCs are based on the 5th percentiles

of NOAELs from chronic animal studies for each of the five substance groups, but an assessment factor of 100 has been applied to these 5th percentiles to extrapolate from rats to humans. Therefore, in order to get the 5th percentile of the NOAELs, the TTC values have to be multiplied by a factor of 100.

NOAEL (5th percentile, class 1-5) = TTC * 100

The 5th percentile of the NOAELs is in principle a conservative starting point. First of all, it concerns the 5th percentile for substances belonging to one of the five chemicals classes (not for species as in the species sensitivity distributions). This means that the value is based on relatively toxic substances within this chemical class. In addition, the NOAELs are based on endpoints that are relevant for human toxicity. These are usually more sensitive than the population-relevant endpoints used for secondary poisoning to birds and mammals.

Since most of the toxicity studies on which the TTC values are based have been performed with rats, the calculation of the PNEC for secondary poisoning is based on a rat weighing on average 250 g. Using an allometric equation (EC, 2018), it can be estimated that a 250 g rat has an energy requirement of 337 kJ per day. With this data, the 5th percentile NOAELs can be converted to an energy-normalised concentration in the rat's diet as follows:

$NOEC_{diet}$ [mg/kJ_{diet}] = NOAEL [mg/kg_{bw}/d] * 0.25 [kg_{bw}] / 337 [kJ/d]

Subsequently, this value is converted into concentrations in leafy vegetables and in worms (wwt) using the standard energy levels for leafy vegetables and worms of 1311 and 1346 kJ/kg, respectively (EFSA, 2009). Finally, a factor of 10 is put on these NOECs in worms and plants. This is the default assessment factor to extrapolate a chronic NOEC for rats to a PNEC for secondary poisoning for terrestrial mammals (Verbruggen, 2014).

$PNEC_{secpois\text{-}worm}$ [mg/kg_{worm}] = NOEC [mg/kJ_{diet}] * 1311 [kJ/kg_{worm}] / 10

$PNEC_{secpois\text{-}leaf}$ [mg/kg_{leaf}] = NOEC [mg/kJ_{diet}] * 1346 [kJ/kg_{leaf}] / 10

The resulting PNECs expressed as concentrations in earthworms and leafy vegetables are shown in Table 21. The only substance specific information required to calculate these values is thus the TTC value. Further conversions are however required as explained in step 2.

Table 20: Tier 1 $PNEC_{secpois}$ for secondary poisoning [mg/kg]

Tier 1 PNECs secondary poisoning		
	Earthworms	Crop leaves
Cramer Class I	0.68	0.29
Cramer Class II	0.20	0.087
Cramer Class III	0.034	0.015
OP and carbamates	0.0068	0.0029
Genotoxic carcinogens	5.6E-05	2.4E-05

4.3.6.3.2 Step 2 Conversion of PEC in pore water to PEC in worms and leaves

The PNECs in earthworms and plants cannot be directly compared with concentrations in soil or pore water. However, the PEC in soil and pore water can be converted to an equivalent concentration in earthworms. The conversion is based on the equations that describe the concentration in earthworms as a function of soil and pore water concentrations and earthworm BCF, and the QSAR that describe the BCF (or BSAF[21]) as a function of the log Kow (ECHA, 2016, ECHA, 2017). Combined, these equations are re-written as

$PEC_{worm} = (PEC_{porew} * (0.84 + 0.012 * K_{ow}) + PEC_{soil} * 0.113)/(1+0.113)$

For uptake in plants, the QSARs are somewhat more complicated. The QSARs for uptake in leaves follow the human toxicological derivation and exposure (see section 4.3.4.1 and Annex F for a detailed description of the formulas).

$PEC_{leaf}= C_{leaf}$ [kg/kg wwt] = BETA.leafR/(ALPHA.R * RHO.plant)

The risk characterisation for secondary poisoning of terrestrial vertebrates via earthworms and plants is defined as:

$RCR_{secpois\text{-}worm} = PEC_{worm} / PNEC_{secpois\text{-}worm}$

$RCR_{secpois\text{-}leaf} = PEC_{leaf} / PNEC_{secpois\text{-}leaf}$

Where the final $RCR_{secpois}$ is the highest of either the $RCR_{secpois\text{-}worm}$ and $RCR_{secpois\text{-}leaf}$.

Depending on the substance properties, one of the two routes will be critical. In general, this will be the worm route for hydrophobic substances and the plant route for more hydrophilic substances.

For biomagnifying substances, the route via the worms is the most critical, but in that case an (estimated) biomagnification factor (BMF) must also be included in the calculations by multiplying it with the RCR. However, the BMF cannot be estimated in a uniform and automated way, and therefore is not part of Tier 1 of this approach.

[21] Note: If experimental BSAF values (kg_{oc}/kg_{lipid}) are used in **higher tiers** this equation changes to:
$PEC_{worm} = PEC_{soil} * (0.012 * BSAF / f_{oc} + 0.113)/(1+0.113)$
With f_{oc} being the fraction of organic carbon in the soil.

5 Fate module, toxicological modules and prioritisation: Results

5.1 Results of fate modeling

5.1.1 Tier 1

Pilot substances were selected based on occurrence data (see chapter 3), see Table 22. The selected soil CECs are categorized in four different substance groups, namely pesticides, PFAS, pharmaceuticals, alkylphenols and PFAS. In this chapter the outcomes of the fate modeling of these selected soil CECs are given. To determine the fate of a substance, chemical properties, emission data and landscape settings were determined. In this project emission data and landscape settings were determined for the PREMISS partners' countries namely Belgium, France and the Netherlands. In the following paragraphs the collection of national emissions and landscape settings are explained, followed by the results per substance group. The collected chemical parameters per substance can be found in Annex D.

Table 21 : Overview of the selected soil CECs, including the CAS number (chemical registration number) and the substance group.

Substance	CAS number	Substance group
Glyphosate	1071-83-6	Pesticide
Imidacloprid	138261-41-3	Pesticide
Metolachlor	87392-12-9	Pesticide
Metolachlor ESA	171118-09-5	Pesticide
Metolachlor OXA	152019-73-3	Pesticide
PFOA	335-67-1	PFAS
PFOS	1763-23-1	PFAS
GenX	13252-13-6	PFAS
PFBA	375-22-4	PFAS
PFHxA	307-24-4	PFAS
PFHxS	355-46-4	PFAS
N-EtFOSAA	2991-50-6	PFAS
Diclofenac	15307-86-5	Pharmaceutical
Triclosan	3380-34-5	Pharmaceutical/biocide
Clarithromycin	81103-11-9	Pharmaceutical
Azithromycin	83905-01-5	Pharmaceutical
4-Nonylphenol	104-40-5	Phenols & Alkylphenols
Bisphenol A	80-05-7	Phenols & Alkylphenols

5.1.1.1 Landscape determination

All fate calculations are specific to one country the regional scale was therefore adjusted to the national scales of The Netherlands, Belgium or France. Belgium land use data was retrieved from the national institute of statistics of Belgium (Statbel, consulted August 2021). Data from the most recent year was used (2019). Dutch land use data was retrieved from the national institute of statistics of The Netherlands (CBS, consulted August 2021). Data from the most recent year was used (2015). The fraction lake water is relatively large in The Netherlands compared to the other countries, due to the presence of the Dutch Markermeer/Ijsselmeer. In Table 23, the collected landscape settings are summarized.

Table 22: Landscape settings per country.

Parameter	Default	Belgium	France	The Netherlands
Area land [km²]	-	30 689	550 000	37 390
Area sea [km²]	-	3 384	57 000	4 153
Fraction lake water	0.0025	0.0032	0.0025	0.053
Fraction fresh water	0.0275	0.0032	0.0039	0.046
Fraction natural soil	0.27	0.44	0.39	0.16
Fraction agricultural soil	0.6	0.35	0.51	0.60
Fraction urban/industrial soil	0.1	0.20	0.093	0.14

5.1.1.2 Fate estimation pesticides

National pesticide emission data were estimated for Belgium based on national average sales in Belgium from 2011-2019 (FPS Health, Food Chain Safety and Environment, Belgium, 2020), see Table 24.

Table 23 : National emissions for glyphosate, imidacloprid and S-metolachlor in Belgium.

Substance	2011	2012	2013	2014	2015	2016	2017	2018	2019	Average
Glyphosate quantity (kg/y)	555 367	701 948	587 042	595 586	511 632	503 275	619 295	475 299	409 151	550 955
Imidacloprid quantity (kg/y)	28 073	25 500	28 801	25 390	19 078	20 280	16 903	14 691	0	19 857
S-metolachlor quantity (kg/y)	73 756	110 028	65 946	82 915	82 655	94 526	60 827	61 343	61 888	77 098

National pesticide emission data was estimated for The Netherlands based on national use of the active ingredients for the years 2012 and 2016. The average was calculated for these two years (CBS, 2020), see Table 25.

Table 24 : National emissions for glyphosate, imidacloprid and S-metolachlor in The Netherlands.

Substance	2012	2016	Average
Glyphosate quantity (kg/y)	414 691	312 035	363 363
Imidacloprid quantity (kg/y)	7 565	1 175	4 370
S-metolachlor quantity (kg/y)	229 516	140 788	185 152

National pesticide emission data was estimated for France based on national sales of pesticides for the years 2011-2019 (BNVD - Banque Nationale des ventes de produits phytopharmaceutiques par les Distributeurs agréés, 2020), see Table 26.

Table 25 : National emissions for glyphosate, imidacloprid and S-metolachlor in France.

Substance	2011	2012	2013	2014	2015	2016	2017	2018	2019	Average
Glyphosate quantity (kg/y)	8 469 993	9 062 117	8 672 989	9 487 045	8 465 720	8 787 138	8 858 783	9 723 436	6 066 719	8 292 600
Imidacloprid quantity (kg/y)	55 087	260 776	261 789	257 055	259 741	271 150	249 903	30 242	1 751	159 760

Substance	2011	2012	2013	2014	2015	2016	2017	2018	2019	Average
S-metolachlor quantity (kg/y)	1 538 449	1 474 469	1 744 172	2 047 957	2 035 928	1 889 255	1 872 292	2 420 550	1 477 142	1 770 994

No national emission data is available for metolachlor ESA and metolachlor OXA. Metolachlor fate in the environment was estimated from measurements in Walloon groundwater: an average of metolachlor repartition between the parent molecule (metolachlor) and its main degradation products (metolachlor OXA and ESA) was made from measurements in Walloon groundwater, from 307 sites where metolachlor ESA (the most abundant form) was quantified. Considering the average measured concentrations, the repartition is: 5% S-metolachlor – 73% metolachlor ESA – 22% metolachlor OXA

Taking into account median measured values, the repartition is similar: 7% S-metolachlor – 76% metolachlor ESA – 17% metolachlor OXA. Based on this second repartition, the emissions of metolachlor, metolachlor ESA and metolachlor OXA were estimated based on the national numbers of S-metolachlor, see Table 27.

Table 26 : Estimated national emissions of selected pesticides for Belgium, The Netherlands and France.

Parameter	Units	Glyphosate 1071-83-6	Imidacloprid 138261-41-3	S-Metolachlor 87392-12-9	Metolachlor ESA 171118-09-5	Metolachlor OXA 152019-73-3
Total emission Belgium	Tons/y	5.51E+02	1.99E+01	5.40E+00	5.86E+01	1.31E+01
Total emission France	Tons/y	8.29E+03	1.60E+02	1.24E+02	1.35E+03	3.01E+02
Total emission The Netherlands	Tons/y	3.63E+02	4.37E+00	1.30E+01	1.41E+02	3.15E+01

The total emissions are divided over the environmental compartments by assuming losses to air (15%), water (1.0%) and soil (84%) (Van de Meent et al., 2020).

In Table 28 the output of the fate calculations for the selected pesticides in Belgium is given, expressed in concentrations per substance in pore water (groundwater), air and soil.

Table 27 : Output data of fate estimation of the selected pesticides in Belgium, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Glyphosate	1071-83-6	1.07E-04	2.44E-09	7.98E-09
Imidacloprid	138261-41-3	3.85E-06	8.36E-11	2.15E-07
S-Metolachlor	87392-12-9	1.03E-06	9.64E-11	9.27E-06
Metolachlor ESA	171118-09-5	1.14E-05	2.45E-10	2.27E-06
Metolachlor OXA	152019-73-3	2.53E-06	5.89E-11	3.15E-06

In Table 29 the output of the fate calculations for the selected pesticides in France is given, expressed in concentrations per substance in pore water (groundwater), air and soil.

Table 28 : Output data of fate estimation of the selected pesticides in France, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Glyphosate	1071-83-6	6.28E-05	4.70E-09	4.70E-09
Imidacloprid	138261-41-3	1.21E-06	8.53E-11	6.77E-08
S-Metolachlor	87392-12-9	9.11E-07	4.00E-10	8.18E-06
Metolachlor ESA	171118-09-5	1.02E-05	7.13E-10	2.04E-06
Metolachlor OXA	152019-73-3	2.28E-06	1.76E-10	2.83E-06

In Table 30 the output of the fate calculations for the selected pesticides in the Netherlands is given, expressed in concentrations per substance in pore water (groundwater), air and soil.

Table 29 : Output data of fate estimation of the selected pesticides in The Netherlands, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Glyphosate	1071-83-6	3.39E-05	1.46E-09	2.54E-09
Imidacloprid	138261-41-3	4.09E-07	1.62E-11	2.28E-08
S-Metolachlor	87392-12-9	1.19E-06	2.63E-10	1.07E-05
Metolachlor ESA	171118-09-5	1.32E-05	5.17E-10	2.63E-06
Metolachlor OXA	152019-73-3	2.94E-06	1.29E-10	3.65E-06

5.1.1.3 Fate estimation PFAS

Reach tonnage bands were available for 3 of the selected PFAS substances, namely PFHxS, PFBA and N-EtFOSAA. The tonnage bands from PFHxS, PFBA and N-EtFOSAA all range from 1-10 tons/year. For PFOA, PFOS, GenX and PFHxA a default range from 0.1-1 tons/year was used as no REACH data was available. To calculate the national use from this tonnage band it is assumed that 13% of the total tonnage is used in France, 2.5% is used in Belgium and 4% is used in the Netherlands.

The total emissions are divided over the environmental compartments by assuming losses to air (8.5%), water (12%) and soil (3.0%). This distribution was determined for REACH chemicals by Van Gils et al. (2020).

The output of the fate calculations for the selected PFAS, expressed in concentrations per substance in pore water (groundwater), air and soil, in The Netherlands, Belgium and France is shown in Table 31, Table 32 and Table 33 respectively.

Table 30 : Output data of fate estimation of PFAS in The Netherlands expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
PFOA*	335-67-1	3.30E-11	7.40E-14	3.32E-08
PFOS*	1763-23-1	3.42E-11	3.21E-14	4.07E-08
GenX*	13252-13-6	3.59E-11	7.88E-14	2.18E-08
PFBA	375-22-4	4.12E-10	8.66E-13	1.33E-09
PFHxA*	307-24-4	5.34E-11	2.60E-14	2.11E-10
PFHxS	355-46-4	5.34E-10	2.62E-13	1.31E-08
N-EtFOSAA	2991-50-6	6.12E-11	3.80E-13	1.39E-06

* Based on default emissions (0.1-1 T/year)

Table 31 : Output data of fate estimation of PFAS in Belgium expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
PFOA*	335-67-1	4.31E-11	5.03E-14	4.33E-08
PFOS*	1763-23-1	4.32E-11	2.25E-14	5.14E-08
GenX*	13252-13-6	4.69E-11	5.34E-14	2.85E-08
PFBA	375-22-4	5.38E-10	5.85E-13	1.73E-09
PFHxA*	307-24-4	6.28E-11	1.85E-14	2.48E-10
PFHxS	355-46-4	6.26E-10	1.87E-13	1.54E-08
N-EtFOSAA	2991-50-6	7.99E-11	2.64E-13	1.81E-06

* Based on default emissions (0.1-1 T/year)

Table 32 : Output data of fate estimation of PFAS in France expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
PFOA*	335-67-1	8.58E-12	4.78E-14	8.63E-09
PFOS*	1763-23-1	9.73E-12	1.88E-14	1.16E-08
GenX*	13252-13-6	9.34E-12	5.08E-14	5.67E-09
PFBA	375-22-4	1.07E-10	5.56E-13	3.45E-10
PFHxA*	307-24-4	1.64E-11	1.22E-14	6.48E-11
PFHxS	355-46-4	1.65E-10	1.24E-13	4.05E-09
N-EtFOSAA	2991-50-6	1.59E-11	2.50E-13	3.60E-07

* Based on default emissions (0.1-1 T/year)

5.1.1.4 Fate estimation pharmaceuticals

REACH tonnage bands were only available for triclosan. The tonnage band from triclosan ranges from 10-100 tons/year. For diclofenac, clarithromycin and azithromycin, Dutch national use data was collected from the GIP databank, which collects data on the prescription of pharmaceuticals. The average pharmaceutical use from 2016-2020 was calculated based on the Defined Daily Doses (DDD's) and the number of DDDs, see Table 34 for the results of the calculations.

Table 33: Estimated national emissions of azithromycin, clarithromycin and diclofenac in The Netherlands.

Substance	2016	2017	2018	2019	2020	Average
Azithromycin	3.99E+00	3.81E+00	3.78E+00	3.38E+00	3.00E+00	3.60E+00
Clarithromycin	1.91E+00	1.82E+00	1.79E+00	1.71E+00	1.38E+00	1.72E+00
Diclofenac	2.31E+00	2.41E+00	2.59E+00	2.74E+00	2.60E+00	2.53E+00

The total emissions were divided over the environmental compartments by assuming human excretion of pharmaceuticals to be 12%, all of which is assumed to be released to WWTPs. The release from WWTP is calculated with the removal efficiency of the specific substances. The removal efficiencies of the pharmaceuticals assessed in this project can be found in Annex C.

In Table 35 the output of the fate calculations is given for the Netherlands, expressed in concentrations per substance in pore water (groundwater), air and soil. The table is an overview of the output, not a comparison. Triclosan is included in this table to be consistent with Chapter 3, where triclosan is categorized as a pharmaceutical.

Table 34: Output data of fate estimation of the selected pharmaceuticals in The Netherlands, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Diclofenac	15307-86-5	1.48E-10	3.63E-13	1.08E-08
Triclosan	3380-34-5	1.97E-11	3.39E-12	5.27E-09
Clarithromycin	81103-11-9	2.33E-09	4.79E-12	2.09E-08
Azithromycin	83905-01-5	1.58E-09	3.32E-12	2.58E-08

In Table 36 and Table 37 the output of the fate calculations of triclosan in France and Belgium is given. Fate calculations of diclofenac, clarithromycin and azithromycin were not performed for France and Belgium as no national numbers were collected.

Table 35: Output data of fate estimation of triclosan in France, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Triclosan	3380-34-5	1,37E-11	2,37E-12	3,68E-09

Table 36: Output data of fate estimation of triclosan in Belgium, expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
Triclosan	3380-34-5	1,27E-11	2,17E-12	3,39E-09

5.1.1.5 Fate estimation alkylphenols

For 4-nonylphenol several CAS numbers can be found, however, chemical property data could only be found on the EPA dashboard for the CAS number 211947-56-7.

REACH tonnage bands were available for both 4-nonylphenol and bisphenol A, however REACH data for 4-nonylphenol was not available for the same CAS number as for which chemical property data was found. The REACH tonnage band for bisphenol A ranges from 100 000-1 000 000 tons/year. The tonnage bands for 4-nonylphenol ranges from 10 000-100 000 tons/year (4-nonylphenol branched CAS number 84852-15-3). To calculate the national use from this tonnage band it is assumed that 13% of the total tonnage is used in France, 2.5% is used in Belgium and 4% is used in the Netherlands.

The emission is divided over the environmental departments by assuming losses to air (8.5%), water (12%) and soil (3.0%), as explained in paragraph 4.2.2.2.

Chemical property data was generated for chemical data from 4-nonylphenol (CAS number 211947-56-7) and emissions data from 4-nonylphenol branched (CAS number 84852-15-3). The output of the fate calculations for the selected industrial chemicals, expressed in concentrations per substance in pore water (groundwater), air and soil, in The Netherlands, Belgium and France is shown in Table 38, Table 39 and Table 40 respectively.

Table 37: Output data of fate estimation of the selected industrial chemicals in The Netherlands expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
4-Nonylphenol	104-40-5	2.78E-06	6.70E-09	5.37E-03
Bisphenol A	80-05-7	4.41E-05	3.83E-08	7.60E-04

Table 38: Output data of fate estimation of the selected industrial chemicals in Belgium expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
4-Nonylphenol	104-40-5	3.63E-06	4.60E-09	7.01E-03
Bisphenol A	80-05-7	5.57E-05	2.45E-08	9.60E-04

Table 39: Output data of fate estimation of the selected industrial chemicals in France expressed in concentration in pore water (groundwater), air and soil.

Substance	CAS nr	C-porew [g/L]	C-Air [g/m3]	C-Soil [g/kg. dw]
4-Nonylphenol	104-40-5	7.23E-07	4.35E-09	1.40E-03
Bisphenol A	80-05-7	1.23E-05	2.09E-08	2.12E-04

5.1.2 Tier 2

5.1.2.1 Direct sources (plant protection products)

Statistics Netherlands (CBS - Statistics Netherlands) collects more detailed information on the use of plant protection products (PPP) than only the total sales or total uses. Once in four years, they organise a detailed inventory of all PPP per hectare for each crop/sector. The surface area of each crop/sector is also reported. See: StatLine - Gebruik gewasbeschermingsmiddelen in de landbouw; werkzame stof, toepassing (cbs.nl).

Glyphosate in the Netherlands as an example

Glyphosate is a herbicide used in different sectors. According to tier 1, the total amount used in the Netherlands in 2016 was 187 tonnes. 84% of the total amount is emitted to soils (4.2.2.2.3), i.e. 158 tonnes, and if we distribute this amount over all agricultural soils in The Netherlands (22,434 km²), one can calculate an average load of 0.07 kg/ha/year.

In Tier 2, the 158 tons are not applied to all agricultural soils, but only to soils where specific crops are grown. This appears to be a much smaller surface than all agricultural soil: 1,548 km². That means that the pesticides load to soils is considerably higher: 1.2 kg/ha/year. When splitting it further into different sectors as shown inTable 41, the maximal calculated load is 1.7 kg/ha/year (in horticulture).

The calculations in SimpleBox assume a long-term pesticides application. Crop rotation will probably result in variable applications to the same plot. Therefore, the average load might be a factor 2-10 lower the values in Table 41 but 0.17-0.85 kg/ha/y is still higher than the calculated amount in tier 1 (0.07 kg/ha/y).

Table 40: Glyphosate data The Netherlands (Statistics Netherlands: StatLine - Gebruik gewasbeschermingsmiddelen in de landbouw; werkzame stof, toepassing (cbs.nl), , last change on 31 January 2020).

Glyphosate	Average Dose (kg/ha/y)
arable farming	1.08
fruit growing	1.58
glasshouse vegetable growing	0.86
grass	1.20
vegetable growing	1.30
horticulture	1.69
glasshouse horticulture	0.68
Average	1.20

5.1.2.2 Indirect sources

Equation 2 requires two types of information: the amounts of materials applied to the soil and the contaminant concentrations in the applied material. The first type of information appeared difficult to obtain. Often, part of the data is available, for example the total amount produced, but it is unknown which part is applied to soils or what surface is applied. We did not distinguish between different types of manure or sludge. First, the amounts of materials applied to the soil, are presented for each country. Second, the amounts of added materials are multiplied by the contaminant concentrations resulting in the yearly load of contaminants (kg/m^2/y).

Belgium - Flanders

The manure data were obtained from 'Cfr. mestrapport 2020 (over 2019)' https://www.vlaanderen.be/publicaties/mestrapport. The total production of manure origins from cattle (60%), pigs (30%) and poultry (10%). The numbers were expressed in kg P_2O_5/ha and kg N/ha. The manure application in kg dry material/ha were calculated based on Dutch data regarding manure composition.

Furthermore, data on digestate in Flanders were available on https://www.vlaco.be/nieuws/afzet-digestaat-verdubbelt-op-periode-van-10-jaar, but it is not clear what the origin of the digestate is (sewage sludge, manure, …). Approximately 85% of the digestated is applied on agricultural soils. The steep increase in Figure 20 suggests a similar increase in application rate.

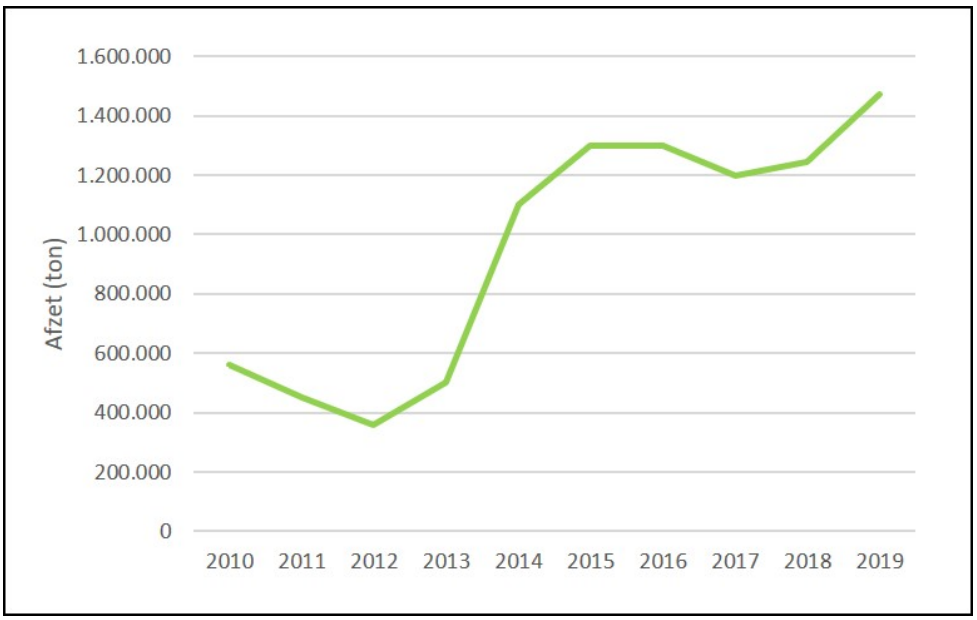


Figure 20: Sales of digestate (as it is) in Flanders. The moisture content can vary a lot so conversion to tonnes dry matter is difficult.

Organic fertilisers/compost was obtained from Wood (2019) who estimated a production of 0.5 million tonnes a year. Most of it is probably applied on agricultural land.

There is no Flemish data available on sewage sludge or dredged material applied on land.

Belgium - Wallonia

Data obtained on manure are from 2008 (CRA-W, 2012). The total amount of manure applied is 2 million tonnes of dry weight, almost all originating from cattle (>95%).

The application of sewage sludge is recorded on a yearly basis (SPGE ; SPW - DGO3 - DSD déclarations des organismes d'assainissement agréés à la SPGE). There is an increase from around 10,000 tonnes dry weight until 2017 up to 35,000 tonnes in 2019 (Figure 21).

Application of dredged materials is not allowed for sediments dredged in navigable waterways. Application of non-navigable watercourses dredged sediment was allowed on the riverbanks but is not anymore. The corresponding volumes have not been recorded. However, this does not represent a large volume of material.

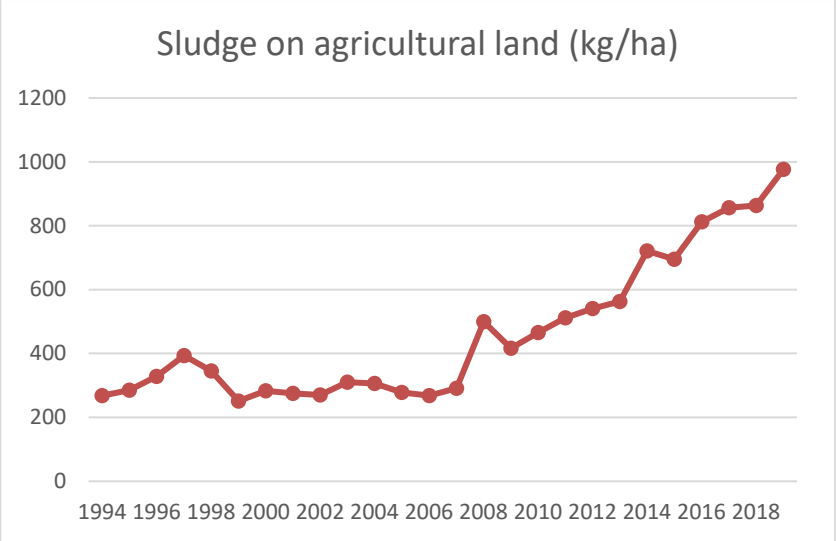


Figure 21: Yearly application of sewage sludge on agricultural land in Wallonia from 1994 to 2019 in kg dry weight per ha assuming that the total amount applied is distributed over 5% of all agricultural land.

France

Data concerning manure application are recorded per region, so data on a national level are lacking. Also data on the application of dredged materials is not available, but is probably a minor source in most of the country.

Regarding the application of sewage sludge: the total volume of spread sludges is around 1 to 2 million tons (dry matter) per year. 70% of the sludge produced are used for agricultural soil amendment. The spreading area is limited to few percent of the agricultural area estimated at 800 000 ha.

Each applied agricultural plot is referenced, and the frequency to return on the same plot is between every 3 and 5 years. To authorize the spread of sludge there is some guidance concerning metals and biological criteria.

Digestate: The Wood-report (Wood, 2019) estimates a production of 5.4 million tonnes a year. Most of it is probably applied on agricultural land.

Organic fertilizer/compost: The Wood-report (Wood, 2019) estimates a production of 2.5 million tonnes a year. Most of it is probably applied on agricultural land, but the number of hectares is unknown. For calculations, we assume that 5% of the agricultural land is treated with compost.

The Netherlands

Manure application is accurately reported in the Netherlands (Velthof et al., 2017), although it is always expressed in N or P per ha. Conversion to dry weight could be done. Most of the manure is from dairy farms (70%). Pigs farms take 12% and the rest is veal calves, chickens, sheep and goats. Because the agricultural plots receiving manure are also registered, the application rate is precisely known.

Sewage sludge application is not allowed in The Netherlands.

Digestate: The Wood-report (Wood, 2019) estimates 2.9 million tonnes a year.

Organic fertiliser/compost: The Wood-report (Wood, 2019) estimates 1.4 million tonnes a year. Most of it is probably applied on agricultural land.

A lot of dredged material is spread on agricultural land in the Netherlands, particularly in the western part of the country. A series of reports has been published in 2006 showing the effects of dredged materials distributed on land (Posthuma et al., 2006).

5.1.2.2.1 Overview of the additives applied in different countries

The result of all information is presented in Table 42. The application rate is valid for the plots that are treated with the specific additive. The total amount of a specific additive also depends on the total surface to which the material is applied. For instance: the total amount of manure (in dry weight) applied in the Netherlands is 50 times the amount of compost and 500 times the amount of digestate.

For some of the additives the application rate is very similar: manure application in Belgium and France is in the same range. Compost digestate applications seem to be higher in the Netherlands and Belgium compared to France. The Netherlands deviates by a higher application of dredged material, but no application of sewage sludge. The application of sewage sludge is relevant for Flanders and France.

Table 41: Application rates of frequently used soil additives in the four countries on plots that are treated.

Applied material (kg/m2/y)	Belgium (Flanders)	Belgium (Wallonia)	France	The Netherlands
Sewage sludge	No data	0.08	0.35-0.7	0
Manure	0.22	0.27	No data	0.17-0.45
Organic fertiliser/compost*	1.4	No data	0.18	1.3
Digestate*	0.22	0.22	0.019	0.13
Dredged material	No data	0	0.05*	5.5

* total amount is assumed to be distributed over 5% of the agricultural land

Contaminant concentrations in the additives

To calculate the contaminant load in soils, we also need to know the contaminant concentrations in the additives. For the occurrence data inventory (see Chapter 3), we collected data of contaminants in sewage sludge and dredged material (see Annex B), but not in manure, digestate and organic fertilizers.

Table 43 shows the obtained data for PFOS in sewage sludge in Wallonia and France, and in dredged material in The Netherlands. There are large differences both in the amounts applied, and the contaminant concentrations. The French fields treated with sewage sludge would result in the highest concentrations of approximately 0.4 µg/kg increase[22] per year in the cultivation layer.

Table 42: Estimated yearly added concentration of PFOS as caused by application of sewage sludge (Wallonia, France) or dredged material (The Netherlands)

Country	Applied material (kg/m2/y)	Amount applied (kg/m2/y)	Concentration (µg/kg)	Added concentration in top 30 cm/y
Be-Wal	Sewage sludge	0.004-0.04	112	0.001-0.01
Fr	Sewage sludge	0.5-1.0	243	0.27-0.54
NL	dredged material	5.5	2.8	0.031

[22] Leaching to groundwater and crop uptake is not included in the approach.

5.2 Results Toxicity module

To test the prioritisation prototype, multiple pilot substances were selected from various chemical classes (see Chapter 3). For these substances the Fate and Toxicity were determined. The substance selection and results of the Fate module are described in section 5.

This chapter describes the results of the determination of toxicity for the pilot substances and the prioritisation performed for the pilot substances for each receptor.

5.2.1 Representative SMILES

The first step of the toxicological module was to determine the representative SMILES for each of the pilot substances. For this, a lookup list was available produced using the QSAR ready workflow described in section 4.3.1. A SMILES code was available for all of the pilot substances. Table 44 provides the SMILES codes used in the toxicity module.

Table 43: SMILES codes for the pilot substances

Substance	SMILES
Glyphosate	OC(=O)CNCP(O)(O)=O
Imidacloprid	[O-][N+](=O)N=C1NCCN1CC1=CN=C(Cl)C=C1
S-Metolachlor	CCC1=C(N(C(C)COC)C(=O)CCl)C(C)=CC=C1
Metolachlor ESA	CCC1=CC=CC(C)=C1N(C(C)COC)C(=O)CS(O)(=O)=O
Metolachlor OXA	CCC1=CC=CC(C)=C1N(C(C)COC)C(=O)C(O)=O
PFOA	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
PFOS	OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
GenX	OC(=O)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F
PFBA	OC(=O)C(F)(F)C(F)(F)C(F)(F)F
PFHxA	OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
PFHxS	OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
N-EtFOSAA	CCN(CC(O)=O)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Diclofenac	OC(=O)CC1=C(NC2=C(Cl)C=CC=C2Cl)C=CC=C1
Triclosan	OC1=C(OC2=CC=C(Cl)C=C2Cl)C=CC(Cl)=C1
Clarithromycin	CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(C)(CC(C)C(=O)C(C)C(O)C1(C)O)OC
Azithromycin	CCC1OC(=O)C(C)C(OC2CC(C)(OC)C(O)C(C)O2)C(C)C(OC2OC(C)CC(C2O)N(C)C)C(C)(O)CC(C)CN(C)C(C)C(O)C1(C)O
4-Nonylphenol	CCCCCCCCCC1=CC=C(O)C=C1
Bisphenol A	CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1

5.2.2 Hazard labels using the ZZS similarity tool

Using the SMILES codes the ZZS similarity tool was used to provide hazard labels for the pilot substances (see section 4.3.3). Each pilot substance was assessed separately in the ZZS similarity tool. The similarity tool provided an overview of which hazard label was associated with a substance that was similar to the pilot substance. Results can either return nothing, a substance with no similarity, or a substance with similarity in one or more of the hazard categories. Only the latter of these options were used to assign

the hazard labels to the pilot substances. Table 45 provides an overview of the pilot substances with their hazard labels.

Table 44: Hazard labels of the pilot substances assigned using the ZZS similarity tool. The acronyms in order are: Persistent, Bioaccumulating, Toxic (PBT); very Persistent very Bioaccumulating (vPvB); Carcinogenic, Mutagenic, Reprotoxic (CMR); Endocrine Disruptive (ED)

Substance	PBT	vPvB	CMR	ED
Glyphosate				
Imidacloprid				
S-Metolachlor				
Metolachlor ESA				
Metolachlor OXA				
PFOA	x	x	x	
PFOS	x	x	x	
GenX	x	x		
PFBA	x	x	x	
PFHxA	x	x	x	
PFHxS	x	x	x	
N-EtFOSAA				
Diclofenac				
Triclosan	x	x		
Clarithromycin				
Azithromycin				
4-Nonylphenol			x	x
Bisphenol A			x	x

As can be seen in the table, most of the PFAS substances were assigned the labels PBT and vPvB. Notably, N-EtFOSAA, a precursor to PFOS, has no labels. This raises a point of discussion namely, the similarity tool only assigns labels based on the substances included in its database, and not based on substance properties. However, substances that are not included in the similarity tool's database may have properties suggesting potential hazard. Additionally, precursors may not be similar enough to their eventual environmental product to be recognized by the similarity tool. **A methodology for PMT assessment (Persistent Mobile Toxic) is under discussion** (Hartmann et al., 2021), and can be implemented into the prototype at a later stage. In particular the i**dentification of ED-label is an ongoing classification**; **some compounds can have a change in the next months**, such as Triclosan (under review, https://echa.europa.eu/fr/ed-assessment).

5.2.3 Human toxicity module

The human toxicity of the pilot substances was assessed using two separate aggregated pathways, namely toxicity through ingestion of soil and crops, and toxicity through direct consumption of groundwater as drinking water (untreated). For both pathways the daily exposure and the tolerable daily intake (TTC) were determined. This section will first describe the results of the Human exposure calculations (see section 4.3.4.1 and Annex J3), before describing the results of the toxicity calculations.

5.2.3.1 Human exposure

Human exposure calculations require substance properties and concentrations used in the Fate module (see section 5). For each country, exposure values were calculated since the environmental concentrations calculated from the fate module vary between the different countries. Table 46, Table 47 and Table 48 provide the results of the exposure calculations for respectively France, Belgium, and the Netherlands. Exposure was not calculated for diclofenac, triclosan, clarithromycin, azithromycin for France and Belgium as no emission data were available.

Table 45: Results exposure calculations for France

Substance	**Groundwater consumption** [ug/kg bw/day]	**Ingestion of soil + crops** [ug/kg bw/day]
Glyphosate	1.80E+00	1.18E+02
Imidacloprid	3.46E-02	2.86E+01
S-Metolachlor	2.60E-02	4.42E-02
Metolachlor ESA	2.92E-01	8.48E+02
Metolachlor OXA	6.51E-02	2.66E+01
PFOA	2.45E-07	5.47E-12
PFOS	2.78E-07	8.07E-07
GenX	2.67E-07	5.28E-12
PFBA	3.06E-06	3.62E-11
PFHxA	4.69E-07	1.58E-02
PFHxS	4.71E-06	5.08E-02
N-EtFOSAA	4.55E-07	2.57E-10
4-Nonylphenol	2.07E-02	1.09E-04
Bisphenol A	3.51E-10	7.00E-09

Table 46: Results exposure calculations for Belgium

Substance	**Groundwater consumption** [ug/kg bw/day]	**Ingestion of soil + crops** [ug/kg bw/day]
Glyphosate	3.05E+00	2.01E+02
Imidacloprid	1.10E-01	9.08E+01
S-Metolachlor	2.95E-02	5.02E-02
Metolachlor ESA	3.24E-01	9.43E+02
Metolachlor OXA	7.24E-02	2.96E+01
PFOA	1.23E-06	2.75E-11
PFOS	1.24E-06	3.59E-06
GenX	1.34E-06	2.65E-11
PFBA	1.54E-05	1.82E-10
PFHxA	1.79E-06	6.05E-02
PFHxS	1.79E-05	1.93E-01
N-EtFOSAA	2.28E-06	1.29E-09
4-Nonylphenol	1.04E-01	5.48E-04
Bisphenol A	1.59E-09	3.17E-08

Table 47: Results exposure calculations for the Netherlands

Substance	**Groundwater consumption** [ug/kg bw/day]	**Ingestion of soil + crops** [ug/kg bw/day]
Glyphosate	9.69E-01	6.40E+01
Imidacloprid	1.17E-02	9.64E+00
S-Metolachlor	3.40E-02	5.77E-02
Metolachlor ESA	3.76E-01	1.09E+03
Metolachlor OXA	8.39E-02	3.43E+01
PFOA	9.44E-07	2.11E-11
PFOS	9.78E-07	2.84E-06
GenX	1.03E-06	2.03E-11
PFBA	1.18E-05	1.39E-10
PFHxA	1.53E-06	5.15E-02
PFHxS	1.53E-05	1.64E-01
N-EtFOSAA	1.75E-06	9.89E-10
Diclofenac	4.24E-06	4.12E-04
Triclosan	5.63E-07	1.13E-07
Clarithromycin	6.67E-05	2.27E+01
Azithromycin	4.52E-05	3.00E+00
4-Nonylphenol	7.94E-02	4.20E-04
Bisphenol A	1.26E-09	2.51E-08

As explained above, the environmental concentration for a large part determines the exposure in the prototype. For the direct consumption of groundwater, this is in fact the only variable in the calculation. When comparing the porewater concentrations derived in section 4.3.4 we can indeed see that the exposure through consumption of groundwater follows a similar pattern, varying only due to different concentrations for the pilot substances. However, for ingestion of soil and crops, other variables also influence exposure due to the uptake by plants. For example, the exposure for groundwater consumption of imidacloprid and S-Metolachlor are of the same order of magnitude, whereas for ingestion of soil+crops the exposure of imidacloprid is 2 orders of magnitude larger (100x) compared to S-Metolachlor. The resulting prioritisation may therefore differ between both aggregated pathways, showing the relevance of splitting the prioritisation of human toxicity into two separate pathways via groundwater and soil. In paragraph 5.3.4 the prioritisation based on the human exposure and toxicity is shown for the three countries.

5.2.3.2 Human toxicity

The HBGVs for human toxicity were determined using the smiles/CAS-number in the OECD QSAR Toolbox (see section 4.3.4.2). It was possible to derive a HBGV for all pilot substances. Contrary to the exposure calculations, HBGV is solely substance dependant and can be used for all countries. Table 49 provides the HBGV for all the pilot substances. The HBGV range from 0.0025 to 9 ug/kg bw/day (3.5 orders of magnitude).

Table 48: HBGV derived through the OECD QSAR Toolbox using the procedure described in section 4.3.4.2.

Substance	**HBGV (TTC)** [ug/kg bw/day]
Glyphosate	0.025
Imidacloprid	0.025
S-Metolachlor	0.025
Metolachlor ESA	0.025
Metolachlor OXA	0.025
PFOA	1.5
PFOS	1.5
GenX	0.0025
PFBA	1.5
PFHxA	1.5
PFHxS	1.5
N-EtFOSAA	0.0025
Diclofenac	1.5
Triclosan	0.0025
Clarithromycin	0.0025
Azithromycin	0.0025
4-Nonylphenol	9
Bisphenol A	1.5

The TTC methodology is a generic method that is, in most cases, a worst-case assessment of the potential toxicity of a substance. However, when compared to measured toxicity data (when available), the TTC methodology may not always lead to a lower HBGV. For example for PFAS the EFSA, using a new methodology based on epidemiological endpoints, lowered the HBGV for PFOS to 4.4 ng/kg bw/week, which translates to 0.00063 µg/kg bw/day. This is four times lower than the most conservative TTC value of 0.0025 µg/kg bw/day assigned to GenX, and differs even more greatly for the other PFAS pilot substances. Nonetheless, the TTC methodology merely provides a first step in the assessment of toxicity, substances may still be more accurately prioritised for tier 2. Inherent to a generic methodology like the TTC approach is that in some cases the worst-case criteria are not met, but it largely provides valid grounds for prioritisation.

5.2.4 Direct ecotoxicity

The direct ecotoxicity of the pilot substances was assessed using ECOSAR 2.0 as described in section 4.3.5. ECOSAR accepts both SMILES and CAS numbers as input. However, the program automatically checks the provided SMILES against its internal database and includes multiple variations (different counter ion or different charge) of the substance into the assessment. This can lead to unexpected results. Therefore, the determination was undertaken first using CAS number. For substances for which there was no output, ECOSAR was run using the SMILES (see Annex L). Table 50 provides the $PNEC_{direct}$ derived for the pilot substances. The estimated ecotoxicity ranges from 5.6E-03 up to 4.96E+05 µg/l (8 orders of magnitude).

Table 49: $PNEC_{direct}$ ecotoxicity derived using ECOSAR 2.0

Substance	**$PNEC_{direct}$** [µg/L]
Glyphosate	4.96E+05
Imidacloprid	2.81E+00
S-Metolachlor	4.40E-03
Metolachlor ESA	1.74E+02
Metolachlor OXA	2.45E+02
PFOA	1.43E+00
PFOS	4.15E+00
GenX	6.06E+01
PFBA	5.97E+02
PFHxA	4.23E+01
PFHxS	1.30E+02
N-EtFOSAA	4.24E-01
Diclofenac	9.10E+00
Triclosan	5.70E-02
Clarithromycin	2.08E+00
Azithromycin	1.87E+00
4-Nonylphenol	5.60E-03
Bisphenol A	1.28E+00

5.2.5 Secondary poisoning

The $PNEC_{secpois}$ for the pilot substances were derived using the methodology described in section 4.3.6. The risks associated with secondary poisoning are assessed using the most critical of two RCR, namely the RCR for consumption of worms, or the consumption of plants. Therefore, the $PNEC_{secpois}$ is calculated for both plants and worms and the PEC used from the Fate module must be transformed into a PEC in worms or plants (see paragraph 4.3.6.3). Since the PEC is dependent on environmental concentration from the Fate module, different PEC values are derived for each country. It was possible to calculate a $PNEC_{secpois}$ for all pilot substances.

Table 51, Table 52 and Table 53 provide both the PEC and the $PNEC_{secpois}$ in earthworms and plants for the pilot substances per country. The $PNEC_{secpois}$, worm and $PNEC_{secpois}$, leaf both range almost 3 orders of magnitude.

Table 50: PEC and $PNEC_{secpois}$ for France.

Substance	PEC-worm	PNEC-worm	PEC-leaves	PNEC-leaf
Glyphosate	4.74E+01	2.43E-01	6.91E+03	2.50E-01
Imidacloprid	9.56E-01	2.43E-01	1.67E+03	2.50E-01
S-Metolachlor	1.54E+01	2.43E-01	2.58E+00	2.50E-01
Metolachlor ESA	9.33E+00	2.43E-01	4.95E+04	2.50E-01
Metolachlor OXA	5.03E+00	2.43E-01	1.55E+03	2.50E-01
PFOA	4.52E-02	1.46E+01	3.19E-10	1.50E+01
PFOS	6.30E-02	1.46E+01	4.71E-05	1.50E+01
GenX	2.65E-02	2.43E-02	3.08E-10	2.50E-02
PFBA	5.76E-04	1.46E+01	2.11E-09	1.50E+01
PFHxA	1.10E-04	1.46E+01	9.21E-01	1.50E+01
PFHxS	9.25E-03	1.46E+01	2.96E+00	1.50E+01
N-EtFOSAA	3.88E+00	2.43E-02	1.50E-08	2.50E-02
4-Nonylphenol	8.50E+03	8.75E+01	6.37E-03	8.99E+01
Bisphenol A	4.50E+02	1.46E+01	2.86E+02	1.50E+01

Table 51: PEC and $PNEC_{secpois}$ for Belgium.

Substance	PEC-worm [ug/kg worm]	PNEC-worm [µg/kg worm]	PEC-leaves [µg/kg wwt]	PNECleaf [µg/kg wwt]
Glyphosate	8.05E+01	2.43E-01	1.17E+04	2.50E-01
Imidacloprid	3.04E+00	2.43E-01	5.30E+03	2.50E-01
S-Metolachlor	1.75E+01	2.43E-01	2.93E+00	2.50E-01
Metolachlor ESA	1.04E+01	2.43E-01	5.50E+04	2.50E-01
Metolachlor OXA	5.59E+00	2.43E-01	1.73E+03	2.50E-01
PFOA	2.27E-01	1.46E+01	1.60E-09	1.50E+01
PFOS	2.80E-01	1.46E+01	2.09E-04	1.50E+01
GenX	1.33E-01	2.43E-02	1.55E-09	2.50E-02
PFBA	2.89E-03	1.46E+01	1.06E-08	1.50E+01
PFHxA	4.20E-04	1.46E+01	3.53E+00	1.50E+01
PFHxS	3.51E-02	1.46E+01	1.12E+01	1.50E+01
N-EtFOSAA	1.95E+01	2.43E-02	7.53E-08	2.50E-02
4-Nonylphenol	4.26E+04	8.75E+01	3.20E-02	8.99E+01
Bisphenol A	2.04E+03	1.46E+01	1.29E+03	1.50E+01

Table 52: PEC and $PNEC_{secpois}$ for the Netherlands

Substance	PEC-worm [µg/kg worm]	PNEC-worm [µg/kg worm	PEC-leaves [µg/kg wwt]	PNECleaf [µg/kg wwt]
Glyphosate	2.56E+01	2.43E-01	3.73E+03	2.50E-01
Imidacloprid	3.22E-01	2.43E-01	5.62E+02	2.50E-01
S-Metolachlor	2.01E+01	2.43E-01	3.37E+00	2.50E-01
Metolachlor ESA	1.20E+01	2.43E-01	6.38E+04	2.50E-01
Metolachlor OXA	6.48E+00	2.43E-01	2.00E+03	2.50E-01
PFOA	1.74E-01	1.46E+01	1.23E-09	1.50E+01
PFOS	2.21E-01	1.46E+01	1.66E-04	1.50E+01
GenX	1.02E-01	2.43E-02	1.18E-09	2.50E-02
PFBA	2.22E-03	1.46E+01	8.13E-09	1.50E+01
PFHxA	3.57E-04	1.46E+01	3.00E+00	1.50E+01
PFHxS	2.99E-02	1.46E+01	9.59E+00	1.50E+01
N-EtFOSAA	1.49E+01	2.43E-02	5.77E-08	2.50E-02
Diclofenac	3.10E-02	1.46E+01	2.40E-02	1.50E+01
Triclosan	2.04E-02	2.43E-02	6.58E-06	2.50E-02
Clarithromycin	3.94E-02	2.43E-02	1.32E+03	2.50E-02
Azithromycin	5.41E-02	2.43E-02	1.75E+02	2.50E-02
4-Nonylphenol	3.27E+04	8.75E+01	2.45E-02	8.99E+01
Bisphenol A	1.61E+03	1.46E+01	1.02E+03	1.50E+01

As can be seen in the tables, both the $PNEC_{secpois\text{-}worm}$ and the $PNEC_{secpois\text{-}leaf}$ follow a pattern comparable to the 5 increments between the TTC values. This is expected as the only variable in the $PNEC_{secpois}$ are these TTC values. For the $PEC_{secpois}$ however, substance properties and the soil, porewater, and air concentrations do play a role. Moreover, the difference in the order of magnitude between the minimum and maximum PEC values for leaves is greater than for PEC values for worms. The calculation for $PEC_{secpois\text{-}leaf}$ makes use of multiple substance properties (i.e. solubility, K_{ow}, Vapour pressure) whereas for $PEC_{secpois\text{-}worm}$ only the K_{ow} is used.

5.3 Results Prioritisation (RCR)

Based on the results of the different Toxicity modules and the Fate module a prioritisation was made for the pilot substances. Per country, for each of the four receptors a separate prioritisation was made, namely for Direct ecotoxicity, Secondary poisoning, and human toxicity separated into direct consumption of groundwater and ingestion of soil and crops. For this chapter only the prioritisation for The Netherlands is shown as for this country, concentrations for the most pilot substances were calculated in the Fate module. Any differences in prioritisation between the countries will be due to differences in the results of the Fate module (see section 5.1). The prioritisations for Belgium and France can be found in section 5.3.4. Note, the figures in the following paragraphs are in log-scale. The results on prioritisation are then discussed.

5.3.1 Prioritisation human toxicity

5.3.1.1 Human toxicity – Consumption of groundwater

Table 54 and Figure 22 show the prioritisation for the pilot substances for the human toxicity through direct consumption of groundwater (see 4.3.4.1). Similar to secondary poisoning the pesticides are at the top of the prioritisation list. This is due to a combination of high environmental concentrations from the Fate section, as well as the sharpest TTC value of 0.0025 µg/kg bw/day.

Table 53: Prioritisation for human health – consumption groundwater for pilot substances in the Netherlands. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Prio	Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
1	Glyphosate	1.94E+03				
2	Metolachlor ESA	7.52E+02				
3	Metolachlor OXA	1.68E+02				
4	S-Metolachlor	6.80E+01				
5	Imidacloprid	2.33E+01				
6	Bisphenol A	4.20E+00			x	x
7	Clarithromycin	1.33E-01				
8	Azithromycin	9.04E-02				
9	4-Nonylphenol	4.41E-02			x	x
10	N-EtFOSAA	3.50E-03				
11	GenX	2.05E-03	x	x		
12	Triclosan	1.13E-03	x	x		
13	PFHxS	5.09E-05	x	x	x	
14	PFBA	3.93E-05	x	x	x	
15	Diclofenac	1.41E-05				
16	PFHxA	5.09E-06	x	x	x	
17	PFOS	3.26E-06	x	x	x	
18	PFOA	3.15E-06	x	x	x	

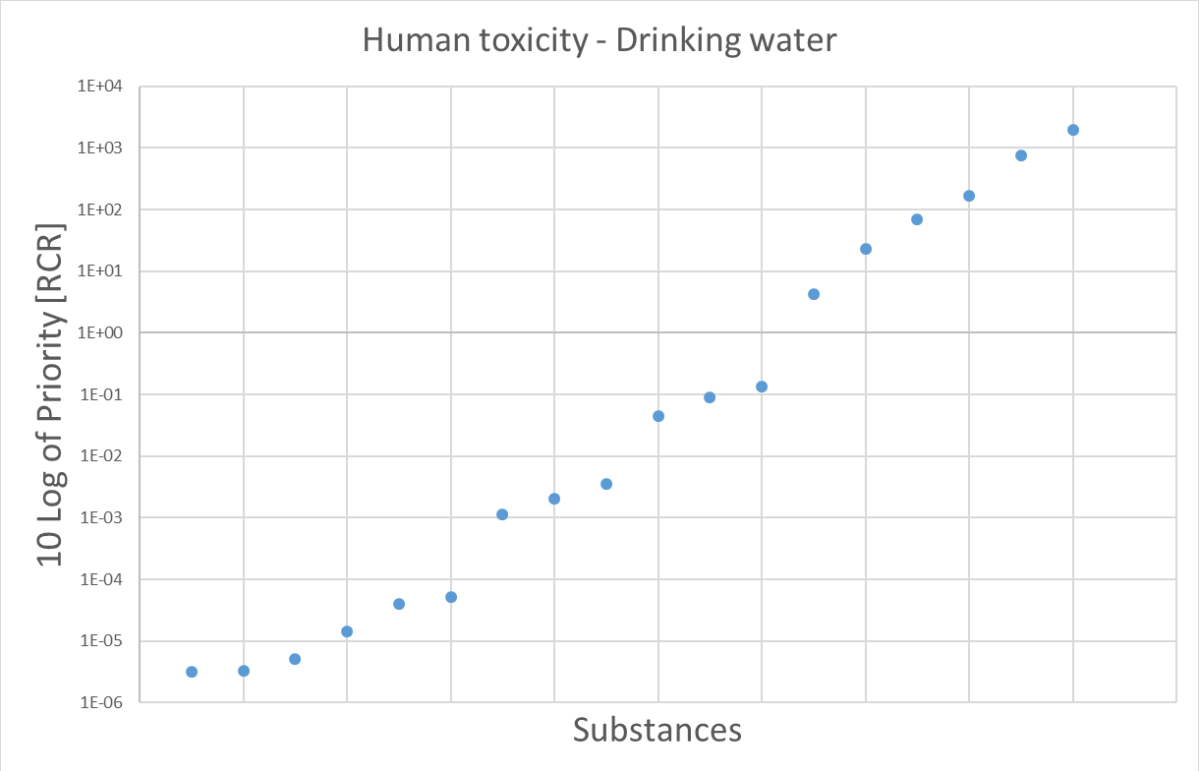


Figure 22 : Graph depicting the prioritisation for human toxicity – groundwater consumption for the Netherlands. The substances are sorted to show the highest (1) priority listed in on the right. The log-scale of the graph shows the trend of the prioritisation.

5.3.1.2 Human toxicity – Ingestion of soil and crops

Table 55 and Figure 23 show the prioritisation for the pilot substances for the human toxicity through ingestion of soil and crops. As for consumption of ground water and secondary poisoning the pesticides are on top of the prioritisation due to the sharp TTC value and high concentrations from the Fate module. The order of substances differs from the groundwater consumption pathway due to differences in exposure calculations.

Table 54: Prioritisation for human health – ingestion of soil and crops for pilot substances in the Netherlands. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Prio	Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
1	Metolachlor ESA	4.37E+05				
2	Glyphosate	2.56E+04				
3	Metolachlor OXA	1.37E+04				
4	Clarithromycin	9.09E+03				
5	Imidacloprid	3.86E+03				
6	Azithromycin	1.20E+03				
7	S-Metolachlor	2.31E+01				
8	Bisphenol A	1.17E+01			x	x
9	PFHxS	1.10E-01	x	x	x	
10	PFHxA	3.43E-02	x	x	x	
11	Diclofenac	2.75E-04				
12	4-Nonylphenol	4.66E-05			x	x
13	Triclosan	4.51E-05	x	x		
14	PFOS	1.89E-06	x	x	x	
15	N-EtFOSAA	3.95E-07				
16	GenX	8.12E-09	x	x		
17	PFBA	9.29E-11	x	x	x	
18	PFOA	1.40E-11	x	x	x	

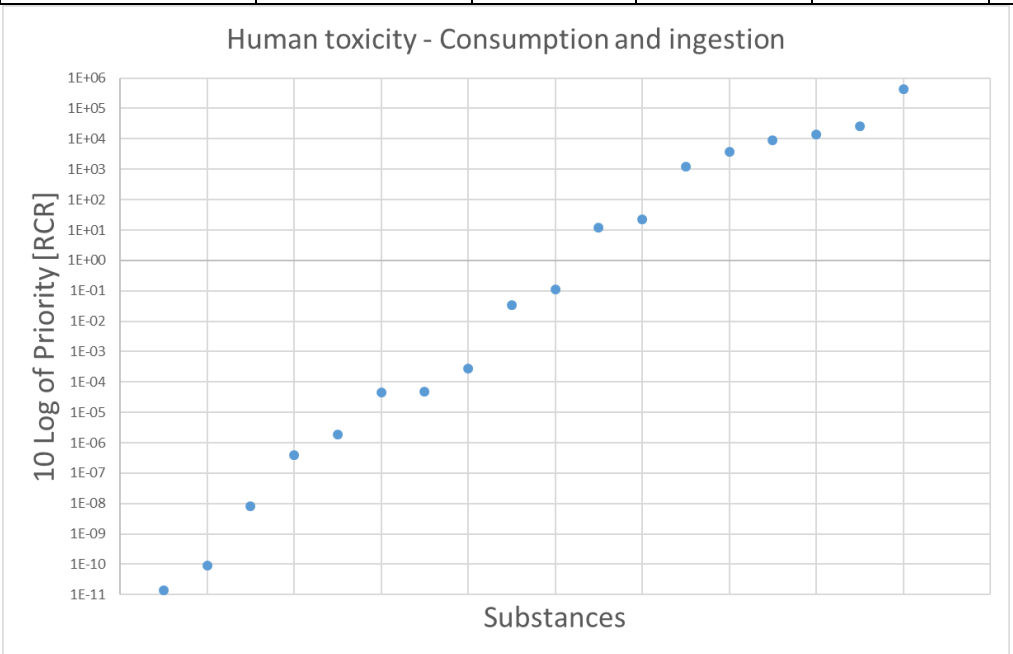


Figure 23 : Graph depicting the prioritisation for human toxicity ingestion of soil and crops for the Netherlands. The substances are sorted to show the highest priority (1) listed in Table 58on the right. The log-scale of the graph shows the trend of the prioritisation.

5.3.2 Prioritisation direct ecotoxicity

Table 56 and Figure 24 show the results of the prioritisation for direct ecotoxicity. The substances are prioritised from high to low RCR. Note, Figure 24 is on a log-scale with the highest prioritised substance at the far right. From the prioritisation figure and table can be seen that two substances (4-nonylphenol and S-metolachlor) are grouped together, with the next three substances having an RCR of 3 orders of magnitude lower.

Table 55: Prioritisation of direct ecotoxicity for the Netherlands. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Prio	Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
1	4-Nonylphenol	4.97E+02			x	x
2	S-Metolachlor	2.71E+02				
3	Bisphenol A	3.44E+01			x	x
4	Imidacloprid	1.45E-01				
5	Metolachlor ESA	7.57E-02				
6	Metolachlor OXA	1.20E-02				
7	Clarithromycin	1.12E-03				
8	Azithromycin	8.46E-04				
9	Triclosan	3.46E-04	x	x		
10	N-EtFOSAA	1.44E-04				
11	Glyphosate	6.84E-05				
12	PFOA	2.31E-05	x	x	x	
13	Diclofenac	1.63E-05				
14	PFOS	8.25E-06	x	x	x	
15	PFHxS	4.12E-06	x	x	x	
16	PFHxA	1.26E-06	x	x	x	
17	PFBA	6.90E-07	x	x	x	
18	GenX	5.93E-07	x	x		

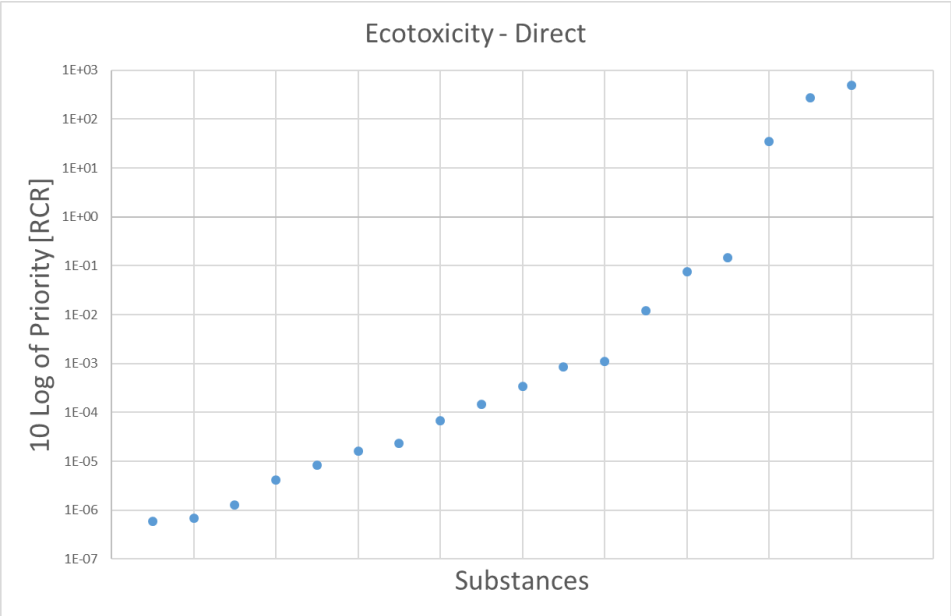


Figure 24 : Graph depicting the prioritisation for direct ecotoxicity for the Netherlands. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

5.3.3 Prioritisation secondary poisoning

Table 57 and Figure 25 show the prioritisation for the pilot substances for secondary poisoning. Compared to direct ecotoxicity, no distinct grouping in the RCR-score of the pilot substances can be identified. Nonetheless, the figure and table do show a large difference in RCR score between the pilot substances. The top 4 substances are pesticides, which is unsurprising as pesticides are expected to be toxic for organisms in the food chain. Additionally, these substances do not have any hazard labels assigned, meaning they are not similar to any substance on the ZZS-list.

Table 56: Prioritisation for secondary poisoning for pilot substances in the Netherlands. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Prio	Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
1	Metolachlor ESA	2.55E+06				
2	Glyphosate	1.49E+05				
3	Metolachlor OXA	8.02E+04				
4	Clarithromycin	5.31E+04				
5	Imidacloprid	2.25E+04				
6	Azithromycin	7.02E+03				
7	S-Metolachlor	8.27E+02				
8	N-EtFOSAA	6.13E+02				
9	4-Nonylphenol	3.73E+02			x	x
10	Bisphenol A	1.11E+02			x	x
11	GenX	4.19E+00	x	x		
12	Triclosan	8.38E-01	x	x		
13	PFHxS	6.40E-01	x	x	x	
14	PFHxA	2.00E-01	x	x	x	
15	PFOS	1.52E-02	x	x	x	
16	PFOA	1.19E-02	x	x	x	
17	Diclofenac	2.13E-03				
18	PFBA	1.52E-04	x	x	x	

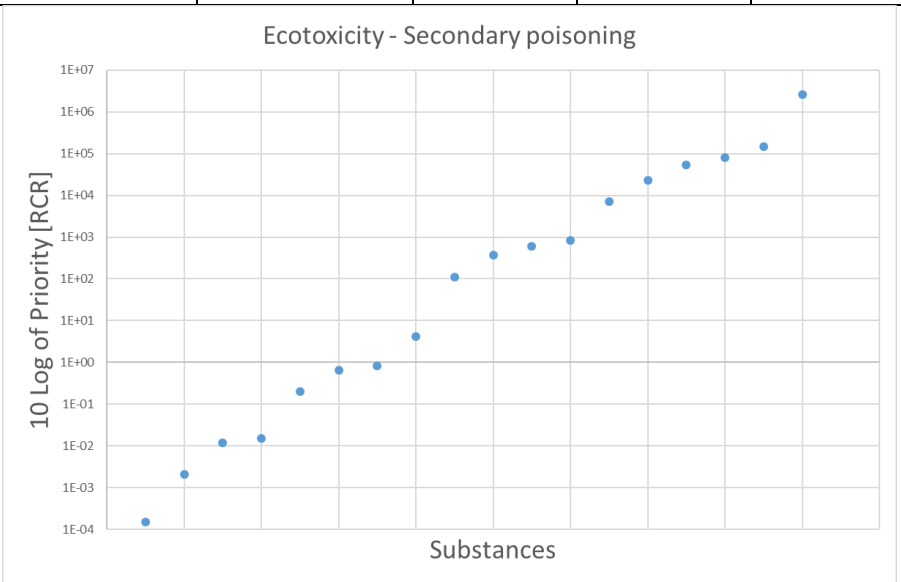


Figure 25 : Graph depicting the prioritisation for secondary poisoning for the Netherlands. The substances are sorted to show the highest (1) priority listed in Table 58 on the right. The log-scale of the graph shows the trend of the prioritisation.

5.3.4 Ranking of substances in prioritisation

Table 58 shows the results of the four prioritisations side by side. Table 59 shows the ranking in the four prioritisations for each substance. All results are based on the fate estimations for the Netherlands, because all example compounds were calculated.

Figure 26 to Figure 29 show for the four endpoints the prioritisations of the Netherlands, Belgium and France in one graph. The substances referred to in the labels can be found in Table 60.

Table 57: Table showing the ranking of substances in the four prioritisations side by side. Industrial chemicals are in blue, pesticides in green, pharmaceuticals in red and PFAS in purple

Priority	Eco-direct	Eco-secpois	Human-drink	human-ingestion
1	4-Nonylphenol	Metolachlor ESA	Glyphosate	Metolachlor ESA
2	S-Metolachlor	Glyphosate	Metolachlor ESA	Glyphosate
3	Bisphenol A	Metolachlor OXA	Metolachlor OXA	Metolachlor OXA
4	Imidacloprid	Clarithromycin	S-Metolachlor	Clarithromycin
5	Metolachlor ESA	Imidacloprid	Imidacloprid	Imidacloprid
6	Metolachlor OXA	Azithromycin	Bisphenol A	Azithromycin
7	Clarithromycin	S-Metolachlor	Clarithromycin	S-Metolachlor
8	Azithromycin	N-EtFOSAA	Azithromycin	Bisphenol A
9	Triclosan	4-Nonylphenol	4-Nonylphenol	PFHxS
10	N-EtFOSAA	Bisphenol A	N-EtFOSAA	PFHxA
11	Glyphosate	GenX	GenX	Diclofenac
12	PFOA	Triclosan	Triclosan	4-Nonylphenol
13	Diclofenac	PFHxS	PFHxS	Triclosan
14	PFOS	PFHxA	PFBA	PFOS
15	PFHxS	PFOS	Diclofenac	N-EtFOSAA
16	PFHxA	PFOA	PFHxA	GenX
17	PFBA	Diclofenac	PFOS	PFBA
18	GenX	PFBA	PFOA	PFOA

Table 58 : Overview of the substance ranking in each of the four prioritisations, including the number of labels assigned using the ZZS similarity tool.

Substance	No. of labels	eco-direct	eco-secpois	Human-drink	Human-ing
4-Nonylphenol	2	1	9	9	12
S-Metolachlor		2	7	4	7
Bisphenol A	2	3	10	6	8
Imidacloprid		4	5	5	5
Metolachlor ESA		5	1	2	1
Metolachlor OXA		6	3	3	3
Clarithromycin		7	4	7	4
Azithromycin		8	6	8	6
Triclosan	2	9	12	12	13
N-EtFOSAA		10	8	10	15
Glyphosate		11	2	1	2
PFOA	3	12	16	18	18
Diclofenac		13	17	15	11
PFOS	3	14	15	17	14
PFHxS	3	15	13	13	9
PFHxA	3	16	14	16	10
PFBA	3	17	18	14	17
GenX	2	18	11	11	16

Table 59 : Substance labels used in the comparison of prioritisations between countries.

Code	Substance
s 1	Glyphosate
s 2	Imidacloprid
s 3	S-Metolachlor
s 4	Metolachlor ESA
s 5	Metolachlor OXA
s 6	PFOA
s 7	PFOS
s 8	GenX
s 9	PFBA
s 10	PFHxA
s 11	PFHxS
s 12	N-EtFOSAA
s 17	4-Nonylphenol
s 18	Bisphenol A

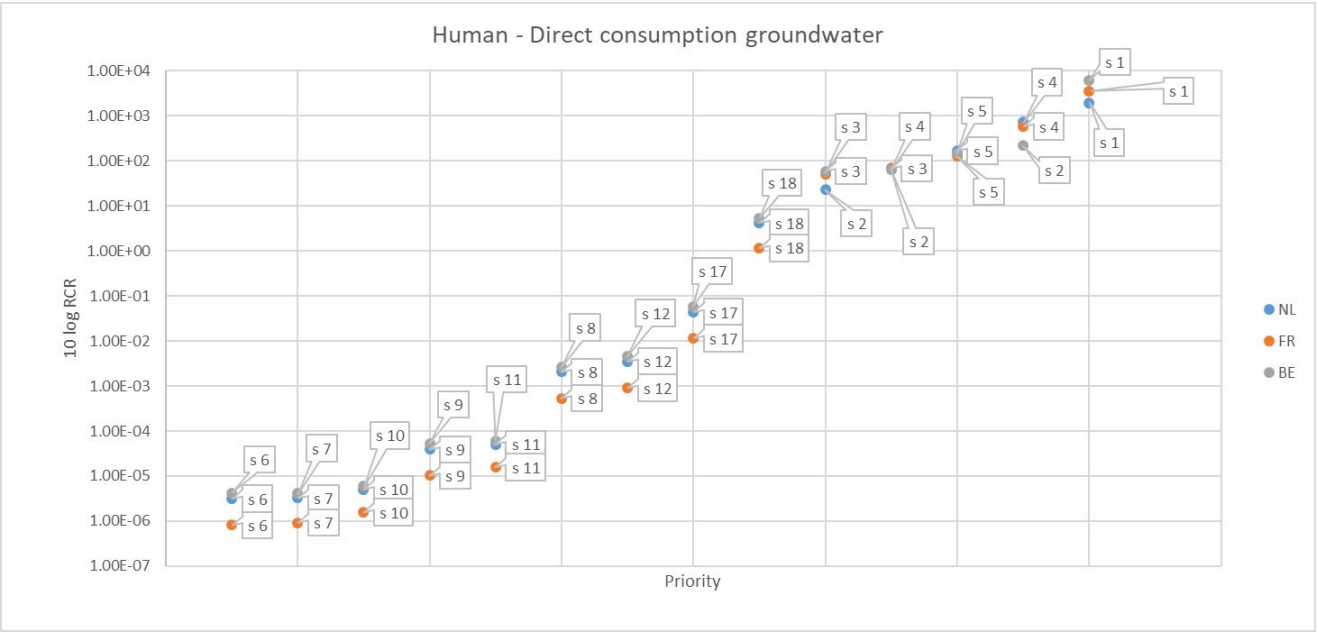


Figure 26 : RCRs for Human toxicity – Direct consumption groundwater for all three countries.

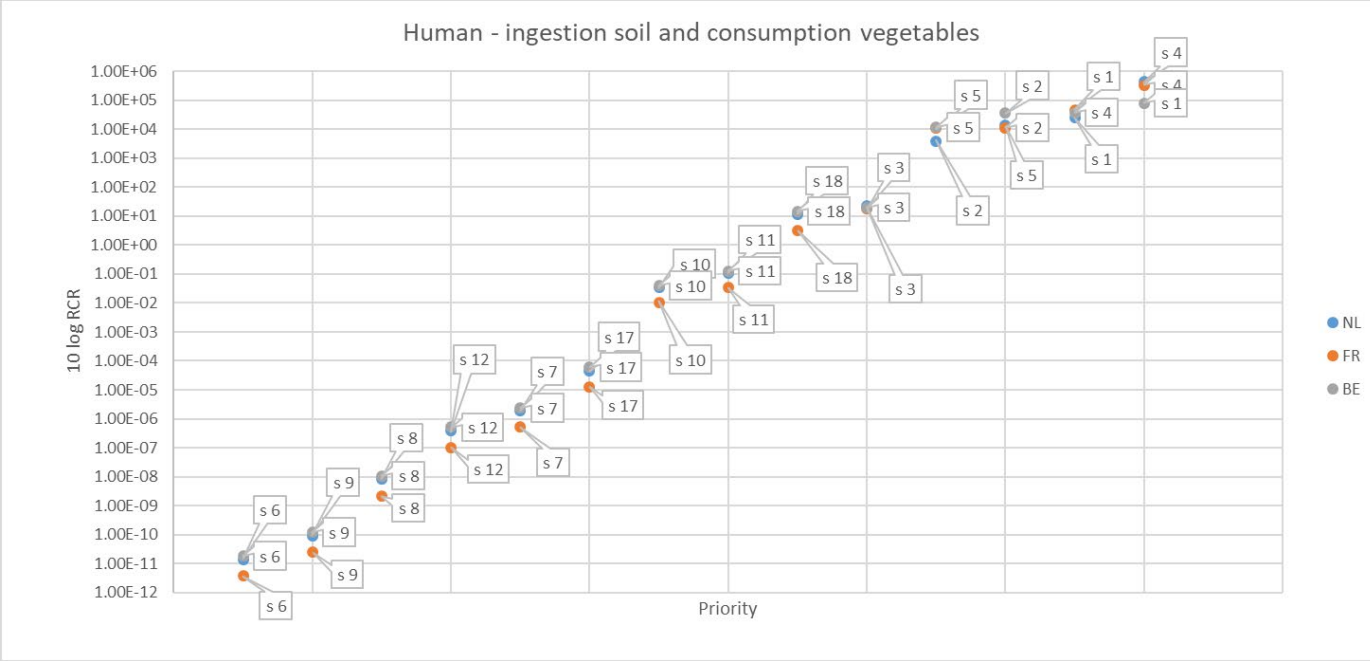


Figure 27 : RCRs for Human toxicity ingestion of soil and consumption of vegetables for all three countries.

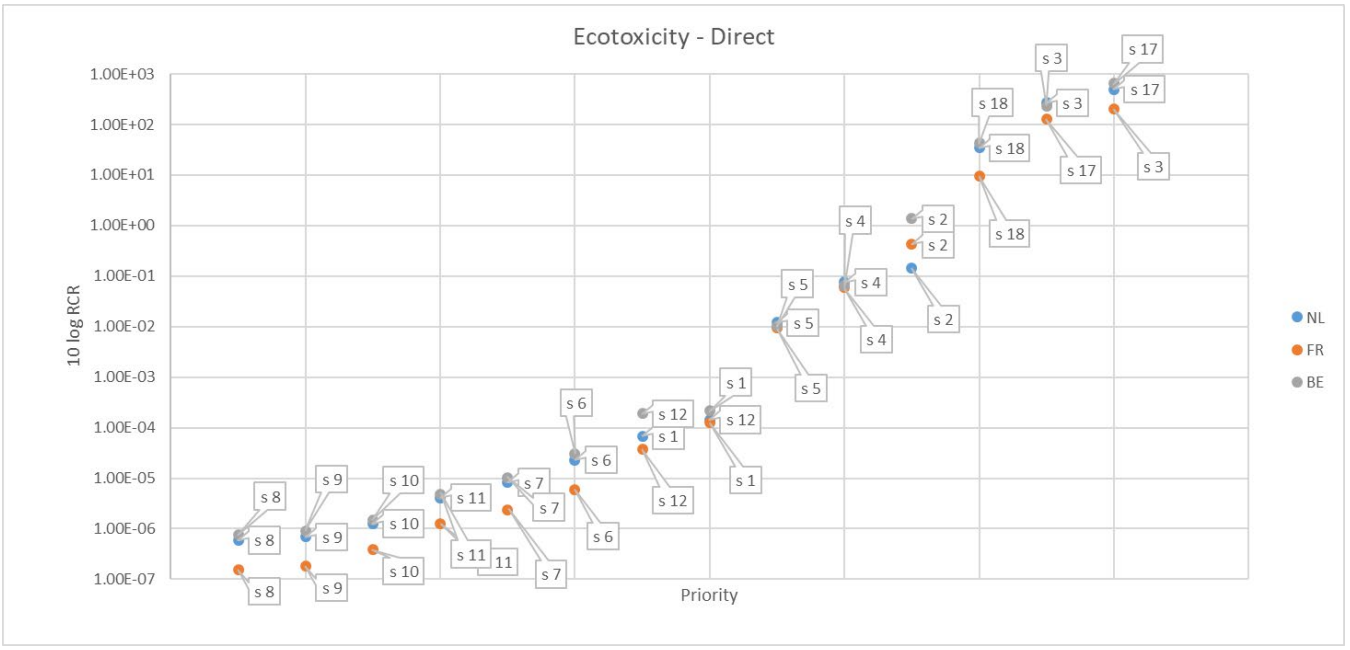


Figure 28 : RCRs for direct toxicity for all three countries.

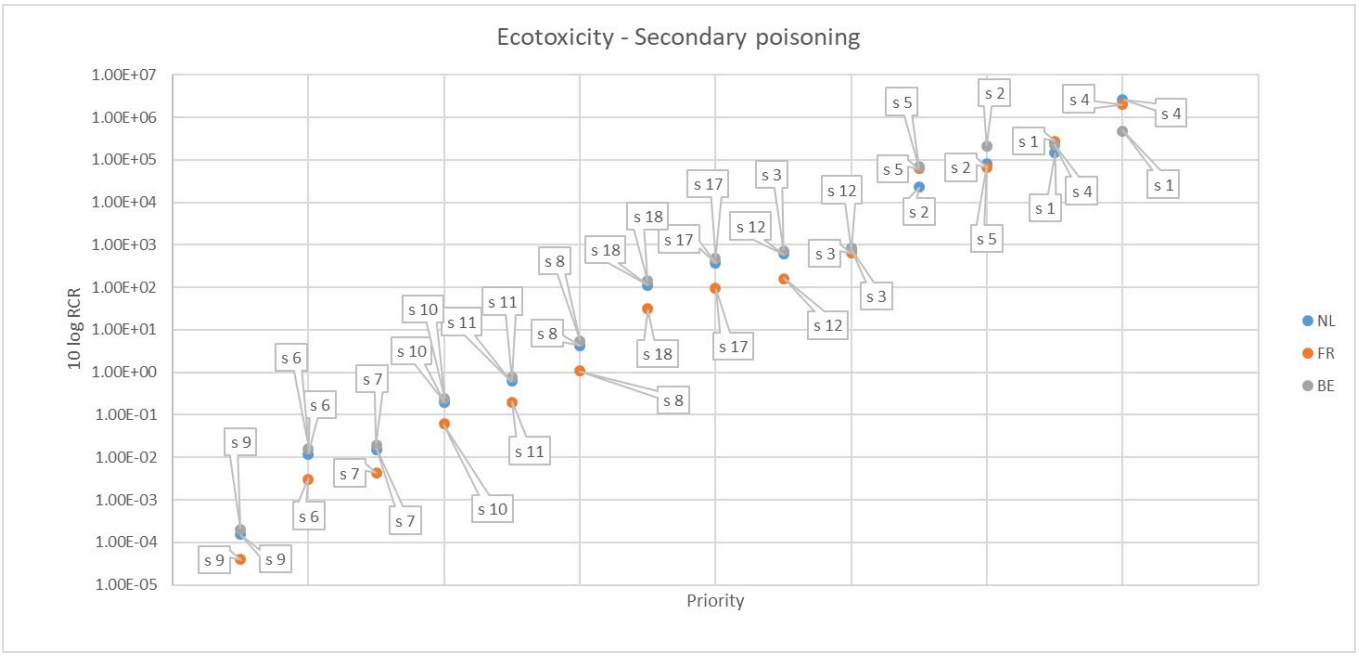


Figure 29 : RCRs for secondary poisoning for all three countries.

5.4 Discussion and Conclusion

5.4.1 Estimation of fate

The first tier in the fate approach includes a number of steps. First of all, the emissions to soil, water and air have to be estimated. The emission to the soils is the most important for this purpose, but emissions to air can be relevant as an indirect source. The estimated load is most reliable for pesticides. The use is well registered, and most of the pesticides are emitted to soils. Also the use of pharmaceuticals is well-known in many countries. The assumption that fixed part of 12% will leave the body can be improved my making this percentage substance specific. The application of sewage sludge is the only indirect source to soils included in the PREMISS prototype tool. The pilot was calculated for the Netherlands, where no sewage sludge is applied to soils. For other countries, information about the percentage of sewage sludge applied to soils is needed. REACH-regulated industrial chemicals are the most difficult compounds to estimate the emissions. The production volumes within the EU are registered in categories (0.1-1 tonnes/year, 1-10, etc.). However, losses to the environment can occur in the whole chain, from production of the substance, via use in (end) products, consumer use, to recycling and waste disposal. The variety in uses is very large. Some industrial chemicals are only used as intermediate, other chemicals are used in many end products. Several attempts to distinguish various groups of chemicals with specific pathways failed. Due to the lack of alternatives, a fixed distribution to surface water, soil and air was used. This is something to improve.

SimpleBox is a steady state model calculating the stable concentration after long-term exposure. Temporal trends (e.g. historic higher emission volumes are not included due to restrictions) and incidental spills cannot be simulated using SimpleBox. The model includes a lot of parameters. Chapter 5.1 focuses on the uncertainty of the various model parameters, such as chemical properties, and landscape characteristics. These landscape characteristics do not have a large uncertainty, but the number of categories is limited, i.e. only natural soil, agricultural soil, and urban/industrial soil are distinguished. The model does not include more specific agricultural sectors. It makes sense to work with long-term load (kg/m^2/y) instead of total amounts distributed over all agricultural soils. This is particularly the case for pesticides, because they are related to specific crops, but it is also relevant if the contaminants are applied to the soil via soil amendments such as sewage sludge, dredged sediments or (organic) fertilisers. That is why we developed a tier 2 which is focused on the specific emissions to soils.

Figure 30 shows that the resulting soil concentrations for all compounds in all countries range from 0.07 ng/kg to 7 mg/kg. Most of the compounds have a concentration of 0.003 to 10 µg/kg (a factor of 3000 difference). There is not direct correlation between calculated concentrations in soils and emission to soil, the log Kow, or the data source of the emissions. Soil concentrations seem to be the result of combined model parameters. The differences between countries are limited compared to the total range.

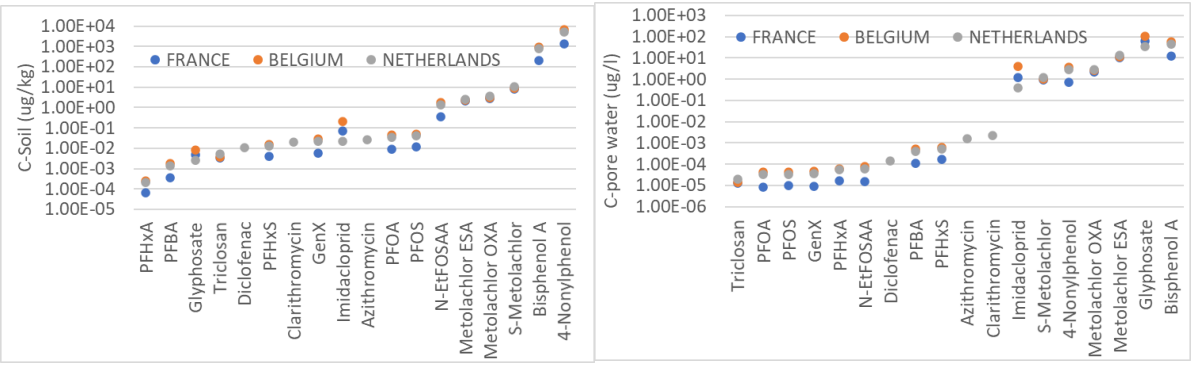


Figure 30 : Calculated soil concentrations (left) and pore water concentrations (right) for all substances in the pilot.

The calculated pore water concentrations show another picture. Most of the compounds have a concentration of 10^{-5} to 10^{-3} µg/l, whereas the five plant protection products and the two alkyl phenols have a concentration ranging from 1 to 60 µg/l. The main reason is the amount of the emissions.

Some specific observations:

- The high concentrations of the alkyl phenols and the three Metolachlor compounds correlate to high emission and an average Kow, whereas the very low Kow of Glyphosate results in a low concentration in soil despite a high emission.
- Most PFAS-compounds, and particularly PFHxA, PFBA and PFHxS, show low concentrations in soils. This is remarkable for PFHxS and PFBA, because they had (together with N-EtFOSAA) a ten times higher production tonnage compared to other PFAS. The low Kow is probably the main reason for low concentration in soils. The porewater concentrations of these PFAS are higher than the PFAS with low production tonnages (GenX, PFOS, PFOA).
- The calculated concentrations in France (except for imidacloprid) are generally a bit lower than in Belgium and the Netherlands. This might be an effect of landscape parameters (size of the country).

The 2nd tier comprises the calculation of losses to soil via soils amendments. This approach requires data on added amounts to the soil and on concentrations in soils amendments. Both type of data is difficult to obtain on a large scale. It might be better to run realistic scenarios based on practical cases. In such cases, amounts per surface unit (kg/m²/y) can be derived. This can be extrapolated to derive realistic input values in the model.

Within this project, contaminant concentrations in dredged sediments, sewage sludge, compost, digestate and manure had been collected giving a first insight in contaminant concentrations in soil amendments. An advanced search for more data (particularly with respect to manure) and a more comprehensive analysis of available data will result in a more complete and more reliable overview. A monitoring program might solve the remaining gaps in the data. The Netherlands is currently working on a program to monitor CEC in soil and sediments, but other soil amendments are out the scope of this monitoring program. Due to the amounts of manure that are used on agricultural land, we recommend putting more efforts in finding contaminant concentrations in manure. The European fertilizer regulation will apply soon but involves no CEC. The Walloon Region is identifying the fertilizers and their potential contamination with pollutants not included in the regulation in order to be able to limit flows considered problematic. A study of CEC in fertilizers is therefore carried out. A monitoring of the flow of fertilizers must also be implemented.

5.4.2 Estimation Toxicity

The approach on the estimation of toxicity is set up in such a way that many different substances can be assessed. For all pilot substances, it was possible to derive a toxicity value (HBGV, PNEC) using the prototype. Additionally, the methodology can be scaled up to a larger number of substances. However, due to the generic approach, a number of uncertainties are present which may influence the results:

- The hazard labels are currently assigned using the ZZS similarity tool, labelling whether a substance is an SVHC or similar to an SVHC. However, when a substance is not similar to any substance on this SVHC list, the label is not assigned even when based on substance properties a hazard label may be warranted. Therefore, future versions of the prototype can use rules based on substance properties to assign hazard labels, while also using the ZZS similarity tool to label substances as 'similar to ZZS' more widely accepted terminology could be "similar to SVHC".
- Human exposure due to ingestion of soil and crops depends on substance properties and the results from the Fate module. Any uncertainties in input data (like emissions and substance properties) will add to the uncertainty of the exposure calculation. An uncertainty analysis would be needed to know if there is a linear relation or not and which parameters have the highest influence on the outcome. Just like for fate the emission level and the $\log k_{ow}$ are important parameters. Additionally, soil-plant relations using the BCF method of EUSES were initially developed for non-ionic substances. The BCF for highly soluble substances may therefore be more uncertain. When available, future developments in modelling soil-plant relations for dissociating substances could be implemented in the prototype.
- Looking specifically at PFOS we know from additional information that the human toxicity is higher than currently estimated with the TTC-approach. This shows that there can be exceptions, in this case due to the exceptional substance properties of PFAS and the more sensitive type of human endpoint.
- PNECs for direct ecotoxicity were calculated using ECOSAR 2.0. In future developments of the prototype integration with the Norman database could be explored to corroborate the PNECs derived using ECOSAR 2.0. However, attention has to be given to not mixing measured PNECs with QSAR-based PNECs. This also applies for mixing the TTC with evaluated HBGV and PNEC for secondary poisoning.
- Secondary poisoning, similar to human health, relies on concentrations and substance properties from the Fate module and for estimating the concentrations in food (plants and earthworms). Any uncertainties in fate input data influence the uncertainty of the PNECsecpois.
- It was found that the use of the QSAR tools (OECD toolbox and ECOSAR) requires some initial setup time for installation. However, after installation, the tools are straightforward in use and can be scaled up to assess a larger number of substances. For human health we recommend creating a scenario in the QSAR toolbox that returns the TTC as a result, removing any need for interpretation on the user's side. For ECOSAR 2.0 we recommend developing a script to return the lowest endpoint as PNEC.

5.4.3 Discussion on prioritisation

For all four receptors the prioritisation returned RCR values differing at least 9 orders of magnitude (direct ecotoxicity and human groundwater consumption, more for human ingestion and secondary poisoning). This difference is large enough for substances with a relative high RCR to be prioritised and with a low RCR to be discarded. Taking into account the effect of uncertainties in parameters, it is not expected that the priority will change from high to low or vice versa. This is also due to the use of worst-case assumptions limiting the impact uncertainties may have on the model outcome. Additionally, some grouping occurred in the RCR scores, notably the pesticides all received similar RCR-scores, whereas for other substance types the RCR-scores could differ multiple orders of magnitude. Within the group of pesticides with a high prioritisation it could be recommended to go to a tier 2 assessment.

The goal of the first tier prioritisation is to assess which substances require further attention in a tier 2 assessment. A clear cut-off point for which substances ought to be prioritised was however not present. Such a cut-off point may depend on other factors than the RCR itself, such as the maximum amount of substances that can be assessed in tier 2 due to time constraints. For example, a top 20 or top 100 of the substances on the prioritisation could be prioritised for tier 2. If different groups of compounds can be identified, the group with the highest RCR could be prioritised in tier 2. It is an important advice to end users (for ex. policy makers)and further discussion on this topic is required.

Figure 26 to Figure 29 show that there is no significant difference between countries. Because the estimated toxicity is the same in each country it can be concluded that differences in the fate calculations for soil and groundwater in different countries are small.

Figure 26 to Figure 29 also show that the order of magnitude in the prioritisation is much higher for the human endpoint of ‘ingestion of soil and crops’ than for ‘consumption of groundwater’. The reason is that the uptake of contaminants from soil into crops give an additional differentiation of compounds. The ranking of groundwater directly follows the estimated groundwater concentration. It also implies that the uncertainties in the prioritisation of the human intake of soil and crops will be higher. In general industrial chemicals have a high score for direct toxicity. 4-nonylphenol for example has the highest concentration in the model leading to a high priority on direct ecotoxicity and for other endpoints a mid-range. This difference can be explained by the expected low human toxicity (Cramer Class 1).

Pesticides have a relatively high priority as a group (see Table 58). This is strongly related to the high estimated concentrations in porewater (see Figure 29) and the high human and ecotoxicity of this group. For pharmaceuticals the prioritisation is more scattered.

The relatively low ranking of PFAS-compounds for all four endpoints has different reasons. First calculation of the fate leads to relatively low concentrations in soil (for PFHxA, PFBA and PFHxS because of a low logKow; GenX, PFOS, PFOA have relatively lower emission tonnage). Secondly the estimated toxicity is highest for GenX and N-EtFOSAA; the other four compounds are in Cramer-class III, a middleclass toxicity range. The recent knowledge on toxicity of PFAS is not part of tier 1; it is expected that using substance specific toxicity data (tier 2) would lead to higher RCR-scores.

Based on the uncertainty analysis of fate discussed in paragraph 6.1 (concentrations in soil and groundwater) the following parameters have a large influence on the prioritisation: logKow and the emission tonnage. Toxicity can also be an important factor, but does for these compounds not lead to a complete change in ranking when starting from the porewater concentration.

Although we did not perform an uncertainty analysis on the prioritisation (RCR) it is possible to indicate parameters that will lead to the differences in prioritisation of the four endpoints (excluding the calculated fate in soil and groundwater). For direct ecotoxicity and human toxicity to drinking water:

only the estimated toxicity is relevant for differences. Due to the methodological approach the human toxicity will be more uncertain than the direct ecotoxicity and human exposure to drinking water, because it is a conservative approach with five classes of the estimated toxicity.

For secondary poisoning and human toxicity consumption & ingestion (of soil and crops) the exposure parameters will also contribute to the uncertainty (Kow, solubility and vapour pressure), additional to uncertainties in the estimated toxicity.

6 PRIORITISATION RESULTS DISCUSSION

6.1 Sensitivity analysis

6.1.1 Fate module

The input parameters of the simple box model are of types: molecule properties and source and site settings.

For all these parameters, an input value is required, except for the degradation rates, as these values are currently set to zero in the prototype.

The sensitivity calculations were performed with diclofenac as example. The sensitivity analysis included variation of individual of substances property or one parameter of source and site settings, as described below:

- logKow: +1, +2, +3, -1, -2, -3
- vapour pressure (Pa): /10, /100, *10, *100
- solubility (mol/m3): +0.005, -0.005
- molecular weight (g/mol): +100, +200, -100, -200
- melting point (K): +100, +200, -100, -200

Regarding sources and site settings, emissions were varied by a factor 10, 100, 0.1 and 0.01 (pharmaceutical pathway). Emission pathways were varied by also using different pathways as input: the REACH pathway and the pesticide pathway. Landscape settings were varied by using Dutch, French and Belgium settings. Soil degradation was varied by using the default degradation rate, default degradation rate/10 and degradation rate*10.

As a result of the sensitivity tests, the following parameters seem to have the biggest impact on the output:

- Emission: output concentration in soil varies with a factor 0.01-100 (one on one relation)
- logKow: output concentration in soil varies with a factor 0.004-40 based on the logKow
- Degradation rate: output concentration in soil varies with a factor 0.13-0.0015 (current calculations therefore really are a worst case, as by including a degradation rate the concentration will always decrease)
- Pathways
- Landscape settings

The following parameters seem to have little impact on the output:

- Vapour pressure: vapour pressure of *100 influences the output concentration in soil by a factor 0.5
- Molecular weight
- Solubility
- Temperature

These results highlight the **strong impact of the emission parameter** that drives a lot the resulting soil concentrations. However, this data is often difficult to estimate, especially at regional and national

scales.

6.1.2 Toxicological and RCR module

Although we did not perform uncertainties analysis on the prioritisation we can indicate some major principles.

For direct ecotoxicity and human exposure to drinking water, as the ranking directly follow the groundwater concentration, difference between measured and predicted concentration are totally transferred to RCR calculations.

For secondary poisoning and human ingestion, in addition to already considered parameter's sensibilities on the predicted soil concentrations, the physicochemical properties also play a role in the methodological approach for the calculations of soil ingestion by human and on the plant uptakes. So we can consider that the uncertainties in the RCR calculation are bigger, adding even more the intrinsic uncertainties due to the estimation of the toxicity.

6.2 Comparison of estimated (WP4) and measured CEC concentrations (WP3)

Considering the outputs of the WP3 and WP4 data of the PREMISS project a comparison of the results and a discussion on the potential impact on the final conclusion of the tool in terms of RCR and *in fine*, on the prioritisation of substances, is proposed.

Some limitations were identified in this attempt to compare the two sets of data. First of all the lack of occurrence data greatly reduces the potential for comparison. The data merged in the WP3 are, due to the low number of investigated sites, very localized, obtained on specific sites, with specific pollution, etc. For this reason, the comparison is focused on the Netherlands data for the tier 1. We have selected PFAS for the comparison, as the largest set of available data on different compartments. It was, as discussed in WP3, very difficult to select only "background data" in the available database mainly because the information "typology of associated pressure" is not available.

Secondly, through WP4 Tier 1 approach, the output is based on European emission, provided as a range of emission tonnages (low accuracy) if available. In France a robust set of information on pesticides sales within the territory is available, that could lead to opportunity for a tool validation. Nevertheless, the lack of measured data for soil hinders any comparison.

Another potential bias is the analytical factor: as monitoring is in constant evolution, some analytical quantification limits are still too high to allow a consistent comparison of data sets.

6.2.1 Case 1: PFAS in The Netherlands (Tier 1)

In this first case, we compared estimated and measured PFAS concentrations in The Netherlands. Estimated concentrations with SimpleBox in Tier 1 were based on REACH emissions data or, if not available, based on a "default" emission rate of 0.1-1 T/year (when the substance is no longer produced for instance) (see WP4 for more details).

Estimated and measured PFAS concentrations in soils and GW are compared in Table 61 and Table 62 respectively. It is important to note that "PFAS achtergrondwaarden DB" contains data relating to background as well as point source contamination. Therefore, when available, data from RIVM (2020) are preferred over PFAS achtergrondwaarden data.

Considering that an estimated range within a factor 10 of the measured concentrations range is a good estimation, PFOS concentrations in soil seem correctly estimated. Estimated PFOA and PFBA concentrations in soils seem only slightly underestimated (at least 10 times lower than the median value). Estimated N-EtFOSAA concentrations are overestimated (by a factor of 20) compared to the median concentrations found in the RIVM study (2020). Estimated GenX concentrations seem overestimated considering GenX was rarely quantified in soils (0% quantification frequency in the RIVM study, 2020, and 2% of the data in the PFAS achtergrondwaarden DB).

Table 60 : Comparison of PFAS estimated and measured concentrations in soils in The Netherlands.

Substance	CAS nr	C-Soil [µg/kg. dw]	Source of emission data	Measured cc in Soils [µg/kg dw] min – aver. – max	Source of measured data*[23]
PFOA	**335-67-1**	0.0332	Default (0.1-1T/year)	0.62 (med) – 1.81 (p95)	RIVM, 2020 (0-20 cm)
				0.1 – 1 – 380	PFAS achtergrond. DB
PFOS	**1763-23-1**	0.0407	Default (0.1-1T/year)	0,42 (med) – 1 (p95)	RIVM, 2020 (0-20 cm)
				< QL – 31 – -	PFAS achtergrond. DB
PFHxA	**307-24-4**	0.000211	Default (0.1-1T/year)	-	-
				< QL – 0.9 – -	PFAS achtergrond. DB
PFHxS	**355-46-4**	0.0131	REACH (1-10T/year)	-	-
				< QL – 0,2 – -	PFAS achtergrond. DB
PFBA	**375-22-4**	0.00133	REACH (1-10T/year)	0,07 (med) – 0,3 (p95)	RIVM, 2020 (0-20 cm)
				< QL – 2,3 – 0,4 (p95)	PFAS achtergrond. DB
N-EtFOSAA	**2991-5056**	1.39	REACH (1-10T/year)	0,07 (med)	RIVM, 2020 (0-20 cm)
				< QL	PFAS achtergrond. DB
GenX	**13252-13-6**	0.0218	Default (0.1-1T/year)	< QL	RIVM, 2020 (0-20 cm)
				< QL – 0.1 – -	PFAS achtergrond. DB

PFHxA was not measured frequently in soils (15% of the samples) with a low p95 value (0.2 µg/kg dw) which is consistent with a low estimated concentration. PFHxS was even less frequently found (5% of the samples) with a lower p95 value (<QL). Higher estimated PFHxS concentrations compared to PFHxA can be related to its higher emission rate compared to the default range and/or to its higher logKow, meaning this compound is more likely to adsorb to soil particles. Measured occurrence data show the opposite trend, meaning the default range is probably not representative of the PFHxA emission rate to the environment over the past years in The Netherlands. In any case, comparison for PFHxA and PFHxS measured concentrations is quite uncertain due to the limited number of measured data.

Even if SimpleBox follows conservative hypotheses (worst-case scenario), estimated PFAS concentrations in soils are globally lower than measured concentrations. This could be related to the chosen default emission rate which could be too low because historical emissions where higher for these persistent compounds (see Chapter 4.2).

PFAS measured concentrations in GW in The Netherlands are only reported for PFOA at present. However, RIVM published a report on groundwater background PFAS contamination (RIVM, 2021) during the redaction of this PREMISS report and some data are given below for comparison (Table 62). Estimated PFOA concentrations are very low, of the order of magnitude of 10^{-5}. Measured PFOA

[23] RIVM, 2020: data from background monitoring / PFAS achtergrondwaarden DB: data from background and contaminated sites.

concentrations in the KWR monitoring network (KWR, 2017) are also very low: amongst the 488 samples collected between 2015 and 2016, PFOA was detected in 33% of the samples with a median value below the QL.

Median values found in the last RIVM study (2021) are lower, of the order of magnitude of 10^{-3}. Except for PFHxS, which estimation is consistent with measured values in the last RIVM study, estimated concentrations for PFOA, PFOS, PFHxA and PFBA are a factor 10 to 100 lower than measured concentrations. Comparison for N-EtFOSAA and GenX is impossible due to the absence of reported data in GW in Dutch reports or DB to date.

Table 61 : Comparison of PFAS estimated and measured concentrations in groundwater in The Netherlands.

Substance	CAS nr	Estimated C-porew [µg/L]	Source of emission data	Measured cc GW [µg/l] min – aver. – max (# of samples)	Source of measured data
PFOA	**335-67-1**	$3.3.10^{-5}$	Default (0.1-1T/year)	< QL - < QL – 0.34 (488) $7.6.10^{-3}$ (med) – $4.3.10^{-2}$ (p95)	KWR Monitoring network RIVM, 2021
PFOS	**1763-23-1**	$3.42.10^{-5}$	Default (0.1-1T/year)	1.10^{-3} (med) – $1.97.10^{-2}$ (p95)	RIVM,2021
PFHxA	**307-24-4**	$5.34.10^{-5}$	Default (0.1-1T/year)	$1.8.10^{-3}$ (med) – $1.5.10^{-2}$ (p95)	RIVM,2021
PFHxS	**355-46-4**	$5.34.10^{-4}$	REACH (1-10 T/year)	6.10^{-4} (med) –7.10^{-3} (p95)	RIVM,2021
PFBA	**375-22-4**	$4.12.10^{-4}$	REACH (1-10 T/year)	$5.5.10^{-3}$ (med) – $2.1.10^{-2}$ (p95)	RIVM,2021
N-EtFOSAA	**2991-5056**	$6.12.10^{-5}$	REACH (1-10 T/year)	-	-
GenX	**13252-13-6**	$3.59.10^{-5}$	Default (0.1-1T/year)	-	-

In conclusion, in general estimated groundwater and soil concentrations are underestimated by the model compared to the measured concentrations. The most probable reason for PFAS is that the emissions are underestimated (because historical emissions are not used). This might at least be the case for PFOA, PFOS and PFHxA which have default emission. The results based on actual emissions as for PFBA and PFHxS reinforce this hypothesis as the comparison seems more reliable.

Moreover, the soil/groundwater concentrations are probably caused by long-term atmospheric deposition, whereas the emissions in the model are based on current REACH data. Another reason can be that measured concentrations are the result of local emissions.

For N-EtFOSAA and GenX, there is no monitoring data to compare estimations with.

6.2.2 Case 2: Pesticides in Belgium (Tier 2)

When looking at estimated concentrations in GW or soils using Simple Box and collected occurrence data in the same media, one could be tempted to notice differences (Table 63 and Table 64). In general, modelled concentrations in groundwater are higher than measured concentrations. On the other hand, modelled concentrations in soil are lower for imidacloprid and glyphosate than measured concentrations. This might indicate that the partition over the solid and solution phase is not calculated

correctly. Kow (or related Koc) in particular plays a crucial role to estimate soil concentrations. Degradation in the topsoil could also play a role.

Modelled concentration in groundwater and collected measured concentrations are not directly comparable because they relate to something different:

- Estimated concentrations apply to pore water. Therefore, dilution and degradation will lead to lower absolute concentrations in groundwater (at e.g. 10 m below soil surface).
- Pesticides fate modelling is based on SPF registered sales for agriculture, but does not include glyphosate used by consumers in their garden nor by public administrations on parks and other public sites. Pesticides used in households are estimated at less than 5% of the pesticide use in Belgium[24].
- SimpleBox assumes a steady state. While EC has banned several neonicotinoids in 2013, amongst which imidacloprid, this substance is still sold in Europe and in Belgium using derogation (for emergency reasons). Nevertheless, imidacloprid sales in Belgium continuously dropped over the last decade. Glyphosate sales are decreasing since 2018 following regional regulations forbidding the sale to non-professional users (June 2018 in Wallonia and October 2018 for Flanders) and forbidding the use in public spaces (June 2019 in Wallonia). SimpleBox Fate model assumes steady state whereas sales may vary considerably. In the PREMISS project, we chose to consider in the second tier of the fate modelling the average sales over the last decade (9 years in Belgium). This decision is supported by taking into account a large period of data. But the drawback is that the representativeness of this period could vary according to the substances and their respective physicochemical properties and regulation changes (for instance, a persistent substance that is banned at the beginning or at the end of the averaging period even if it has been in use for a much longer period). The way the fate model can handle historical releases of chemical substances could be improved in the next version of the model.
- Furthermore, comparison of estimated concentrations with data obtained from the same database is more reliable than a comparison over different substance groups/databases.

Nevertheless, an indicative comparison is made here to assess the relevance of the estimated concentrations for pesticides in Belgium. Estimated glyphosate concentration in GW (Table 63) are higher than measured ones (by a factor ~1000) whereas estimated soil concentrations (Table 64) are underestimated by a similar factor. This could be related with its low logKow (-3.12). Regarding imidacloprid, estimated concentrations in soils are in the same range as measured concentrations, whereas they are overestimated in GW. Estimated concentrations for metolachlor in GW are in the same range as maximum measured concentrations but higher than average concentrations with a factor 100. Comparison for metolachlor in soils is impossible due to the absence of reported data in soils in Belgian reports or DB to date.

[24] SPW, 2020 – Etat de l'Environnement wallon – Indicateurs environnementaux - http://etat.environnement.wallonie.be/home.html (consulted on the 18th of october 2021)

Table 62 : Estimated versus measured pesticides concentrations in groundwater.

Substance	CAS nr	Estimated C-porew [µg/L]	Source of emission data	Measured cc GW [µg/l] min – aver. - max	Source of measured data
Glyphosate	1071-83-6	107	national average sales in Belgium from 2011-2019[25]: 550 955 kg/y	<0.05 – 0.095 – 2.6 / - 0.001 – 0.097	SPW ESO DB BIODIEN
Imidacloprid	138261-41-3	3.85	national average sales in Belgium from 2011-2019: 19 857 kg/y	<QL - <QL - 0.02	BIODIEN
Metolachlor	87392-12-9	1.03	national average sales in Belgium from 2011-2019[26]: 77 098 kg/y * 5%	<QL – 0.011 – 3.7	SPW ESO DB
Metolachlor ESA	171118-09-5	11.4	national average sales in Belgium from 2011-2019[14]: 77 098 k/y * 73%	<QL – 0.11 – 7.1	SPW ESO DB
Metolachlor OXA	152019-73-3	2.53	national average sales in Belgium from 2011-2019[14]: 77 098 kg/y * 22%	<QL – 0.03 – 1.5	SPW ESO DB

Table 63 : Estimated versus measured pesticides concentrations in soils

Substance	CAS nr	C-Soil [µg/kg. dw]	Source emission data	Measured cc in Soils [µg/kgMS] min – aver. – max (# samples)	Source measured data
Glyphosate	1071-83-6	7.98E-03	national average sales in Belgium from 2011-2019: 550 955 kg/y	<2 – 4.9 – 100 (50)	OVAM, 2021
Imidacloprid	138261-41-3	2.15E-01	national average sales in Belgium from 2011-2019: 19 857 kg/y	0.72 – 0.84 – 0.96 (50)	OVAM, 2021
Metolachlor	87392-12-9	9.27	national average sales in Belgium from 2011-2019[27]: 77 098 kg/y * 5%	No data in soils Data in sediments from France: <QL - 5 – 478 (5 031)	-
Metolachlor ESA	171118-09-5	2.27	national average sales in Belgium from 2011-2019[15]: 77 098 k/y * 73%	No data in soils	-
Metolachlor OXA	152019-73-3	3.15	national average sales in Belgium from 2011-2019[15]: 77 098 kg/y * 22%	No data in soils	-

[25] Federal Public Service - Health, Food Chain Security Safety and Environment (Belgium)
[26] Assuming metolachlor in GW is distributed at 5% for the parent molecule, 73% for metolachlor ESA and 22% for metolachlor OXA.
[27] Assuming metolachlor in GW is distributed at 5% for the parent molecule, 73% for metolachlor ESA and 22% for metolachlor OXA.

7 MODALITIES OF USE AND LIMITATIONS

While taking into account prototype uncertainties and sensitivity described in Chapter 6.1, it is also very important to understand the current limitations of the prioritisation prototype and its modalities of use in order to ensure exploitable results.

7.1 Modalities of use

7.1.1 Importance to choose scenarios according to substance type and use

Scenario refers here to the Source – Pathway – Receptor scheme which describes how the substance may be emitted, enter the environment, migrate and reach the targeted receptor(s). In order to have a proper risk-based approach, it is crucial to select the scenario(s) that are relevant to the substance type and use.

PREMISS studied three scenarios for tier 1 or 1+2 depending on the type of substance:

- *(REACH) industrial substances pathway* using selected PFAS and Alkylphenol as pilot substances and REACH emission. The following assumptions were made on the REACH emission data: 25% of the tonnage are potentially released to the environment; this environmental emission is weighted by national activity to define national emission; the derived national emissions are assumed to partition in surface water, soil and air according to a set ratio (12%, 3% and 8.5%).
- *Waste water treatment pathway* considering that the substance enters the environment through substance consumption, and that part enters the waste water treatment system inducing sludge production and its application on agricultural land. Two tiers for fate were tested for this pathway:
    - *Tier 1:* The studied substances were pharmaceutical products for which emission data were Dutch national emission data or REACH (for triclosan). Ratio between drug consumption and volumes of sludge applied to agricultural land were calculated to evaluate the emission of the substances to soil.
    - *Tier 2:* The studied substance was PFOS. PFOS concentration in sludge was approximated from the inventory of occurrence data. Based on national quantity of sludge applied on agricultural soil, soil concentration was estimated.

- *Pesticides / Plant Protection Product application on agricultural field.* Two tiers for fate were tested for this pathway:
    - *Tier 1:* National database of pesticides use quantities was considered as an input for emission, which was considered homogeneous over the overall national agricultural surface area. The distribution of pesticides in surface water, soil and air was set according to a fix ratio (1%, 54% and 15%).
    - *Tier 2:* Dutch statistical data on the use of PPP (glyphosate) according to crop types were used. This data specified pesticides distribution according to crop specificity.

For each substance or substances family of interest, it is necessary to draft a Source-Pathway-Receptor scheme through which the substance may pose a risk to the receptor. The substance may come from multiple sources, follow multiple pathways and reach the same receptor. Therefore, it is important to

draft all the SPRs relevant to a substance.

Currently, PREMISS prioritisation prototype can run the three tested scenario. The prototype could be developed to include any other necessary scenario.

7.1.2 Scale of application

In principle, PREMISS prioritisation prototype can be used from European to local scale, as long as the input data are available at the chosen working scale and the SPR scheme is set in the prototype.

In the course of the project, PREMISS tool was mainly tested at national scale, either using REACH data from which national emissions were derived or using national emission data and considering that the distribution was homogeneous over the country (according to landscape setting and agricultural surface area). Regional, local or site-scale need to be further tested to validate their application.

7.1.3 Data input

It is important to recall that the prioritisation approach developed in PREMISS aims to undertake a **relative prioritisation approach among** substances and not an absolute prioritisation approach. Moreover, the quality of a **prioritisation depends on the quality of the RCR** (which is directly linked to the sources of data used to estimate emissions, fate and toxicity). This is why:

- **A lower quality RCR** based on more uncertain data leads to **a prioritisation with a high uncertainty.**
- Results of prioritisation between substances using same data sources to assess substance fate and risks, i.e. results based on data having same scale and (ideally) similar uncertainties range are more reliable and comparable between substances.
- Results from prioritisation between substances having various RCR quality (high, medium, low) shall be taken with caution, as they contain heterogeneous uncertainties, which may impede the rating of the substances, because of systematic differences.

In any case, caution shall be raised when prioritizing substances having different use and pathway.

In order for prioritisation results to be exploitable (e.g. comparable to each other) attention should be paid to input data as follows:

- **Not to mix** different type of **emission data (**source, scale, etc.) for the same scenario / pathway
- **Not to mix different toxicological data** (measured PNECs & QSAR based PNECs, TTC & evaluated HBGV and PNEC for secondary poisoning)

As stated above, input data origin and scale are very important in order to understand the meaning of the RCR and to assess whether or not substance prioritisation is comparable. Therefore, throughout the process, it is necessary to **ensure the traceability of the input data by specifying the data input source, scale and date**.

7.2 Limitations of the prototype

The prioritisation prototype developed in PREMISS is based on existing tools developed in previous projects. Certain assumptions were used and chosen in the SOLUTIONS project for the distribution among different compartments (as described in 4.2) and adapted in order to assess CECs for soil, sediment, sludge and groundwater. The overall objective was to develop a robust methodological and calculation approach to screen a wide range of substances to identify potential CECs, according to their fate and risk. The approach was tested (and validated) in PREMISS on a selected set of 18 pilot substances and for 3 selected SPR. After one-year of development, the current prototype has still some shortcomings, which can be improved in the future development steps. These limitations are described below.

7.2.1 Data input

The methodology gives guidance on how to collect input data, e.g. emission from REACH, physico-chemical properties from EPA dashboard, QSAR from ECOSAR. However, in PREMISS the input data were collected manually by the project partners for each substance from these external databases. This was a good way to test the efficiency of the data collection methodology. However, this manual process is not very user-friendly and quite time consuming (which was fine for the few pilot substances that were planned to be tested in PREMISS). In order to be able to prioritise a large amount of substances, easing or automatizing the collection of input data is needed. This may consist in assessing the possibility to connect the prototype tool to current databases (according to the most suitable databases) to automatically feed the prototype with the data for all substances of interest at once.

Moreover, some input data were missing (e.g. REACH data for banned substances or substance of low tonnage). These missing data were approximated, by making assumptions, but no proper methodology was designed in the project duration for dealing with data gap.

7.2.2 Implementation of the fate and transport model

7.2.2.1 Soil degradation rate

Degradation in soil was not included in the prototype, as no degradation rates were available in the database. As a consequence, the substance persistence assessment did not include degradation and was overestimated.

Two ways of improvements are suggested to overcome this shortcoming: 1) Developing a methodology to include the degradation rate (in soils) in the calculation of the fate model, 2) Include soil degradation rate as part of Tier 2 fate assessment (ie on CECs selected from Tier 1).

7.2.2.2 Emission duration/Substance accumulation

Emission duration of the substance over the years in the media is not taken into account in the model. As it is a steady–state model, it is assumed that the emission is constant over time (until the steady state is reached; time is not taken into account). However, as emissions values are a very impacting factor for fate, it is important to consider the emission (and its variation) over time and to take into account substance accumulation. IF emission values are available over the emission duration, emission value may be taken as the total emission over the emission duration (eg average emission value / y x nb of year of emission or the sum (over the years) of yearly emission values on the emission period).

7.2.2.3 Historical / banned substance

For historical or banned substances, past emission may be no longer available. As an example, for PFOS,

there is no longer REACH emission data available online, as PFOS production is banned. In PREMISS, when REACH emission data was missing for a substance, the emission value was set to 0.1 to 1 T/year. However, this assumption may clearly underestimate the emission, especially if the substance accumulated over decades when it was released and registered under REACH (e.g. PFOS). In order to overcome this shortcoming, it is suggested to develop a methodology to deal with historical substances (to be linked with substance accumulation methodology) and to possibly get historical emission data from (former) environmental permits.

7.2.2.4 Distribution of the substances' emission in surface water, soil and air

As the objective of SIMPLEBOX is to rapidly screen substances, the SIMPLEBOX tool works with default values for the substance emission distribution to air, water and soil. For the (REACH) industrial emission pathway, it is considered that 25% of the emissions in the environment are distributed by default between surface water (12%), soil (3%) and air (8.5%) for any substances, without taking into account substance physico-chemical properties. However, these set assumptions on distribution may induce a bias in the prioritisation, as it does not take into account the solubility or the volatility of the substance (which are important parameters for partitioning in various environmental media).

Introducing these criteria (solubility and Henry coefficient), despite it may be complex, may improve the prioritisation of substances among themselves.

7.2.3 Implementation of the toxicological module

Toxicity was assessed according to generic toxicological values, which may induce some uncertainties. In order to reduce uncertainties, methodology to refine and improve determination of hazard label, BCF, PNEC and TTC may be developed. Development of a tier 2 approach is also important.

7.2.4 Scenario: Source Pathway Receptor scheme

As stated before, the prioritisation prototype was tested for three scenario (Tier 1 or Tier 1&2 for fate). It shall only be used for these scenarios to this date. Additional scenario may be developed and tested to take into account more SPR schemes.

8 Expectations & feedback from the stakeholders on CECs prioritisation

The prioritisation approach which is developed in PREMISS aimed to be useful and meaningful for foreseen users. This is why PREMISS promoted stakeholders' involvement over the course of the project by engaging with stakeholders twice:

- A first stakeholders' meeting was organised within the first months of the project to discuss stakeholders' demands (their needs and expectations) on prioritisation. Following the meeting, the project team assessed which demands could be included in PREMISS work and which could not (mainly due to the limited duration and resources of the project).
- A second stakeholders' meeting was organised in the last month of the project in order to get some stakeholders' feedback on the work performed in PREMISS and to give perspectives on the prototype development and exploitation.

In order to engage with stakeholders, a stakeholders group was formed. This group included stakeholders from Belgium (Wallonia and Flanders), the Netherlands and France who may have to deal with CECs in soil and sub-surface. These stakeholders covered a wide range of professionals, encompassing problem owners (site manager, natural resources manager, industry), regulators, service providers (consultant, contractor and laboratories), funders and researchers. The same stakeholders' group was involved in both meetings in order to guarantee the follow-up and continuity of the project.

8.1 Stakeholders' demands

Expectations were discussed at the first stakeholders' meeting, which facilitated national discussion groups. Three parallel sessions (French, Belgian and Dutch sessions) were organised to gather national stakeholders' demands on CECs prioritisation in soil and sub-soil, by questioning the stakeholders on :

- their current state of knowledge on CECs in soil and sub-surface;
- their demands & expectations on prioritisation of CECs in soil;
- how they could exploit the prioritisation outputs. Detailed information on this first meeting is available on Annex N.

8.1.1 General expectations and demands

CECs prioritisation was found to be useful as it enables to define which substances SKH shall spend their time and efforts on. CECs prioritisation was seen as a means to save time: it is important to bring focus in CECs activities in order to take targeted actions. It takes a lot of time to regulate a substance (enabling prevention and prohibition), the faster you can prioritise the faster restrictions can be imposed for the substances that are really problematic.

CECs prioritisation was also deemed necessary to enhance cost effectiveness. Indeed, it is not economically viable to investigate all CEC families. As resources are limited, it is important to select the actions with most effect at reasonable cost, prioritising on contaminations that are actually (or with high probability) causing risks to humans or the environment.

The overall actions/ aims of CECs prioritisation include:

- To accelerate prevention and regulation:
    - To prioritise efforts in policy approach (prevention of risks)
    - To focus on preventing emissions of CECs before they start or become larger
    - To set up a warning system
- To gain insights on risk assessment (was considered as a priority):
    - To understand potential risks from CECs (toxicology, behaviour in soil and in groundwater, exposure, …). Can the substance become a problem somewhere else? Is there a need to take action by looking at the impact/risk of a substance, not only at the concentration. Assess how the risks compare to the usefulness/essential use of a substance.
    - To properly undertake soil investigation, monitoring and risk assessment
- To develop a robust management approach based on a limited number of substances:
    - To develop a good methodology focusing on a few substances, that can be used for similar substances;
    - To start managing some new CECs in order to gain experience and to be able to give rise to a legal framework.
    - To develop a methodological approach which enable CECs management in various contexts.
    - To develop a methodological approach which goes beyond the substances screening process as far as risks assessment and management of CECs.
- To identify knowledge gaps and point out where additional knowledge can improve the prioritisation. Identify where more information is needed. Indeed, with the present tool, the user may face the problem of insufficient information (eg. on substance behaviour or toxicology) to perform the prioritisation.

CECs prioritisation shall give insights on which pollutants it is necessary to develop activities. Such as services (laboratory, consultancy, remediation, others), economic activities and R&D activities.

8.1.2 Specific demands for prioritisation tool

The stakeholders also raised specific demands on prioritisation. These demands are summarised in the tables below according to the theme they deal with (scenario (SPR conceptual scheme), substances (sources and emissions); toxicity/risk assessment). Additionally, the last column indicates if (and how) the specific demand was taken into account or not in the development of the prioritisation made.

Demands	Priority/ included
Scenario	
• CECs emission (pesticides) -> soil -> impact trophic chain	Yes
• CECs emission -> Soil -> biodiversity (soil, hunted fauna or other fauna)	Yes
• CECs emission -> soil -> drinking water	Yes
• CECs emission -> soil -> groundwater (DW or "good ecological status")	Yes
• WWTP Sludge / sediment -> agricultural soil (quality, quantity of CECs present in soil)	Yes
Site scale:	
• Industrial emission (Accidental)-> Soil -> Receptors	No
• Industrial emission (Leak)-> Soil -> Receptors	No
• CECs emissions -> urban soils (large scale)	No
• Flooding: Sediment deposition -> agricultural soils	No
• Sediment Management: dredged sediments, sediments deposits due to hydraulic installations / production units	(Yes)

Demands	Priority/ included
Substances	
• How to take into account substances which are NOT registered in REACH (substances not more used or produced, pesticides)?	• Only tier 2
• Difficulties to estimate emission: emission depends on the type of emissions (accidental, production, leak) and the production process which may vary overtime -> Use of probability factor (depending on type of emission) to better estimate emission	• No
• Include current and past emission.	• Only current
• Include both local and diffuse pollution.	• Yes diffuse and regional
• How to link REACH emissions (which are not site scale) and the different scale of exposure (global, site scale)?	• Reach converted to national scale
• How to link activity and substances at site-scale?	• In tier 2 overwrite reach-emission with local data
• How to take into account degradation/ transformation product of CECs?	• Not taken into account for soil (absence of DT50)
• Individual substances versus mixture of substances and co-effects?	• Only individual
• Substances selection based on:	
- Toxicity / bio-accumulation (& emissions) and not necessarily on occurrence	• Label PBT/PMT
- Persistence & exposure routes	• Yes
- Widely produced	• Yes
- Exposure routes & end-points:	
Bio-accumulating substances – trophic chain	• Yes
Mobile substances – drinking water	• Yes
- Pay attention to recirculation of substance due to circular reuse	• No

Demands	Priority/ included
Demands toxicity • How to take into account subjective criteria for risk assessment. Such as sensitivity of target • Have you different approaches for toxicity estimation between urban soil/agricultural soil/industrial polluted soil? • Need for the toxicity / ecotoxicity values for CECs • Secondary poisoning important to consider for trophic chain	• Three separate endpoints • No • Yes • Yes

Other demands
• Fate and Transport: Take into account geology to predict fate of CECs in soil and sub-soil
• Prioritisation may be based:
  • on use, persistence, emission
  • on worst-case scenario, in absence of data – only to discriminate some substances
  • on laboratory capacity - not very relevant as services developed when needed.
  • on previous prioritisation experience eg NL PFAS
	• No, one soil type
	• Yes
	• Yes
	• No
	• No

Table 64 : Specific stakeholders' demands on prioritisation and how it was included in the development of the prioritisation prototype

8.2 Feedback on PREMISS outcomes

Feedback on PREMISS results were discussed at the second stakeholders' meeting, through two discussion groups. Two parallel sessions (one French speaking group and one Dutch speaking group) were organised to gather stakeholders' views on potential exploitation of the prioritisation prototype and its possible technical improvement. Prior to these working sessions the project outcomes were presented to the audience. It is important to note that the outcomes of the project were presented as concisely as possible (not going into much details on tools) and that it is based on this information that stakeholders were asked to give their feedback.

8.2.1 Application & Exploitation of the prioritisation approach (occurrence and prototype)

Further to PREMISS outcomes presentation, stakeholders generally thought that the prioritisation prototype could be useful to them. However, most of them stated that it could be only partially useful as they were questioning the assumptions made in the prototype model, the input data quality and the associated representativity and interpretation of the prioritisation results. Therefore stakeholders raised the need to focus more on model uncertainties and assumptions when prioritising and carefully communicate associated limitations of current knowledge, data and used tools, and consequences in RCR results. Moreover, limitations of the models should be properly described and communicated according to the tier level. One stakeholder considered that the prioritisation prototype was too up-front from its day-to-day work (contaminated land management consultancy) based on complying to existing regulatory framework.

A wide range of potential uses for the prioritisation approach was spotted by the stakeholders:

- Regulation:
  - Prioritise substances
  - Target substances for which intervention or remediation values in soil need to be define. This raised the issue of availability of physico-chemical and toxicological data necessary to derive new standard.

- Prevention:
  - Early warning prevention
  - "Instructions for use": Provide insight on which actions can be taken to reduce the impact of substance (restrictions on use), develop legislation, etc.;

- Monitoring:
  - Screen substances which shall be looked at (initial approach)
  - Set national or EU scale monitoring for selected substances and cross check the monitoring results with the prediction of the prioritisation approach

- Management:
  - Prioritise Contaminated Land management (sites)
  - Provide orientations for CECs management: Analytical development & what types of actions need to be developed

The **scale of application** was discussed thoroughly by the stakeholders. The prioritisation approach was deemed useful for diffuse contamination (which was the scale at which the tool was demonstrated). Its application for point-source scenario was questioned. If tests were performed for point-source, it was deemed necessary to specify any uncertainties associated with assumptions and results. The use of the prototype to prioritise sites and sources among multi-sites and multi-sources was mentioned. Stakeholders showed interest for this application.

The prototype was deemed useful to provide insight into the kind of measures that could be taken to deal with CECs. In any case, it was stressed that **uncertainties** associated with the input data and the prioritisation results **had to be assessed in more insight and managed**.

8.2.2 Improvements towards a full-scale prioritisation prototype

Most of the stakeholders mentioned that the prioritisation prototype met partially their expectations. From the concise and dense presentation of the results, some stakeholders stressed that it was difficult for them to make an opinion on the prototype. The results presented were considered sufficient as they were results from the prototype. Further developments (new scenarios…) need to be addressed and uncertainties further commented.

Prior to listing improvements for the prototype tool, the French speaking stakeholders emphasized that the future development of the tool depended strongly on the objectives of the prioritisation and its scale. The following examples were given: classification of substances (banned or not); macro scale development (including many substances, generic input data) for policy purposes; diffuse pollution versus point source pollution.

The stakeholders suggested the improvements for the prioritisation prototype as follows:

- Tool development:

- Include substances degradation & by-products
- Collect / acquire more accurate toxicity data (update Cramer?)
- Include specific SPR and end-points for PFAS, which shall be considered as a distinct group.
- Take into account historical emissions (especially for substances which are persistent and had been emitting for a long time)
- Include PMT (Persistence-Mobile and Toxic) classification in the prototype
- Develop Tier 2 for fate and toxicological assessment
- Include heterogeneity across the area and depth in the soil

- Tool validation:

  - In-depth sensibility analysis
  - Discuss results with occurrence and measured data
  - Discuss relevance of Simple Box to model some scenario
  - Test tool with known substances (for which there are numerous data) in order to validate the model

- Tool "instructions for use":

  - Clear indications of current uncertainties, shortcoming of the prototype
  - Clearly state that this tool is at the "prototype" stage
  - Methodological guidelines to interpret the results

As for **inventory of occurrence data**, many soil data are collected at local scale (site or municipality) encompassing mainly "known" substances. Gathering this data from diverse local sources of information may be very challenging and not very relevant (if "known" substance). In order to organise soil data collection of CECs, it was suggested to **pre-target the CECs already** identified and measured other media (such as surface water).

The prioritisation approach was considered useful for policy makers. However, the **way to exploit results towards a policy instrument needs to be developed**.

Eventually, stakeholders recommended to **share** knowledge and methodology **and collaborate with European institutions** (such as JRC, EEA) or **EU network** (such as NORMAN).

9 Recommendations

9.1 General recommendations on CECs prioritisation

9.1.1 Recommendations on occurrence data

PREMISS outcomes (inventory of occurrence data and stakeholders' involvement) enabled to draw the following recommendations on occurrence data at national levels and EU level.

- Data inventory and compilation could be facilitated by **harmonisation** of substance international signalling, of data treatment and associated metadata. This will also contribute to achieving FAIR[28] data treatment,one of the EC goals for Europe.
- **Central storage** of existing WWTP solid effluents, manure, compost and digestate quality data shall be organised.
- Available data in soils for the selected CECs are scarce (a few in the Netherlands and Flanders, hardly any in France or Wallonia). **(Prospective) soil monitoring** has to be developed in order to acquire CECs data in soils (and identify CECs of interest and confirm/ infirm prioritisation) and orientate further regulations. Prospective monitoring in WWTP solid effluents, manure, compost and digestate should also be organised.
- CECs monitoring shall be encouraged by several existing and upcoming policy initiatives under the European Green Deal (the Chemical Strategy, the new Soil Strategy, the Zero Pollution Action Plan) which provide a European framework to protect land and soil from pollution. However, a **more coherent EU policy framework on soil** would further reinforce efforts towards a sustainable soils management. Besides, the new EU Regulation on Fertilizer (coming into force in July 2022) does not cover CECs.
- **Promote CEC data collection in soil and storage** in common database as initiated by the LUCAS survey and beyond. The relevance of easing soil data collection of CECs by pre-targeting the substances based on CECs identified and measured in other media (such as surface water) shall be assessed.

9.1.2 Recommendations for prioritisation prototype application and exploitation

Prioritisation prototype need to be used according to **its modalities of use** (type of scenario, scale of application and data input) and keeping in mind **its limitations** (input data, fate and toxicological modules and scenario) described in section 7.

Prior to any prioritisation prototype application, it was deemed necessary to have better insight on uncertainties associated with the input data and model assumptions and to have clear guidance on results interpretation. Application of the prioritisation prototype is foreseen in various fields including **regulation, prevention, monitoring and management**. However, the **way to exploit and transfer results towards a policy instrument and monitoring or management guidelines needs to be developed**.

Regarding **application scale**, the prioritisation approach was considered useful for diffuse contamination (which was the scale at which the tool was demonstrated). Its application for point-

[28] In 2016, the 'FAIR Guiding Principles for scientific data management and stewardship' were published. They intend to provide guidelines to improve the **F**indability, **A**ccessibility, **I**nteroperability, and **R**euse of digital assets by both humans and machines.

source contamination or for multi-sites and multi-sources application was of interest, but need to be demonstrated.

9.1.3 Recommendations for the prioritisation of emerging contaminants and link to the other EU initiatives

The knowledge and tools that have been developed in PREMISS, and data that were gathered are connected to other EU initiatives. In the future, new initiatives should have benefits from reusing and applying the knowledge, data and tools developed in PREMISS.

Examples of projects and initiatives that are connected to PREMISS

- The recently started HORIZON 2020 project in support of the European Green Deal PROMISCES (Preventing Recalcitrant Organic Mobile Industrial chemicalS for Circular Economy in the Soil-sediment-water)
- Recent launch of the European mission A Soil Deal for Europe

PREMISS is also strongly linked with the new EU Soil Strategy and the EU Soil Observatory (EUSO) which are themselves integrated into a diverse regulatory framework that comprises the "Zero emission action plan", the "Circular Economy action plan", the "Chemical strategy", the "Biodiversity Strategy for 2030", the "Farm to Fork strategy", the "Forest strategy". More specifically, the EU Soil Strategy for 2030 raises the need for significant progress on identifying contaminated sites, restoring degraded soils, defining the conditions for their good ecological status, introducing restoration objectives and improving the monitoring of soil quality. Key actions must be taken to achieve these objectives and PREMISS can help to elaborate strategies of actions. In particular, it is essential to improve the risk assessment of chemicals on soil quality and of soil contaminants on human health and the environment. The PREMISS prioritisation tool lays the foundations for a global and harmonized scheme for the selection of chemicals of concern in soil in a circular economy context. The toxicological module of the PREMISS prototype addresses the risk-assessment of chemicals in soils with a first attempt on some specific source/pathway/receptor routes. These first results raise the need for further developments, in particular for diffuse pollution and high background levels, or related with mixture of contaminants, bioaccessibility and links with epidemiological studies. These recommendations can feed into future works of European strategies for soil quality.

One of PREMISS WP3's outputs is to recommend a European DB and national DB for CECs occurrence data soils. LUCAS is the first attempt to build a consistent spatial DB on soils across the EU. The 2009 survey focused on soil physico-chemical properties. The ongoing LUCAS survey will cover some CECs (pesticides and antibiotics). In parallel and pending the results of this latest LUCAS survey, Member states should centralise their soil data in harmonised DB according to FAIR principles in order to make the best use of it for future research and/or policies.

One of PREMISS WP4's recommendations is putting more efforts in CECs occurrence data in fertilizers (WWTP sludge, manure, etc.). In the desired Circular Economy, prevent the spread of pollutants by adding fertilizers to the soils is indeed of major importance. This is one of the goals of the European Fertilizer regulation (UE 2019/1009), which will soon come into force (July 2022). Unfortunately, this regulation does not cover CECs yet. Improving knowledge on CECs occurrence data in fertilizers is still needed.

Eventually, stakeholders recommended to **share** knowledge and methodology **and collaborate with European institutions** (such as JRC, EEA) or **EU network** (such as NORMAN). The project has been already presented to the EUSO working group but other exchanges can be planned

9.2 Recommendations for prioritisation tool improvement

Recommendations presented in this paragraph include:

- PREMISS project team recommendations suggested by PREMISS partners over the course of the one-year project (during development prototype)

- Stakeholders' demands which could not be included in the prototype within the limited time and resources of the project and stakeholders' feedback on the prototype results.

The recommendations are divided into 3 categories: technical development, technical validation and user-friendly interface development. It is very important to note that the recommendations proposed are very dependent of the overall prioritisation ambitions. This is why the following recommendations may be more or less relevant depending on overall prioritisation objectives.

9.2.1 Technical tool development

In this section, we propose technical recommendations to enlarge the application fields of the tool (additional scenarios), to better manage the uncertainties associated with data gaps and with the assumptions and limitations of the fate or toxicological / prioritisation modules.

9.2.1.1 Design and study additional scenarios – SPR schemes

PREMISS prototype includes three main scenarios (see sections above) having as receptor agricultural soil and its associated end-users. These scenarios were run at the national or regional scale.

Scenarios having a focus on urban and industrial soils and encompassing several scales may be further developed and tested in the prioritisation tool.

The following additional scenarios could be trialled to meet the demands and feedback which was expressed by the stakeholders, such as:

- Site scale industrial emission (Accidental)-> Soil -> Receptors
- Site scale industrial emission (Leak)-> Soil -> Receptors
- Large scale CEC emissions -> urban soils -> Receptors
- Sediment deposition due to flooding -> agricultural soils
- Specific SPR and end-points for PFAS (especially if used as fire-fighting foam), which shall be considered as a distinct group.

Local and site scale SPR shall also be tested in order to assess the applicability of the prototype at small scale.

9.2.1.2 Data gaps management

Within PREMISS pilot substance testing, some emission data were missing (or could not be collected). As for the substance having no the REACH emission data (and under REACH regulations), the emission value was assumed to be in the lower range of 0.1 – 1 t/y. If the prototype is applied to a wide set of substances, it is likely that some physico-chemical properties or toxicological (QSAR) data may be missing, even though the databases selected in this prototype are as robust as possible.

For any data gaps, it is important to further define **a methodology to manage data gaps**. This methodology shall be able to explain how to deal with data gaps (and associated uncertainties). It may

consist in compiling existing scattered data, in easing access to existing databases, in making assumptions for missing data. The first step of the methodology could be, according to the scenario (SPR), to specify which data are specifically important for the SPR and therefore on which data, data gaps management shall be made.

9.2.1.3 Fate module

The fate module could be further developed by refining emissions, improving persistence assessment and introducing flexible options to some input data. The recommendations are summarised below:

- Emission:
  - Include past emission, in order to take into account historical emissions (especially for banned substances which are persistent and had been emitting for a long time)
  - Include both local and diffuse pollution / emission.
  - For all emission types, include emission over the all range of emission duration
- Persistence:
  - Include soil degradation rate and associated CECs transformation products.
- Other parameters:
  - Soil type: Include various soil types in order to take into account geology to predict fate of CECs in soil and sub-soil
  - Under the REACH SPR, distribution over air, soil, water introduce flexible ratio depending on the substance main properties (solubility, volatility) and emission pathways of relevant processes.
  - In general, develop Tier 2 for fate

9.2.1.4 Toxicological and prioritisation module

Toxicological module could be further developed by assessing the possibility and relevance to:

- Collect / acquire more accurate toxicity data:
  - improve determination of hazard label, BCF, PNEC and TTC
  - compound specific PNECs can be used that are derived using the SOLUTIONS SSD database. This database contains Species Sensitivity Distributions (SSD) that are derived from experimental aquatic ecotoxicity data.
  - develop a database on HBGV
- Include PMT (Persistence-Mobile and Toxic) classification in the prototype when the criteria are available
- Soil type: take various approaches for toxicity estimation depending on soil type eg urban soil/agricultural soil/industrial polluted soil?
- Develop a tier 2 for toxicological assessment , in which mixture toxicity assessment can be useful for prioritisation of locations with estimated or measured concentrations (not for prioritisation of substances).

9.2.2 Technical tool testing and validation

Some sensitivity analyses were undertaken on the fate module in the course of the PREMISS project. However, because of the limited time and resource of PREMISS, the project team is aware that additional testing of the tool is necessary to illustrate the robustness of the tool. When the stakeholders gave their feedback on the prototype and the prioritisation results, they thought that the prototype was useful as an initial step towards CECs screening, but they stressed the **uncertainties** associated with the

input data, and point out that the model and the prioritisation results **should be assessed in more insight and managed**.

This is why, the following actions are recommended for the tool verification:

- More extensive sensitivity and uncertainties analysis.
- Comparison of fate results with new measured occurrence data.
- Comparison of prioritisation results with current previous prioritisation experience (eg PFAS in the Netherlands).

Additional tests of the prototypes can be proposed in order to better characterize the uncertainties and validate its fate module. Additional tests may include:

- Testing the tool with known substances (for which there are abundant occurrence data): The tool could be used with monitored substances, allowing to deeper consider impact of different factors on the tool output. These substances should be selected among substances present in the different databases identified during PREMISS project. To this end, a collaboration should be initiated in France with the GIS-SOL (https://www.gissol.fr/). At European level, exchanges with EUSO could give access to other datasets.
- Testing the tool with new emission dataset on a national level: For France, an ongoing study will allow to make available new occurrence data for pesticide in soils. This study, organised by the French Agency for Food, Environmental and Occupational Health Safety (ANSES) is a great opportunity to assess the relevance of the PREMISS tool, even if data are made available through national (GIS-SOL) or European database.
- Testing the tool for additional SPR (Discuss relevance of Simple Box to model some scenarios)
- Testing the tool for additional countries: new participating countries integrating the project could compile and add their occurrence data to enrich the test.
- Testing the tool for larger set of substances
- Testing the tool for small scale scenarios

9.2.3 Development of end-user friendly interface

At present, the entry data was collected manually by the partners and input encoded manually in the prototype by the model developer, which could be time consuming. This was feasible as solely a few pilot substances were tested. However, if a large set of substances is tested, for the development of the full tool it is recommended to **automate the access and the filling of input data**.

The current prototype is a set of excel spreadsheets which are only usable by their developer. In order to enable the use of the tool by stakeholders, it is necessary to **develop a user-friendly interface according to stakeholders' needs and uses**. The user interface could encompass entry such as substance type, substance scenario, scale, etc..). The need to develop several interfaces depending on the stakeholders' needs and prioritisation objectives has to be assessed.

Finally, stakeholders express their need of "**user's guide**", which shall give clear indications of current uncertainties, shortcoming of the prioritisation tool and methodological guidelines to interpret the results.

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ANNEX

Annex A : List of sources of occurrence data and list of CECs included in the PREMISS inventory and quantification frequencies

i. List of national databases

SOIL

- The French soil quality databases (RMQS for agricultural soils and BD-Solu for urban background levels) have been consulted, but no data dealing with pilot shave been identified.
- OVAM Mistral-databank: DB of the public waste agency of Flanders containing analytical results of contaminants in soil and groundwater. This DB contains almost exclusively contaminants linked to risk activities and general screenings.
- PFAS Achtergrondwaarden DB: project in which concentrations of 113 substances included in the Dutch soil standards were measured to ascertain the background level of these substances in natural soil. This DB includes measurements taken at various depths. The background level plays a role in the application of soil in The Netherlands regulation.

SEDIMENT

- OVAM Hotspot verkenner: data inventoried in the ongoing sediment Hotspot study in Flanders.
- Public Service of Wallonia (SPW) Sediment DB: analytical results from the Walloon navigable and non-navigable waterways sediment monitoring network corresponding to the WFD monitoring network sampling sites (73 sites).
- "Naïades" is the French national DB on surface water quality. The data made available in Naïades are produced by organisations (stakeholders) to meet a need (study, regulation, research, etc.) then stored in reference banks which can store data from several producers and meet several needs.
- Dutch Water Authorities: monitoring data of dredged sediments (maintenance dredging 2018-2019) collected by the regional water authorities since it was compulsory to analyse 30 PFAS compounds.

SEWAGE SLUDGE

- The SuPREMA DB is dedicated to collect results from French prospective monitoring exercises in sewage sludge.

GROUNDWATER

- GIDAF is the French application (for Computerized Management of Frequent Self-Monitoring Data) for the operators of industrial installations which may impact the environment to report online and transmit environmental data to the Inspectorate of Classified Installations and to the Water Agencies. Indeed, by law these installations operators must self-monitoring of emissions with regard to the characteristics of their discharges and in particular the flows emitted into the environment. Self-monitored data are banked in GIDAF.
- ADES is the French national groundwater DB which collects on a web site - https://ades.eaufrance.fr - all the groundwater quantitative and qualitative public data. The main objectives of this DB are to elaborate a public data storage tool, to collect all the national groundwater data, with a large range of producers and partners and to facilitate statistical

treatments and mapping presentations. These data were expected to provide information and basic input to hydrological investigations relating to resources inventory, management, and planning of the water resource. It's a privileged tool for assessing the quality and quantity of heritage groundwater within the framework of the WFD.

- OVAM Mistral-databank (see above, in soil)
- SPW Groundwater (ESO) DB: analytical results from the Walloon groundwater monitoring network to respond to the WFD (EC/2000/60 Directive). 350 sites were sampled in 2019 from a total of 450 sampling sites for the groundwater network.
- The REWAB (Drinking water companies database on water quality) database drinking water companies report on the groundwater quality used for drinking water (RIVM, 2020).
- VMM Geoloket (Geoloket waterkwaliteit, www.vmm.be)

ii. List of national reports:

The complete reference of the reports can be found in the Reference section

SOIL

- ExpertisePFAS Centrum: Several studies were performed by the ExpertisePFAS Centrum in 2017 and 2018, focusing on PFAS contamination in The Netherlands.
- OVAM, 2018: Analytical results originating from an exploratory study carried out on behalf of the public waste agency of Flanders into the presence of PFAS in soil, groundwater and sediment at risk locations (such as producers of PFAS, producers of fire extinguishing foam, fire service training sites and fire incidents sites) in Flanders. A total of 35 drillings were carried out at 24 selected sites in Flanders and 40 soil samples and 1 sediment sample were collected for PFAS analyses. 47 monitoring wells were also sampled and analysed for PFAS.
- OVAM, 2021: Analytical results originating from a study carried out on behalf of the public waste agency of Flanders into the presence of PFAS and other selected emerging contaminants in soil at background locations in Flanders. 28 PFAS were analysed on 50 samples from the top layer (0-20 cm) of Flemish unsuspected (uncontaminated) soils. Background concentrations values were derived based on the 90-percentile values. The same soil samples were analysed for a number of other emerging contaminants. This includes pesticides, several of which are no longer available or allowed to be applied, but which may still be present in soil, sediment and groundwater.
- RIVM, 2018. In March 2018, soil and irrigation water samples were sampled in 11 locations around the DuPont/Chemours factory (+ 1 control in Bilthoven).
- RIVM, 2020. RIVM investigated the concentrations of 29 PFAS substances in the soil at 100 agricultural and natural locations throughout the Netherlands. Based on their concentrations, background values have been determined for two commonly occurring PFAS: PFOS and PFOA. In addition, soil samples were also analysed from 100 built-up areas, in order to obtain a complete national overview of the concentrations of PFAS in the soil.
- TNO/Alterra 2004: Database of 100 representative soil sites in the Netherlands collected around the year 2000. Many parameters were analysed by a specialized laboratory to obtain low limits of quantification.

SEDIMENT

- CSO Advies 2010: monitoring data of dredged sediments (maintenance dredging 2000-2010) collected by all Dutch water authorities

- OVAM, 2018 (see above, in soil)
- Sullied Sediment project: Data collected from 18 surveys across three river catchments over 30 months between 2017 and 2020.

SEWAGE SLUDGE

- CARIBOUH project: 52 substances, including 5 PFAS, 12 alkylphenols, 13 phenols and 15 personal care products, were analysed in 29 wastewater treatment plant (WWTP) sludge in 2020 (1 to 12 samplings per year per WWTP) in Wallonia. A confirmatory screening was undertaken at the beginning of the project on 29 WWTP (a single sample was collected at each WWTP).
- FARO Advies 2020: Analysis of CECs in one sample of Dutch sewage sample.
- INERIS, 2014 (Report DRC-14-115758-08437A): Sewage sludge from 12 WWTP (rural and urban) were sampled between 2011 and 2014, before or after treatment (digested or limed or dried and/or composted) in France. 114 substances were analysed: 33 pharmaceuticals substances and 81 non pharmaceuticals emerging compounds (amongst which 5 phenols/alkylphenols and 2 PFAS (PFOA + PFOS). No pesticides were included.
- The JRC report (2012) presents the results of a Pan-European Screening Exercise (FATE SEES) which aimed at identifying and prioritising among relevant compounds to be considered in European regulation dealing with Sewage Sludge. In total, 63 samples originating from 15 countries were assessed for 92 organic compounds including ingredients of personal care products and pharmaceuticals. 9 of the sampled WWTPs were located in Belgium.

GROUNDWATER

- BIODIEN project: Data collected in groundwater from 122 sampling sites in 2015 and 2016 in Wallonia. The project searched for 74 substances of industrial and/or domestic use and 122 pesticides in water (groundwater, surface water, WWTP effluents).
- IMHOTEP project: Data collected in groundwater from 195 sampling sites in 2015 and 2016 in Wallonia.
- OVAM, 2018 (see above, in soil)
- RIVM, 2021. Current status of Dutch drinking water sources (in Dutch). RIVM report 2020-0179

iii. List of CECs occurrence date in environmental media - Quantification frequencies for PFAS
iv. List of CECs occurrence data in environmental media – Quantification frequencies for phenols and alkylphenols
v. List of CECs occurrence data in environmental media – Quantification frequencies for pesticides
vi. List of CECs occurrence data in environmental media – Quantification frequencies for pharmaceuticals

Annex B : Complete set of occurrence data for 18 pilots CECs

Annex C : Chemical Database SimpleBox

Annex D: Predicted chemical properties

Overview of predicted averages of chemical properties, retrieved from the EPA dashboard.

Substance	CAS nr	LogKOW	VP [Pa]	TempMelt [K]	MW [g/mol]	S [mol/m3]
Glyphosate	1071-83-6	-3,12E+00	6,53E-06	4,54E+02	1,64E+02	3,22E-04
Imidacloprid	138261-41-3	4,27E-01	3,67E-06	4,27E+02	2,56E+02	5,68E-04
S-Metolachlor	87392-12-9	3,15E+00	1,76E-03	3,06E+02	2,84E+02	5,71E-04
Metolachlor ESA	171118-09-5	2,09E+00	3,84E-05	3,84E+02	2,80E+02	1,45E-03
Metolachlor OXA	152019-73-3	2,09E+00	3,84E-05	3,84E+02	2,80E+02	1,45E-03
PFOA	335-67-1	5,68E+00	3,24E+01	2,97E+02	4,08E+02	1,33E-03
PFOS	1763-23-1	5,77E+00	3,31E-04	3,57E+02	5,00E+02	1,76E-03
GenX	13252-13-6	5,41E+00	3,49E+01	3,01E+02	3,31E+02	1,27E-03
PFBA	375-22-4	2,60E+00	2,11E+03	2,70E+02	2,04E+02	2,91E-03
PFHxA	307-24-4	2,71E+00	1,09E-06	4,22E+02	3,99E+02	4,69E-03
PFHxS	355-46-4	3,69E+00	1,09E-06	3,59E+02	3,99E+02	4,69E-03
N-EtFOSAA	2991-50-6	7,35E+00	5,53E-01	3,67E+02	6,04E+02	5,75E-04
Diclofenac	15307-86-5	4,27E+00	8,40E-06	4,72E+02	2,98E+02	9,17E-04
Triclosan	3380-34-5	4,97E+00	1,67E-03	3,84E+02	2,93E+02	6,13E-04
Clarithromycin	81103-11-9	3,47E+00	1,93E-08	4,68E+02	7,41E+02	3,85E-04
Azithromycin	83905-01-5	3,47E+00	1,93E-08	4,68E+02	7,41E+02	3,85E-04
4-Nonylphenol	104-40-5	6,03E+00	4,48E-02	3,16E+02	2,23E+02	4,35E-04
2-chlorophenol	95-57-8	2,15E+00	1,52E+02	2,96E+02	1,29E+02	7,58E-04

Annex E: Removal efficiencies pharmaceuticals Tier 1

Annex F: SMILES and PubChem

Within PubChem, the search result gives a “best match” which will often be the substance that the user is looking for. Nevertheless, sometimes multiple “correct” compounds will result (e.g. different stereo-isomers that all have the same CAS registry number, or different salts of a similar substance). The user will have to decide which PubChem compounds the best representation of the substance(s) that needs to be prioritised[29]. By selecting this compound (often the ‘best match’) and scrolling down to section 2.1.4 Canonical SMILES of the chemical information the user can copy and paste the given SMILES code and use this as input for the model software indicated in the different sections below.

For the simple example of the single component aniline, when using the chemical name as search criterion we get the results as shown in screenshot 1. The subsequent Canonical SMILES given in section 4.3.1 for aniline is then the following text string: **C1=CC=C(C=C1)N**

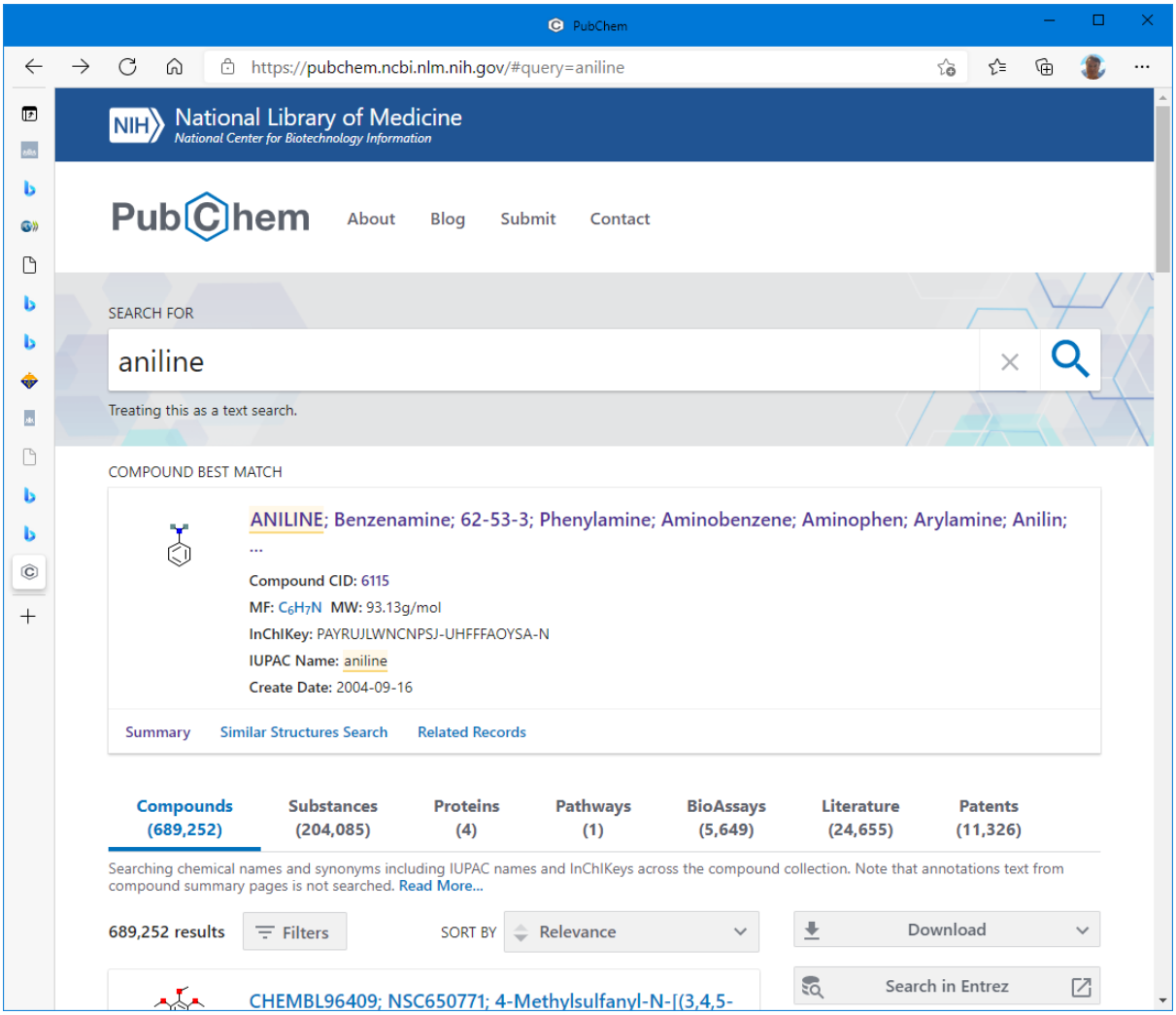


Figure F.1 . Pubchem result result for search-term “Aniline”. By selecting (clicking) on the Compound Best Match the available information (including a SMILES code) is given. The Canonical SMILES (section 4.3.1) can be copied and pasted into other SMILES-aware software used for the PREMISS Tier1 Prioritisation (the OECD QSAR Toolbox, ECOSAR, EpiSuite, SVHC Structure Similarity Tool).

[29] Automation is possible for single species chemicals. However, when mixtures, UVBC products, or technical products are considered the most relevant structure can differ per receptor. Users should therefore manually select the most relevant structures from the available information on the composition.

Annex G: Workflow of the ZZS similarity tool.

The (online) identification of SVHC-alerts status of a substance is achieved by entering the SMILES code (section 4.3.1) in the RIVM Similarity tool website [ZZS-similarity tool | Risico's van stoffen (rivm.nl)]

The result after entering the SMILES code for aniline as an example is given in Figure I.. Aniline itself is not identified as an SVHC substance, but has a high structural similarity to a number of recognised SVHC substances which is reason to flag aniline for potentially having SVHC-properties. The SVHC substance with the highest similarity to aniline are given, with the first being 2-naphtylamine, CAS 91-59-8. The concern is given under possible toxicity: C, i.e. 2-naphtylamine is considered a potential carcinogen. This SVHC status screening is not yielding any quantitative measure that can be compared to an exposure estimate, but those substances that are identified as SVHC, or being flagged as potentially having SVHC-properties, should be marked as priority, because exposure to these substances is unwanted. The similarity of aniline to PBT like structures (following the CMR similarity result) does not yield any sufficiently similar SVHC substances. Therefore, the only potential SVHC concern for aniline would be carcinogenicity.

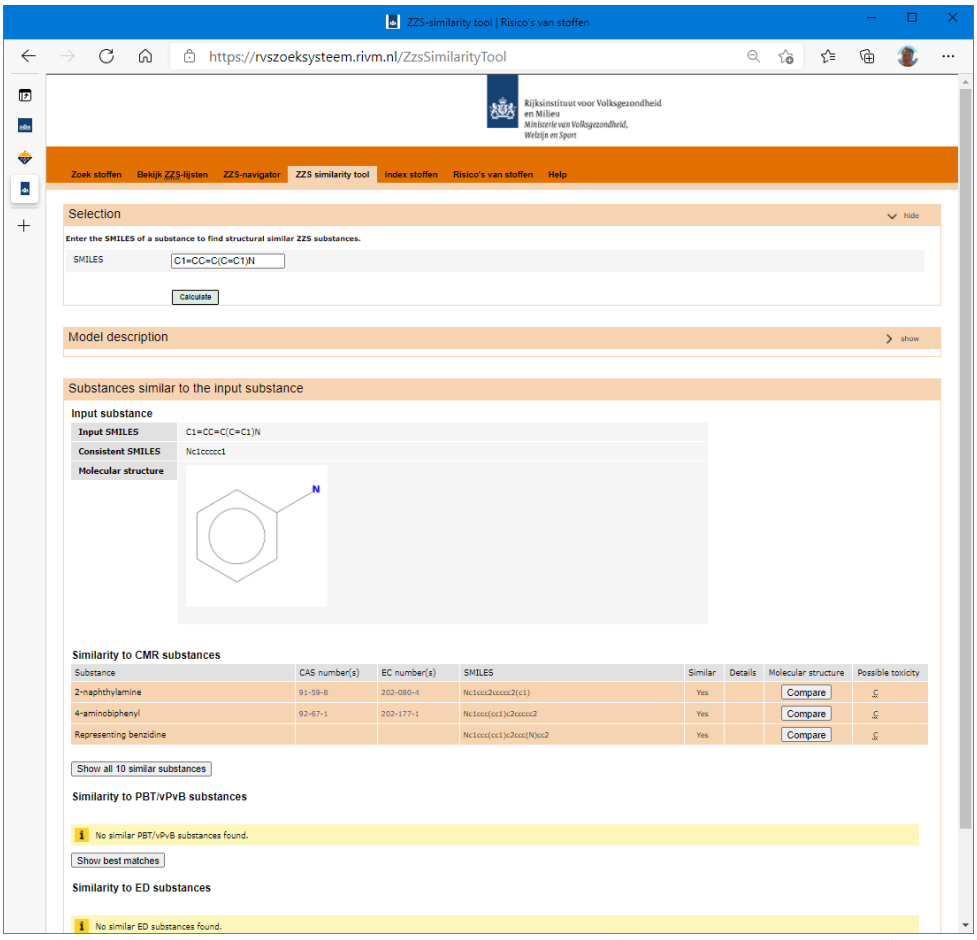


Figure G.1 ZZS similarity tool on the RIVM website [https://rvszoeksysteem.rivm.nl/ZzsSimilaritTool]

Annex H: Formulas Human exposure

The formulas used to calculate human exposure are more extensively described in the background information of the EUSES model (Lijzen and Rikken, 2004) and the CSOIL2020 model (Van Breemen et al., 2020).

Soil ingestion

EXPing [$kg.kg_{bw}^{-1}.d^{-1}$] = (Cs * Fa * AIDa) / BW

EXPing: Exposure through soil ingestion [$kg.kg_{bw}^{-1}.d^{-1}$]

Cs:	Concentration in soil (fate module)	[$kg.kg_{dw}^{-1}$]
Fa	Relative absorption fraction (1)	[-]
AIDA:	Daily amount soil ingestion (0.00005)	[$kg_{dw}.d^{-1}$]

Direct consumption of groundwater

EXPdw [$kg.kg_{bw}^{-1}.d^{-1}$] = (QDW * CPW) / BW

QDW:	Water consumption (0.002)	[$m^3.d^{-1}$]
BW:	Bodyweight (70)	[kg]
CPW:	porewater concentration (Fate module)	[$kg.m^{-3}$]

CROP consumption

Concentration in vegetables

Concentration in Root:

Croot [kg/kg wwt] = K.Plantwater * CPW/RHO.plant

Croot:	Concentration in root	[$kg.kg_{wwt}$]
K.Plantwater:	Partition coefficient plant-water	[$m^3.m^{-3}$]
CPW:	Pore water concentration (Fate module)	[$kg.m^{-3}$]
RHO.plant:	Density of plant material (700)	[$kg_{wwt}.m^{-3}$]

K.Plantwater = Fwater.plant + Flipid.plant * Kow^B

Fwater.plant:	Fraction of water in plant (0.65)	[$m^3.m^{-3}$]
Flipid.plant:	Fraction of lipid in plant (0.01)	[$m^3.m^{-3}$]
Fair.plant:	Fraction of air in plant (0.3)	[$m^3.m^{-3}$]
Kow:	Octanol water partition coefficient (Fate module)	[-]
B:	Correction for differences between plant lipids and octanol (0.95)	[-]

Concentration in leaf

Cleaf [kg/kg wwt] = BETA.leafR/(ALPHA.R * RHO.plant)

BETA.leafR:	Source term of differential equation	[$kg.m^{-3}$]
ALPHA.leafR:	Sink term	[d]
RHO.plant:	Density of plant material (700)	[$kg_{wwt}.m^{-3}$]

Beta.leafR:

BETA.leafR = CPW*TSCF*Qtransp/V.leaf + (1-Fass.aer)*CSA * g.plant*AREA.plant/V.leaf

CPW: porewater concentration (Fate module) [$kg.m^{-3}$]

CSA = Concentration in air (Fate module) [$kg.m^{-3}$]

Constants

Qtransp:	Transpiration stream (1)	[$dm^3.d^{-1}$]

V.leaf: Volume of leaves (2) [dm^3]
g.plant: Conductance (86.4/ (3600*24)) [$m.s^{-1}$]
AREA.plant: Surface area of plant (5) [m^2]

TSCF: Transpiration-stream concentration factor [-]
LogKow <-.5 → TSCF = 0.0931
LogKow >4.5 → TSCF = 0.0378
ELSE
TSCF = 0.784*EXP(-((logKow – 1.78)^2)/2.44)

Fass.aer: Fraction associated with aerosol [-]
Fass.aer = CONjunge * SURF.aer / (VP.L + CONjunge * SURF.aer)

CONjunge: Junge's constant (0.01) [$Pa.m^{-1}$]
SURF.aer: Surface area of aerosol particles (0.01) [$m^2.m^{-3}$]
VP.L : Subcooled liquid vapour pressure [Pa]

TEMPmelt ≤ TEMPenv →

VP.L = VPtemp.env
ELSE
VP.L = VPtemp.env/(exp(6.79* (1-TEMPmelt/TEMPenv)))
TEMP.env: Temperature of environment (285) [K]
TEMP.melt: Temperature of meltingpoint (Fate module) [K]

ALPHA:
ALPHA = (AREA.plant * g.plant) / (K.leafair * V.leaf) +kelim.plant + kgrowth.plant

AREA.plant: Surface area of plant (5) [m^2]
g.plant: Conductance (86.4/ (3600*24)) [$m.s^{-1}$]
V.leaf: Volume of leaves (2) [dm^3]
Kgrowth.plant: Growthrate of plant (0.035) [d^{-1}]

k.leafair = Fair.plant + K.plantwater / K.air.water

Fair.plant: Fraction of air in plant (0.3) [$m^3.m^{-3}$]

K.Plantwater = Fwater.plant + Flipid.plant * Kow^B

K.Plantwater: Partition coefficient plant-water [$m^3.m^{-3}$]
Fwater.plant: Fraction of water in plant (0.65) [$m^3.m^{-3}$]
Flipid.plant: Fraction of lipid in plant (0.01) [$m^3.m^{-3}$]
Fair.plant: Fraction of air in plant (0.3) [$m^3.m^{-3}$]
Kow: Octanol water partition coefficient (Fate module) [-]
B: Correction for differences between plant lipids and octanol (0.95)[-]

K.air.water = HENRY / (GasConst * TEMPenv)

K.air.water: Partition coefficient air-water [$m^3.m^{-3}$]
GasConst: Gas constant (8.314) [Pa.m3.mol-1.K-1]

TEMP.env: Temperature of environment (285) [K]

HENRY = VPtemp.env / (SOLtemp.env / MOLW) [$Pa.m^{-3}.mol^{-1}$]

VPtemp.env: Vapour pressure at environmental temperature [Pa]
Soltemp.env: Solubility at environmental temperature [$kg.m^{-3}$]
MOLW: Molecular weight [$kg.mol^{-1}$]

Kelim.plant [d^{-1}] = Kmetab.plant + kphoto.plant

Kelim.plant:	Elimination rate plant	[d^{-1}]
Kmetab.plant:	Rate of metabolisation(0)	[d^{-1}]
Kphoto.plant:	Rate of photosynthesis (0)	[d^{-1}]

Exposure through vegetable consumption

EXPOSURE PARAMETERS CONSUMPTION

EUSES:

Daily intake of leaf crops:	1.2	[$kg.d^{-1}$]	Qleaf
Daily intake of root crops:	0.384	[$kg.d^{-1}$]	Qroot
Daily intake of meat:	0.301	[$kg.d^{-1}$]	Qmeat
Daily intake of fish:	0.115	[$kg.d^{-1}$]	Qfish
Daily intake of dairy:	0.561	[$kg.d^{-1}$]	Qdairy
Bodyweight:	70	[kg]	BW

Exposure through consumption of leafy vegetables

EXPleaf [$kg.kg_{bw}^{-1}.d^{-1}$] = (Qleaf * Cleaf)/ BW

Exposure through consumption of root vegetables

EXProot [$kg.kg_{bw}^{-1}.d^{-1}$] = (Qroot * Croot)/ BW

Exposure through vegetable consumption

EXPveg [$kg.kg_{bw}^{-1}.d^{-1}$] = Qroot + Qleaf

Annex I : Screenshots Toolbox & technical considerations

Considerations for software and hardware

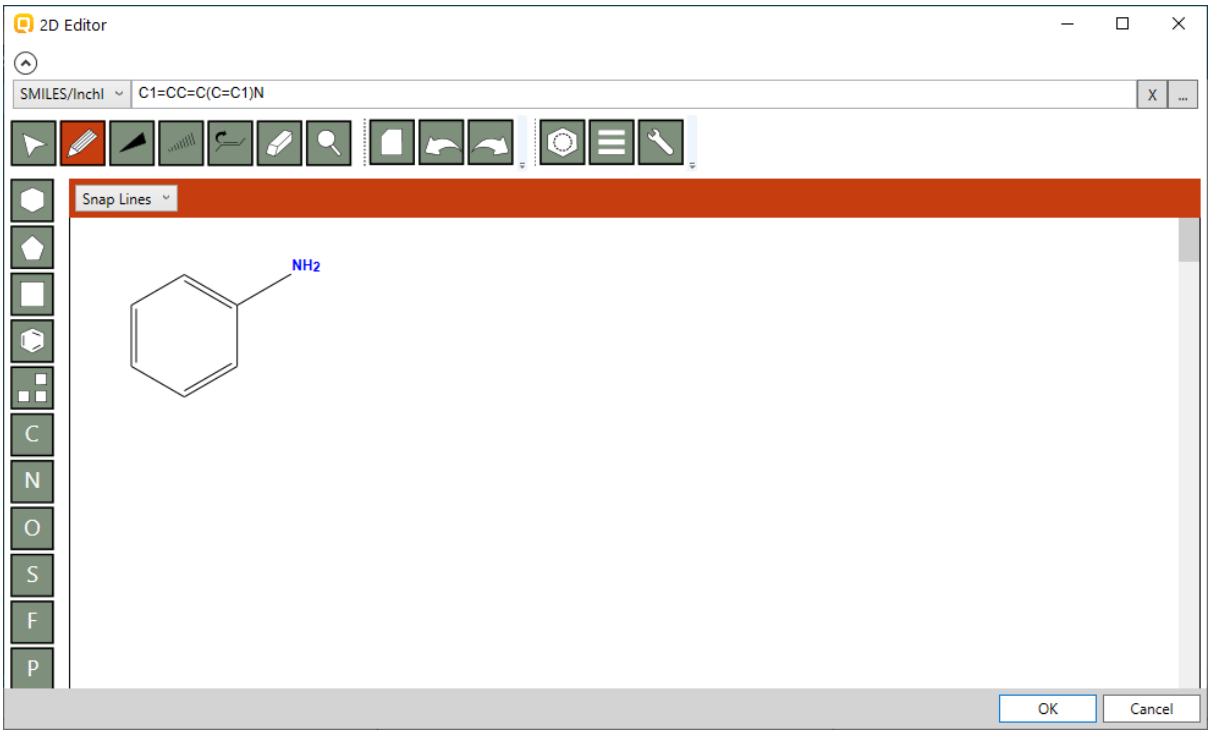
OECD QSAR Toolbox.

Installation of the OECD QSAR Toolbox software requires ~2 GB of free space and both download and installation of the software (after free registration) can take a considerable time. Moreover, users require full admin rights on their operating system for the program to install and function. Large batches of chemicals can be processed in the software and results can be exported as excel tables.
The Toolbox also allows for custom scenario's to be created. Currently a custom scenario is created to assess step 2 (OP-ester and Carbamate) of the TTC approach. However, the TTC values have to be manually assigned. In the future a scenario can be developed that can determine the TTC values directly.

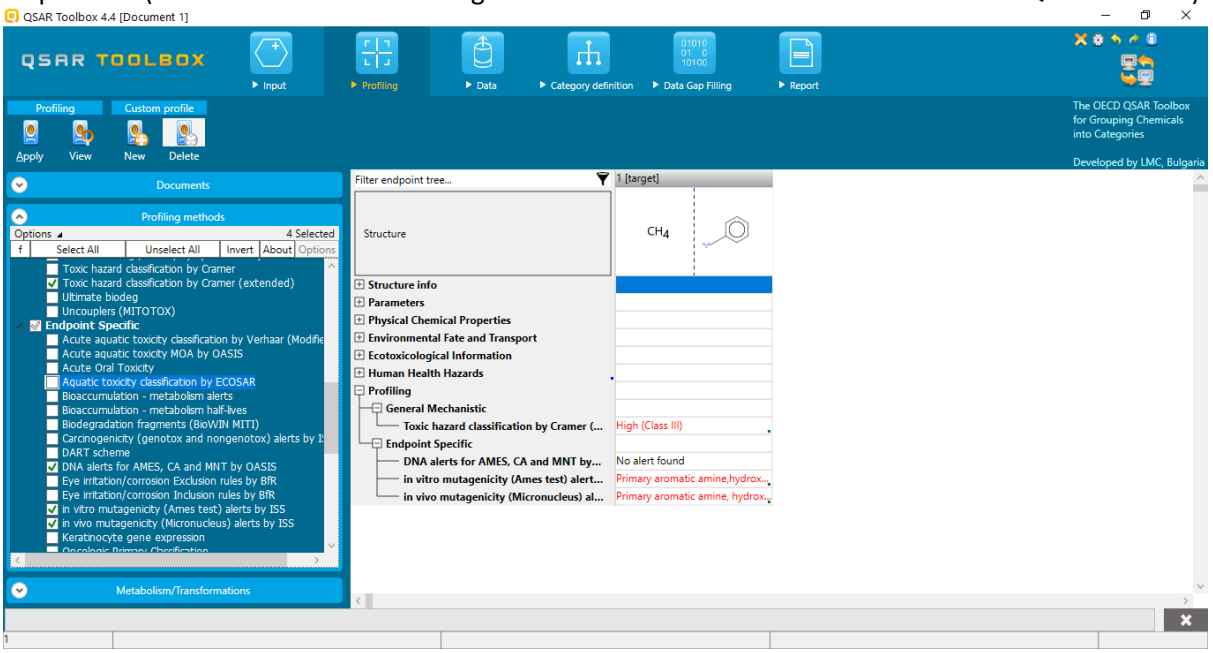
ZZS Similarity tool.

The web-version of the similarity tool only allows the comparison of one substance at a time. However, when provided with a list of SMILES codes, the authors of the tool can perform a batch run to generate the required output. Additionally, For batch generation of Structural Similarity with the appropriate similarity measures either working R-scripts or a KNIME workflow (KNIME software, KNIME | Open for Innovation) of the similarity tool are already available for future prototype developments and can be obtained from the authors (Pim Wassenaar or Emiel Rorije) at RIVM.
An update of the RIVM similarity tool is foreseen for beginning of 2022 that would allow to run batches of structures (SMILES) online and would also allows the input of CAS-numbers.

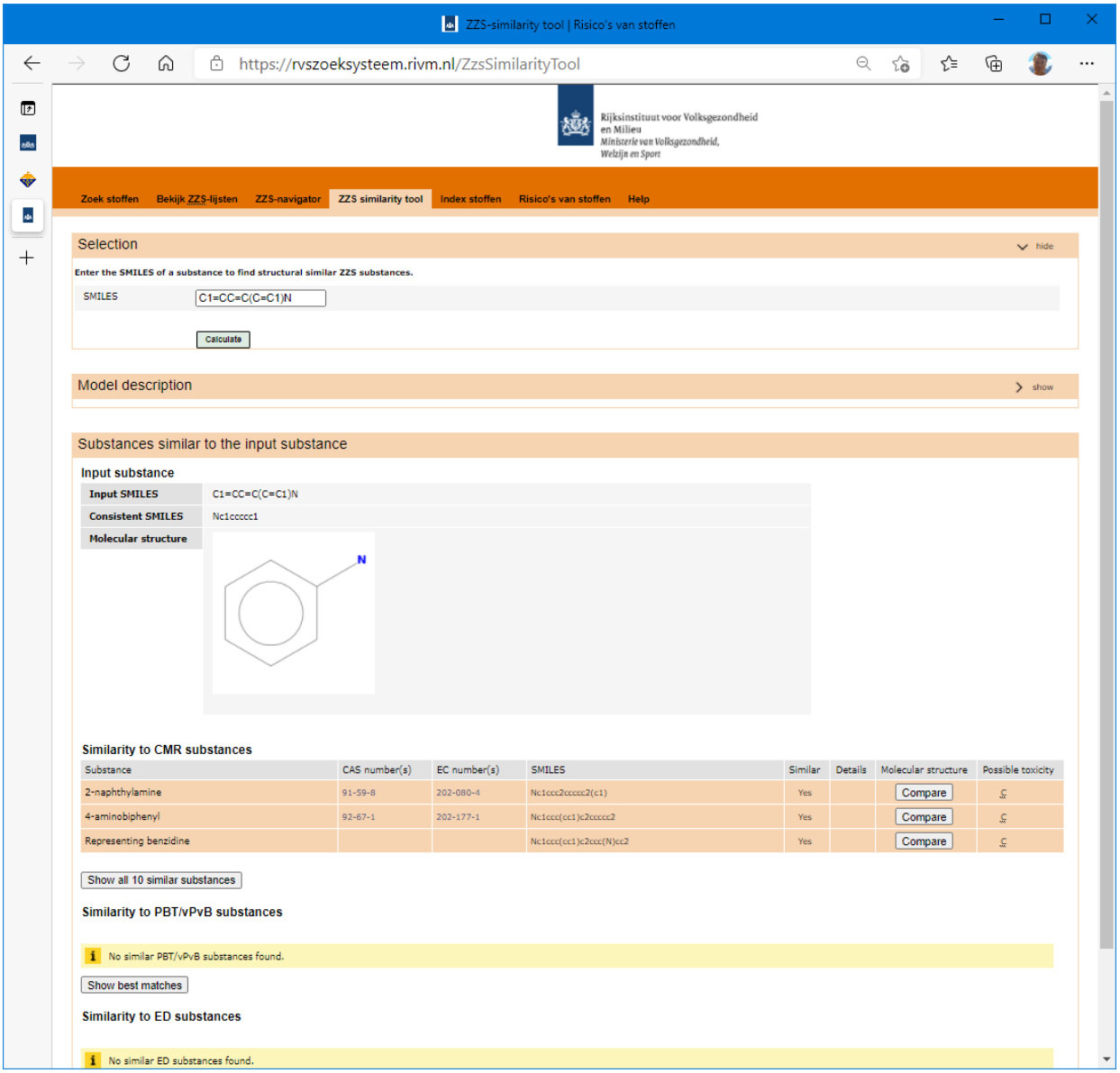
Screenshots QSAR OECD Toolbox



Screenshot 1 – OECD QSAR Toolbox SMILES entry, after selecting the "Structure" button under the "Input" tab (which is the default starting screen in the Classical interface of the OECD QSAR Toolbox).



Screenshot 2 – OECD QSAR Toolbox Profiling result for Aniline, selecting the "Toxic hazard classification by Cramer (extended)", the "DNA Alerts for AMES, CA and MNT by OASIS" the in vitro mutagenicity (Ames test) by ISS" and the "In vivo mutagenicity (Micronucleus) alerts by ISS" Profiling methods (left part of the screen) and pushing "Apply".



Screenshot 3 – ZZS similarity tool at the RIVM website https://rvszoeksysteem.rivm.nl/ZzsSimilaritTool

Annex J : Working with Ecosar

Basics of working with ECOSAR

ECOSAR can be downloaded from the program's website[30]. The installation and use of the program are described in detail in the Operations Manual (US EPA, 2017). Some basic steps are described for illustration.

After accepting the license agreement, the input screen appears as shown below (Figure K.1).

Figure J.1. Screenshot ECOSAR

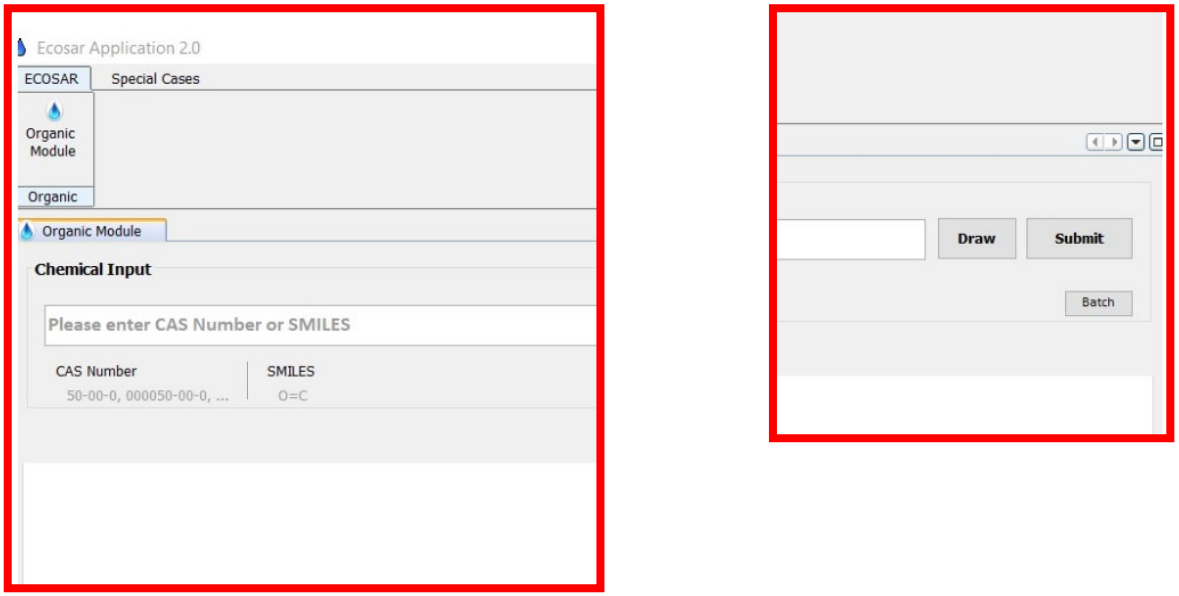


Figure J 2: Input screen of ECOSAR 2.0 with input of chemical identifiers at the left hand side and alternative input options at the right hand side.

Chemicals can be entered using CAS (with or without dashes) or SMILES-code. Alternatively, the Draw-option allows for manual input of specific chemical structures. In case of entering a SMILES-code, ECOSAR may return several options. Required chemical(s) can be selected via the checkbox. Batch input

[30] Ecological Structure Activity Relationships (ECOSAR) Predictive Model | Predictive Models and Tools for Assessing Chemicals under the Toxic Substances Control Act (TSCA) | US EPA

via .txt files is also possible, as further explained in the manual.

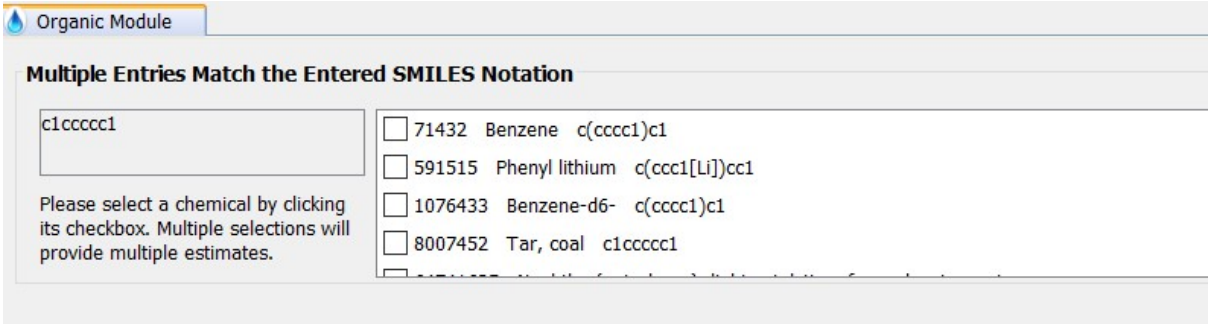


Figure J.3: ECOSAR 2.0 returning different options after entering a SMILES-code.

After entering a chemical identifier (CAS 71432 for benzene in this example), pressing the Submit button will immediately return the results screen (Figure H-3). The different sections of the results screen are briefly explained in the next figures.

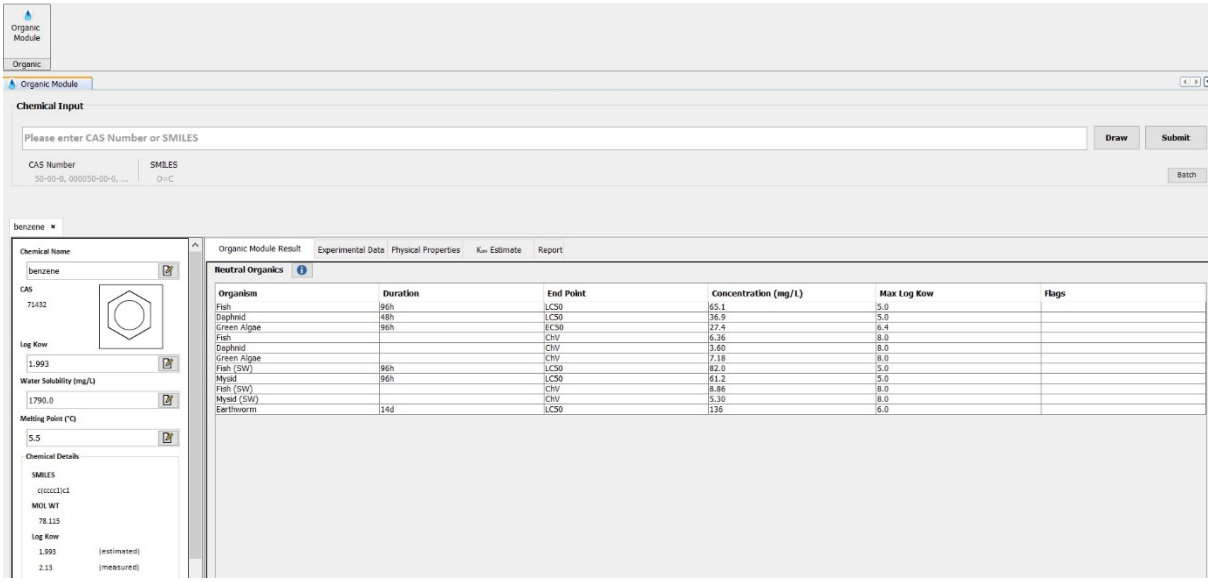


Figure J.4: Lay out of the results screen of ECOSAR 2.0

By default, the result screen opens with the QSAR results displayed in the tab 'Organic Module Result'. The window on the left hand side shows the chemical identity and physico-chemical characteristics used by ECOSAR. Selecting the tab 'physical properties' shows additional experimental physico-chemical data (Figure H.4). The tab 'K_{ow} Estimate' gives the estimated log K_{ow} that is used by ECOSAR as shown on the left. In principle, it is possible to replace the values by user-defined data, e.g. the experimental log K_{ow} shown in the physical-properties tab. However, it is recommended to use the ECOSAR-values, because these were also used in the QSAR training set. Moreover, It is highly preferable for the prioritisation if both the Fate module and ECOSAR use the same log K_{ow} value (either estimated or experimental). By default this is the case since the K_{ow} values used in ECOSAR and in the Fate module are both based on the PHYSPROP database ((EPA, 2012)). When different K_{ow} values are used the difference for most substances will be very small, but occasionally large deviations can be encountered between estimated and measured octanol-water partition coefficients. Even between two separate experimental determinations of log K_{ow} large variation can be observed. For the prioritisation the same log K_{ow} should therefore be used throughout the different steps of the prioritisation process (e.g. in fate modeling and in estimating the ecotoxicological hazard and human exposure).

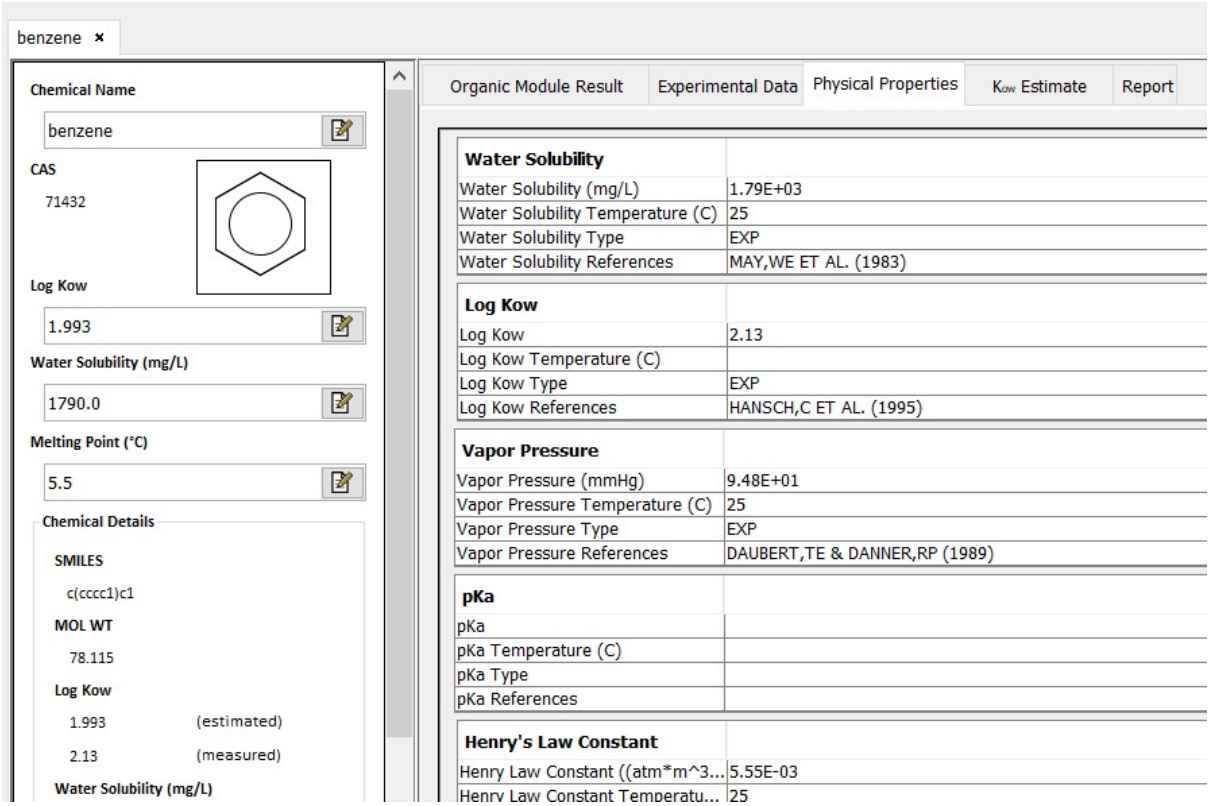
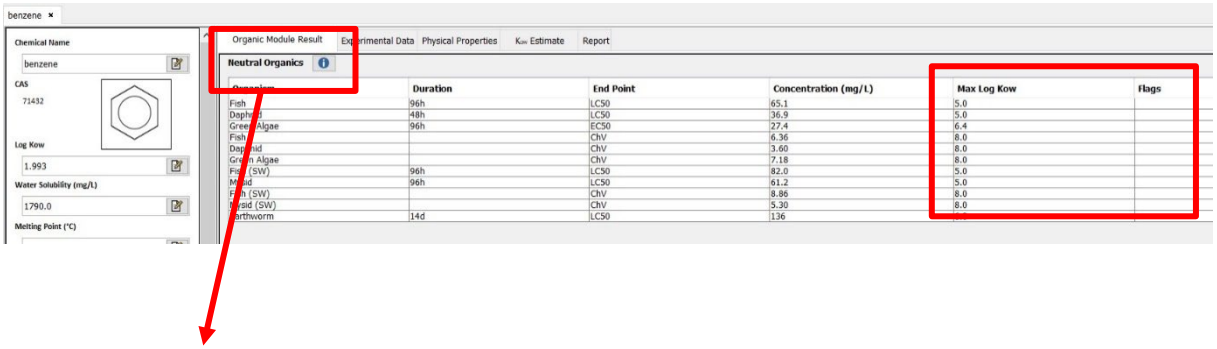


Figure J.5: Identification and physico-chemical properties used by ECOSAR 2.0. The left hand side window shows the properties used by ECOSAR, the tab Physical properties gives background information.

The actual QSAR-results are displayed in the 'Organic Module Result' tab (Figure H.6). The chemical class identified by ECOSAR is given and additional information is shown when clicking the info-button. The column on the right gives the maximum log K_{ow} for which the QSAR is applicable. The flag column is empty in this example, but an exclamation mark will be shown to flag e.g. cases where no effect is expected at the maximum water solubility. Mouse pointing the flag will show a pop-up window with additional information.



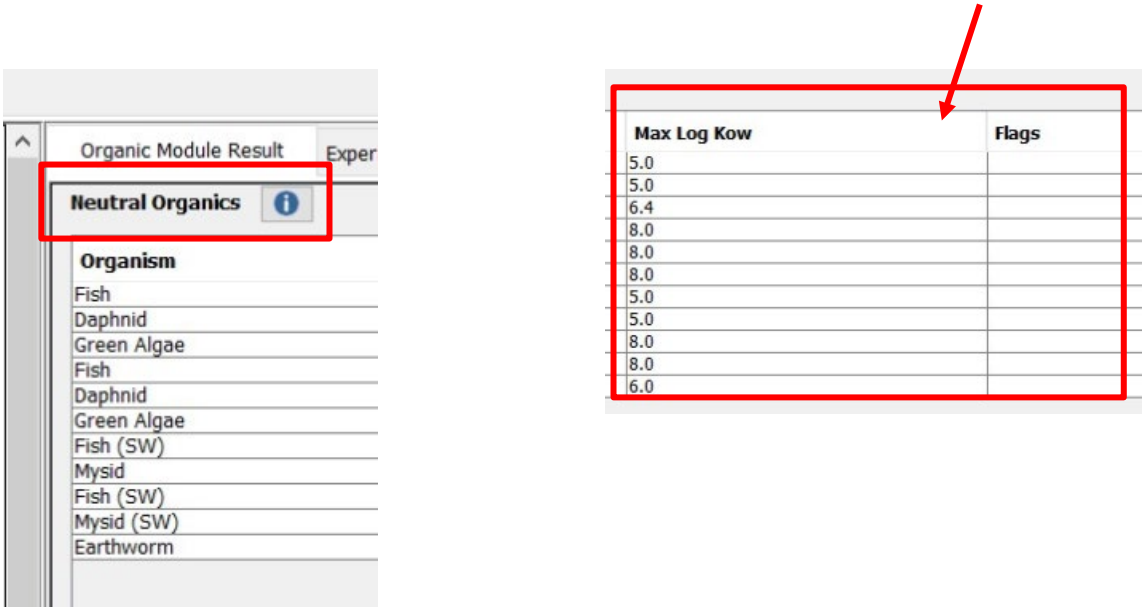


Figure J.6: Example of QSAR results page generated by ECOSAR 2.0. The top three rows give the $L(E)_{50}$ for fish, Daphnids and algae (Figure J.7). In this case, the lowest value of 27.4 mg/L would be selected as the critical value for PNEC-derivation, resulting in a PNEC of 27.4 µg/L when applying the AF of 1000. Underlying experimental aquatic ecotoxicity data are shown in the tab 'Experimental data'. If data are shown in this tab, substance-specific data for the compound under investigation were used to establish the QSAR, which may be assumed to increase the reliability of the prediction for such a compound.

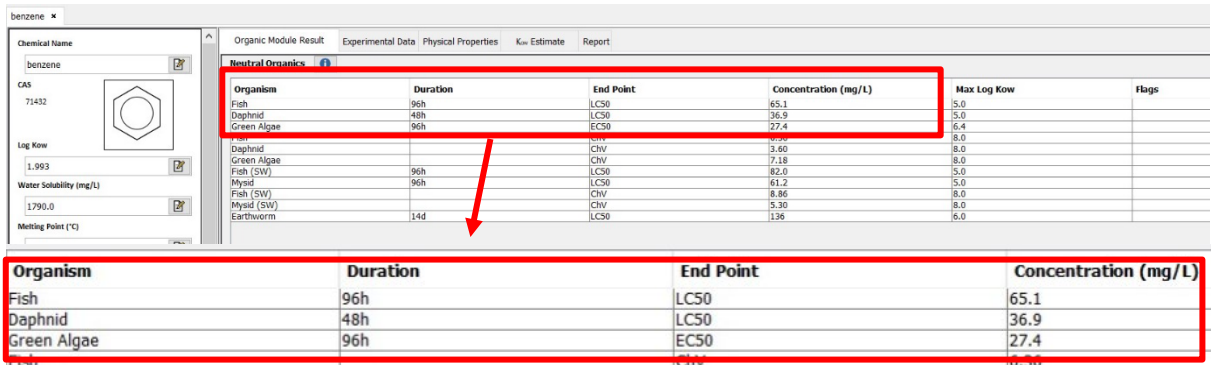


Figure J.7: Acute ecotoxicity values generated by ECOSAR 2.0.

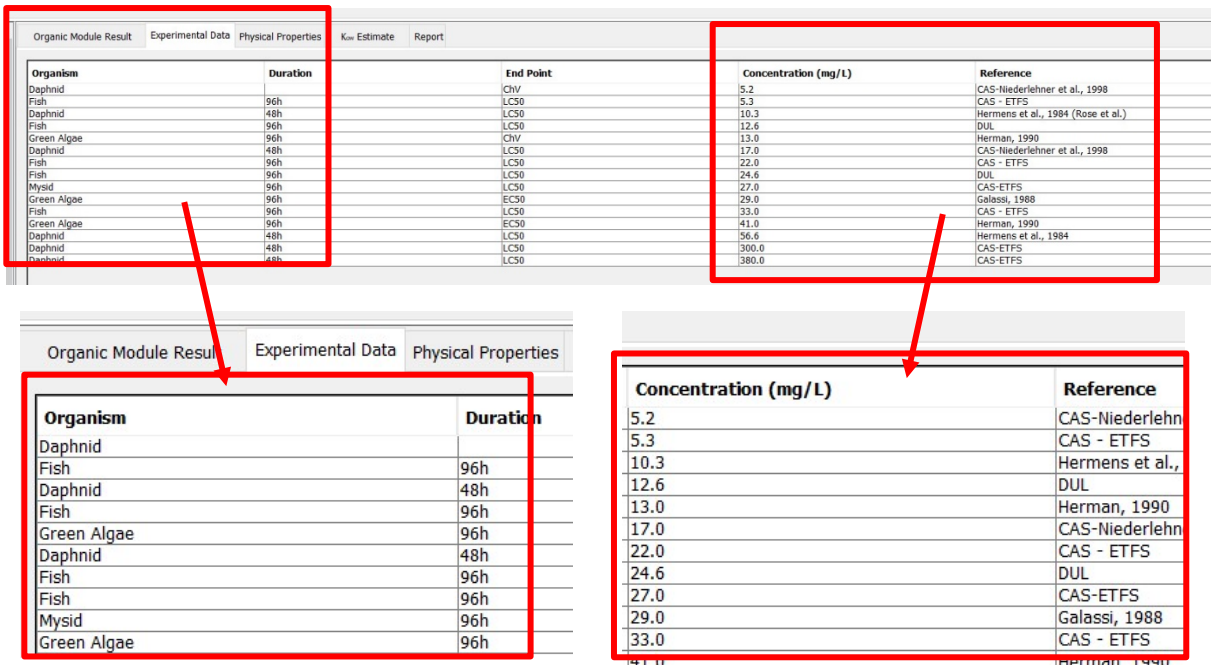


Figure J.8 Experimental ecotoxicity values for the compound of interest included in ECOSAR 2.0.

Finally, clicking the report tab opens a report generator which produces a summary document (Figure H.10) that can be saved or printed (to pdf). When running ECOSAR in batch mode, export to excel is also possible.

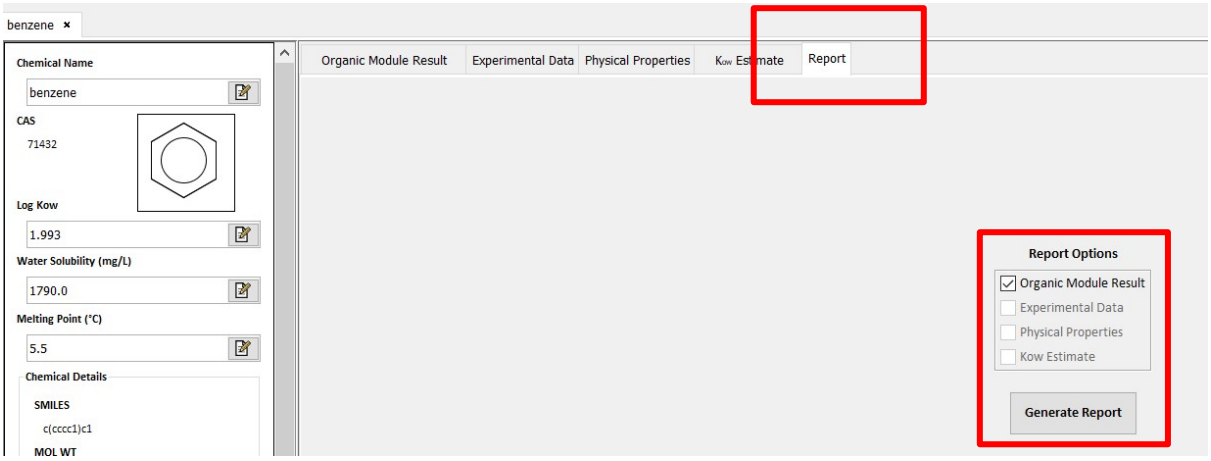


Figure J.10 Report options in ECOSAR 2.0.

The Operations Manual gives an example on how to proceed if the program provides results for multiple substance classes (US EPA, 2017). In the case of permethrin, ECOSAR gives results for esters, vinyl/allyl/propargyl halides, and pyrethroids. Clicking the information icon next to class name gives access to the QSAR class supporting information which can be used to assess structural features of the query compound. From this information, the user needs to determine how many molecular features fit each class definition and whether that class is the most specific available in ECOSAR for this chemical. ECOSAR creates sub-classes for compounds with larger, more complex structural moieties (such as pyrethroids) for which toxicity differs from the more general classes (esters, vinyl/allyl/propargyl halides), even though those simple molecular features are present in the complex compounds. To decide whether or not the sub-class QSAR should be used, the robustness and applicability domain of the respective QSARs should be examined. In the case of permethrin, the QSAR results for esters and

vinyl/allyl/propargyl halides are flagged because the log K_{ow} of permethrin is outside the applicability window of these QSARs. Moreover, the pyrethroid QSAR gives much lower toxicity estimates which are consistent with the experimental data underlying the QSAR. In case of results for multiple substance classes, it is proposed to select the lowest toxicity value. However, for compounds that rank high in Tier 1, expert judgement is always needed, in particular when results from the critical QSAR are flagged or when a less critical QSAR is based on relevant experimental data.

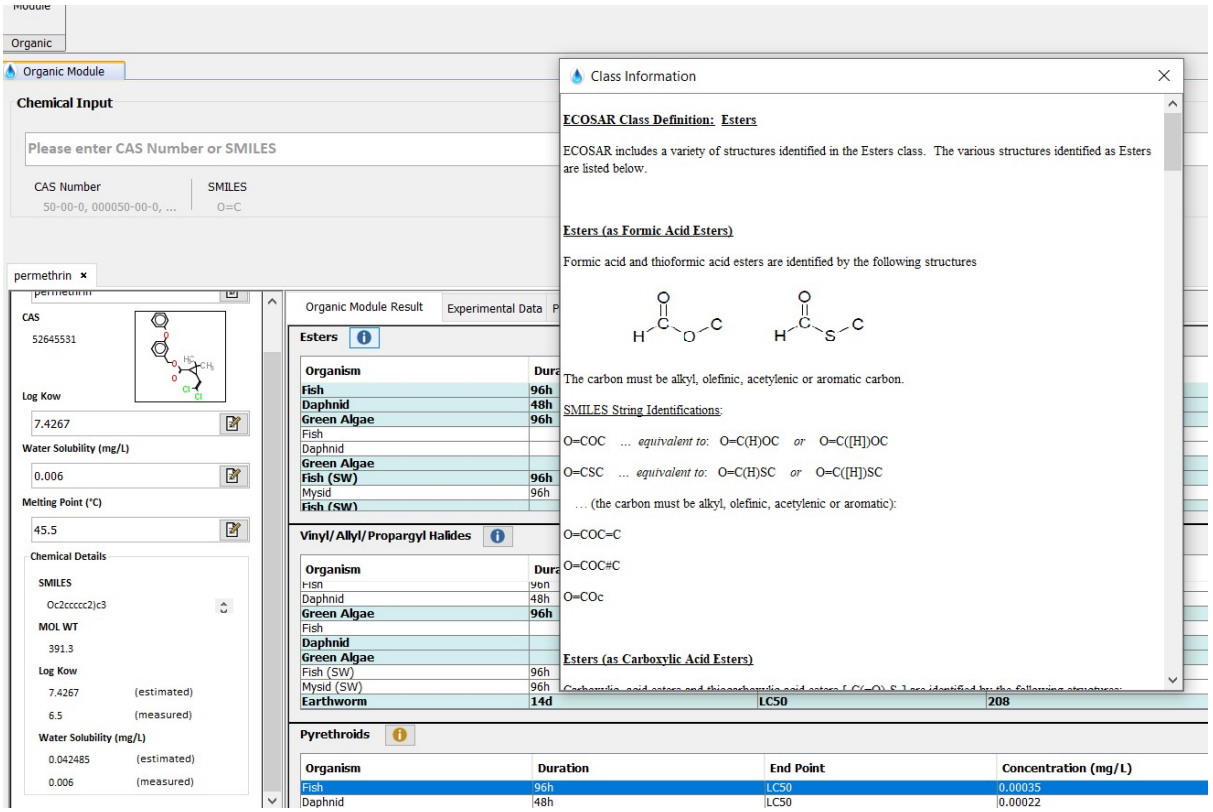


Figure H.11: Example of the ECOSAR 2.0 results window for a substance belonging to multiple chemical classes. Information on class definition is displayed when clicking the information button next to the class name.

Considerations for software and hardware

Ecosar

ECOSAR 2.0 can be downloaded from the US EPA website at https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model. Admin rights are required to install and run the program. In order to use ECOSAR 2.0 in batch-mode a small workaround is advised which requires both CAS-nrs and SMILES codes to function properly.

For the prototype the PNECs were manually chosen from the ECOSAR output one chemical at a time. However, it is possible to develop a script that can assign the PNECs automatically. This will require more work in future projects.

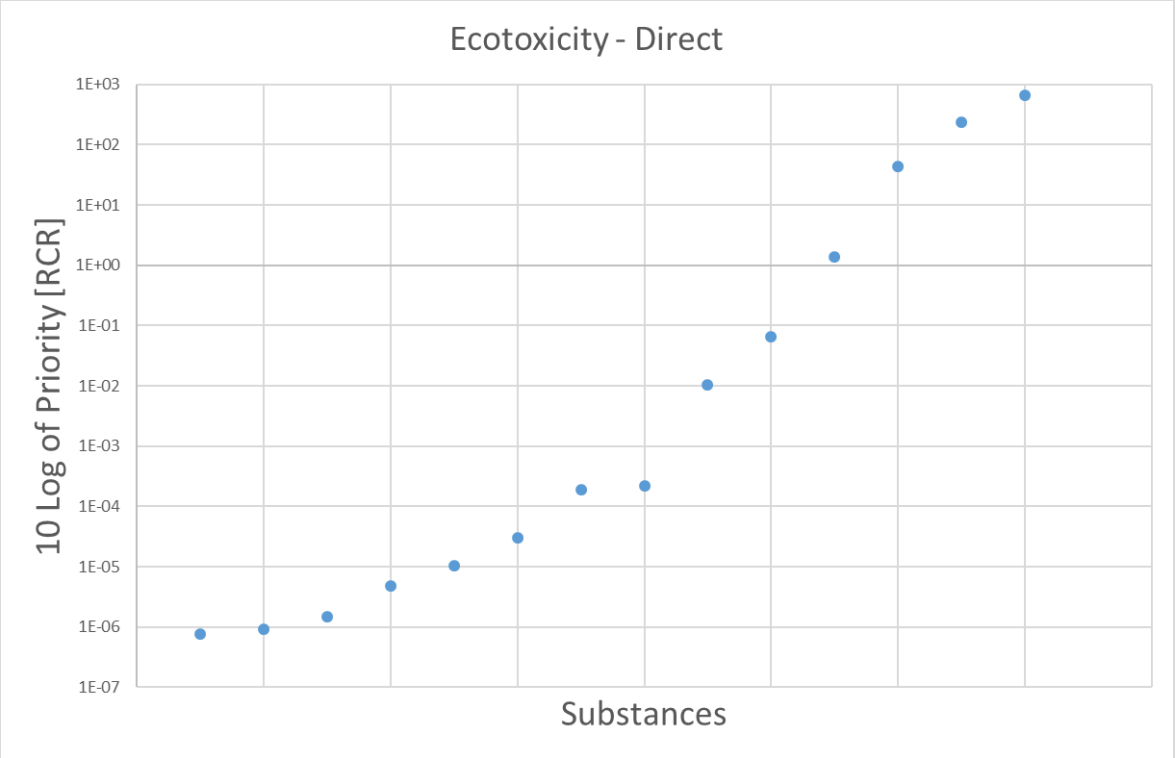
Annex K : Prioritisation results for Belgium and France

Prioritisation Belgium

Direct ecotoxicity

Table 1. Prioritisation of direct ecotoxicity for Belgium. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
4-Nonylphenol	6.48E+02			x	x
S-Metolachlor	2.35E+02				
Bisphenol A	4.35E+01			x	x
Imidacloprid	1.37E+00				
Metolachlor ESA	6.53E-02				
Metolachlor OXA	1.03E-02				
Glyphosate	2.15E-04				
N-EtFOSAA	1.88E-04				
PFOA	3.02E-05	x	x	x	
PFOS	1.04E-05	x	x	x	
PFHxS	4.83E-06	x	x	x	
PFHxA	1.48E-06	x	x	x	
PFBA	9.01E-07	x	x	x	
GenX	7.74E-07	x	x		

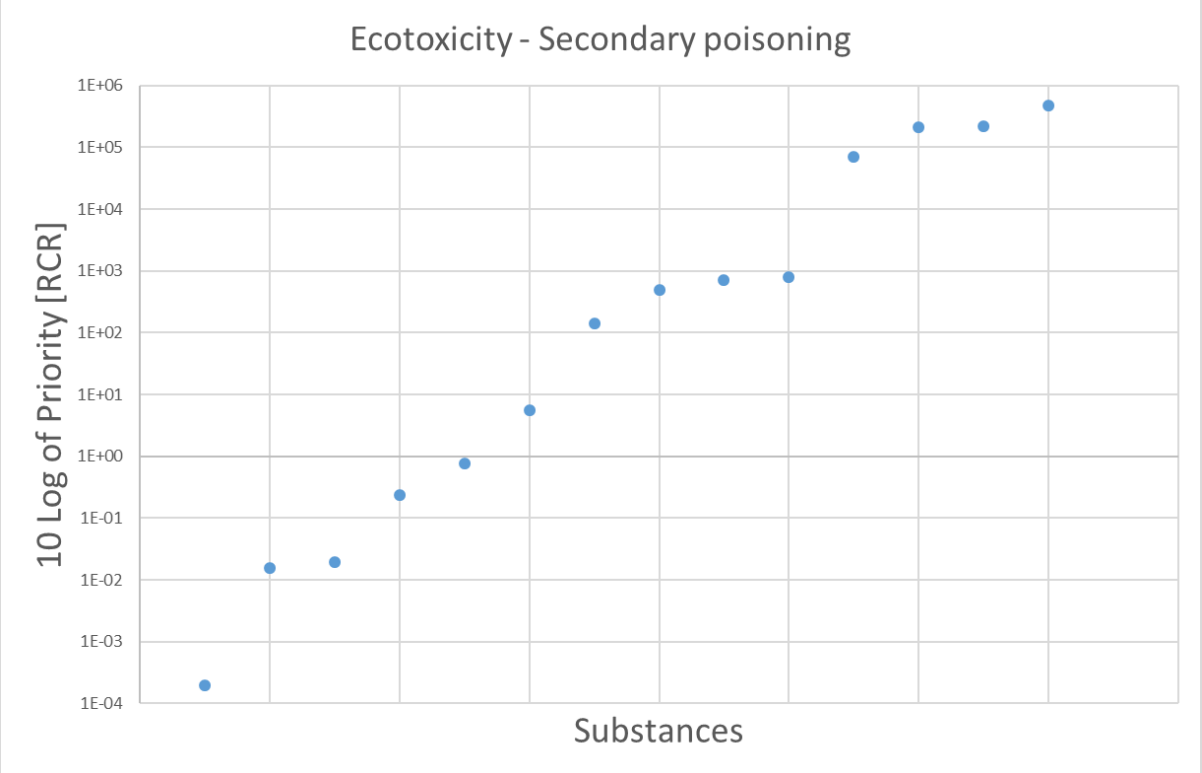


Graph depicting the prioritisation for Direct ecotoxicity for Belgium. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Secondary poisoning

Prioritisation of secondary poisoning for Belgium. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	4.70E+05				
Metolachlor ESA	2.20E+05				
Imidacloprid	2.12E+05				
Metolachlor OXA	6.92E+04				
N-EtFOSAA	8.01E+02				
S-Metolachlor	7.18E+02				
4-Nonylphenol	4.87E+02			x	x
Bisphenol A	1.40E+02			x	x
GenX	5.47E+00	x	x		
PFHxS	7.51E-01	x	x	x	
PFHxA	2.35E-01	x	x	x	
PFOS	1.92E-02	x	x	x	
PFOA	1.56E-02	x	x	x	
PFBA	1.98E-04	x	x	x	

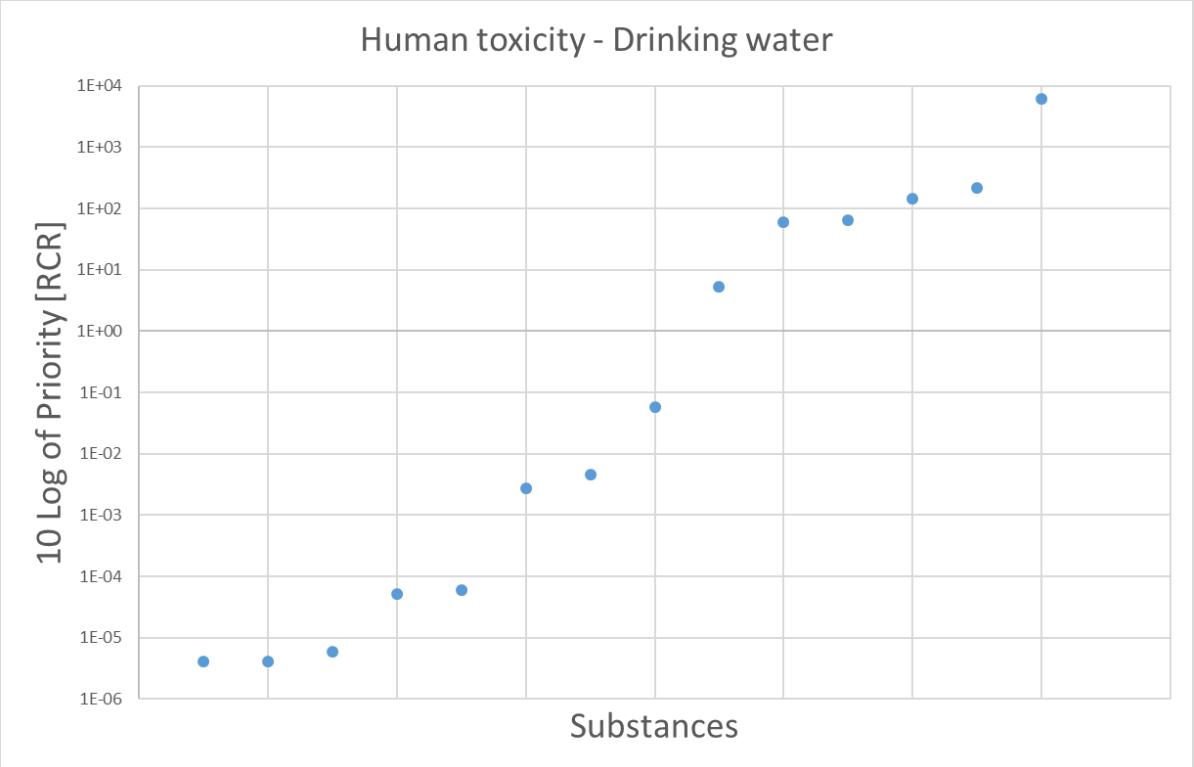


Graph depicting the prioritisation for secondary poisoning for Belgium. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Human toxicity – Groundwater consumption

Prioritisation of human toxicity – groundwater consumption for Belgium. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	6.09E+03				
Imidacloprid	2.20E+02				
Metolachlor OXA	1.45E+02				
Metolachlor ESA	6.49E+01				
S-Metolachlor	5.91E+01				
Bisphenol A	5.31E+00			x	x
4-Nonylphenol	5.76E-02			x	x
N-EtFOSAA	4.56E-03				
GenX	2.68E-03	x	x		
PFHxS	5.97E-05	x	x	x	
PFBA	5.13E-05	x	x	x	
PFHxA	5.98E-06	x	x	x	
PFOS	4.12E-06	x	x	x	
PFOA	4.11E-06	x	x	x	



Graph depicting the prioritisation for human toxicity – groundwater consumption for Belgium. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Human toxicity – ingestion of soil and crops

Prioritisation of human toxicity – ingestion of soil and crops for Belgium. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

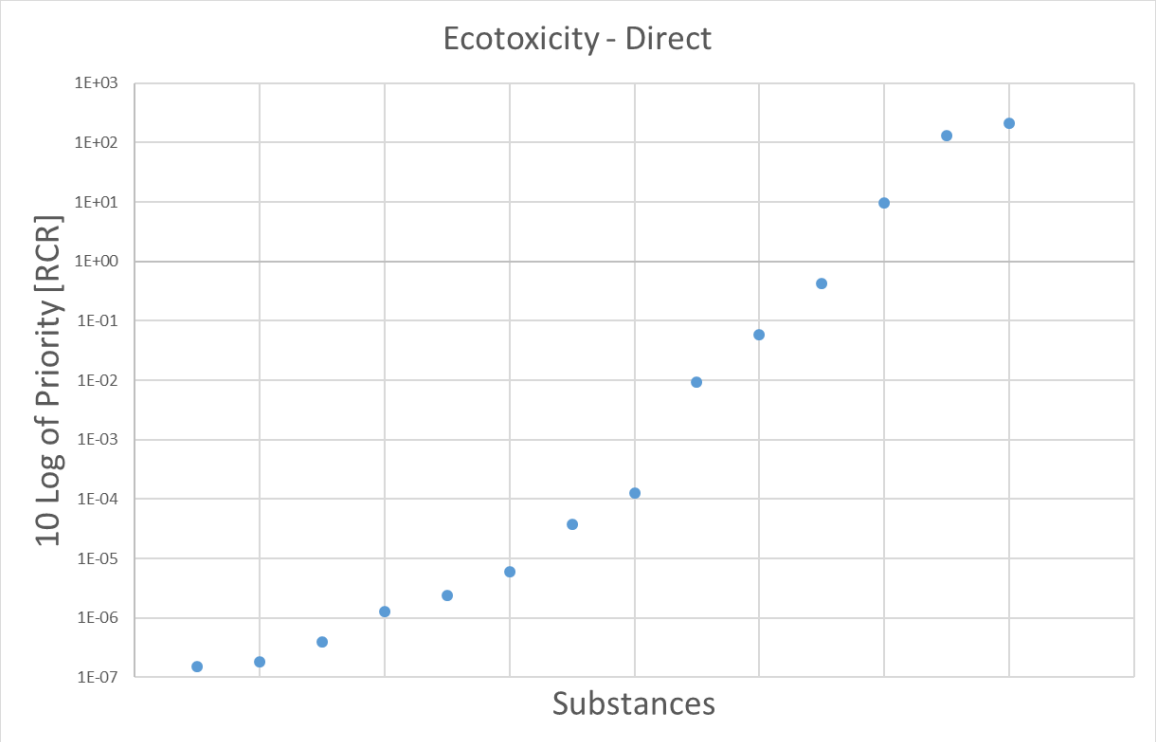
Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	8.04E+04				
Metolachlor ESA	3.77E+04				
Imidacloprid	3.63E+04				
Metolachlor OXA	1.18E+04				
S-Metolachlor	2.01E+01				
Bisphenol A	1.48E+01			x	x
PFHxS	1.29E-01	x	x	x	
PFHxA	4.03E-02	x	x	x	
4-Nonylphenol	6.09E-05			x	x
PFOS	2.39E-06	x	x	x	
N-EtFOSAA	5.16E-07				
GenX	1.06E-08	x	x		
PFBA	1.21E-10	x	x	x	
PFOA	1.83E-11	x	x	x	

Prioritisation for France

Direct ecotoxicity

Prioritisation of direct ecotoxicity for France. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
4-Nonylphenol	6.48E+02			x	x
S-Metolachlor	2.35E+02				
Bisphenol A	4.35E+01			x	x
Imidacloprid	1.37E+00				
Metolachlor ESA	6.53E-02				
Metolachlor OXA	1.03E-02				
Glyphosate	2.15E-04				
N-EtFOSAA	1.88E-04				
PFOA	3.02E-05	x	x	x	
PFOS	1.04E-05	x	x	x	
PFHxS	4.83E-06	x	x	x	
PFHxA	1.48E-06	x	x	x	
PFBA	9.01E-07	x	x	x	
GenX	7.74E-07	x	x		

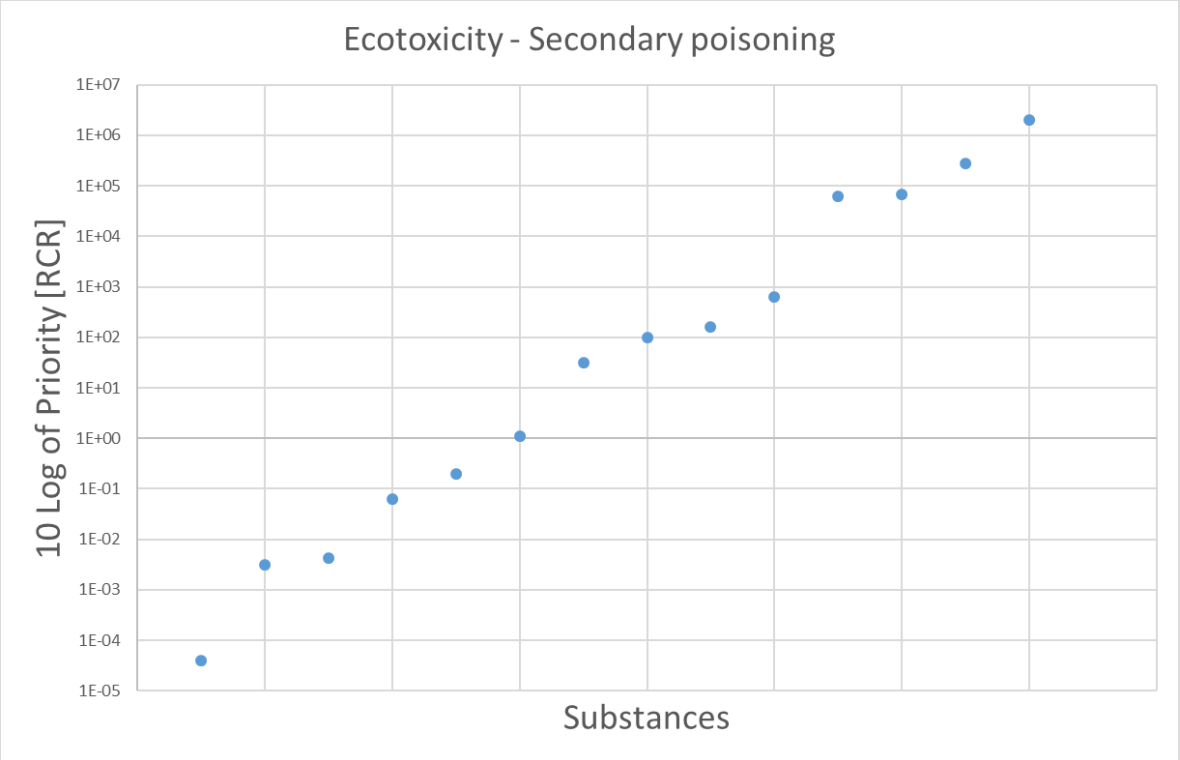


Graph depicting the prioritisation for Direct ecotoxicity for France. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Secondary poisoning

Prioritisation of secondary poisoning for France. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	4.70E+05				
Metolachlor ESA	2.20E+05				
Imidacloprid	2.12E+05				
Metolachlor OXA	6.92E+04				
N-EtFOSAA	8.01E+02				
S-Metolachlor	7.18E+02				
4-Nonylphenol	4.87E+02			x	x
Bisphenol A	1.40E+02			x	x
GenX	5.47E+00	x	x		
PFHxS	7.51E-01	x	x	x	
PFHxA	2.35E-01	x	x	x	
PFOS	1.92E-02	x	x	x	
PFOA	1.56E-02	x	x	x	
PFBA	1.98E-04	x	x	x	

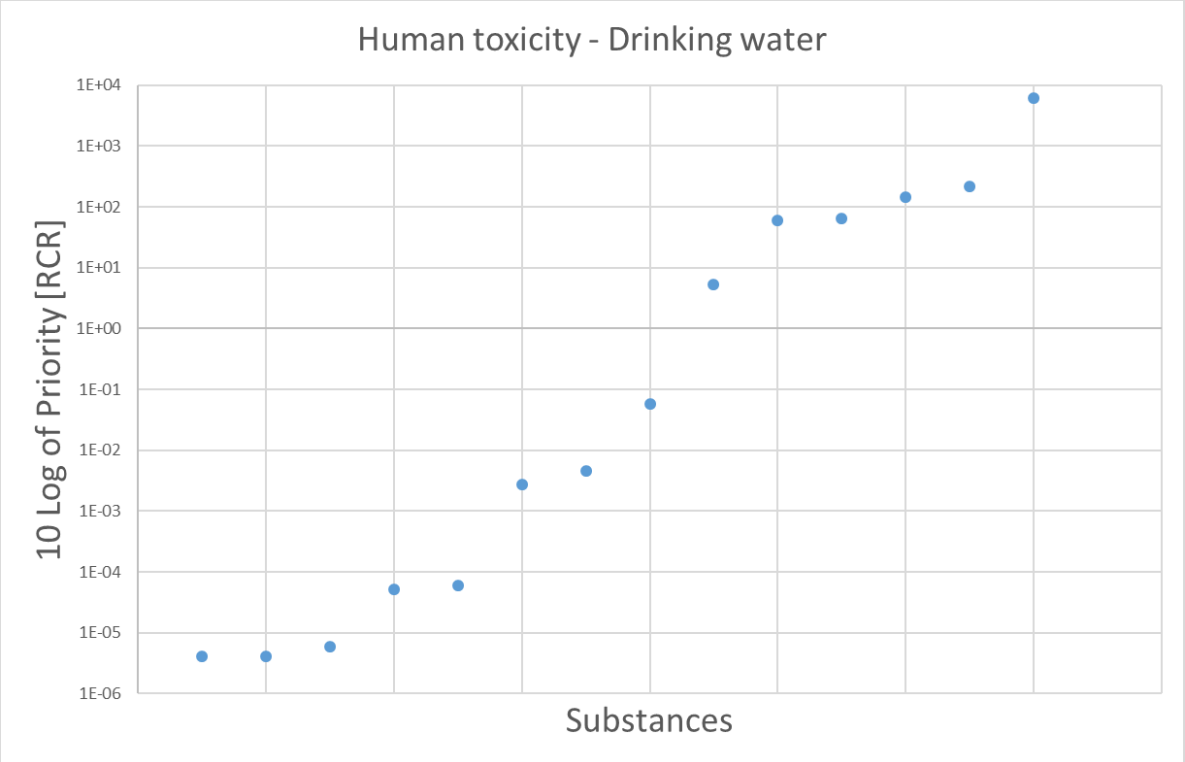


Graph depicting the prioritisation for secondary poisoning for France. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Human toxicity – groundwater consumption

Prioritisation of human toxicity – groundwater consumption for France. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	6.09E+03				
Imidacloprid	2.20E+02				
Metolachlor OXA	1.45E+02				
Metolachlor ESA	6.49E+01				
S-Metolachlor	5.91E+01				
Bisphenol A	5.31E+00			x	x
4-Nonylphenol	5.76E-02			x	x
N-EtFOSAA	4.56E-03				
GenX	2.68E-03	x	x		
PFHxS	5.97E-05	x	x	x	
PFBA	5.13E-05	x	x	x	
PFHxA	5.98E-06	x	x	x	
PFOS	4.12E-06	x	x	x	
PFOA	4.11E-06	x	x	x	

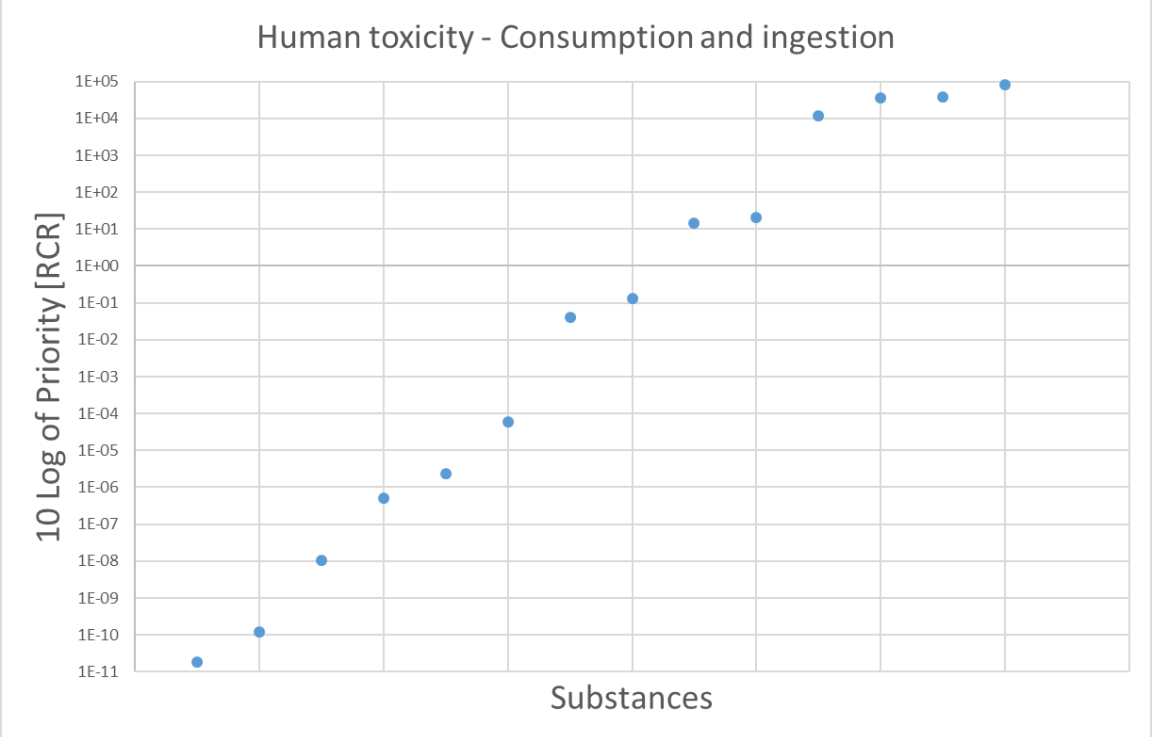


Graph depicting the prioritisation for human toxicity – groundwater consumption for France. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Human toxicity – ingestion of soil and crops

Prioritisation of human toxicity – ingestion of soil and crops for France. The hazard labels are also included. The priority in this table goes from high to low, with the first substance having the highest priority.

Substance	RCR-score	Label PBT	Label vPvB	Label CMR	Label ED
Glyphosate	8.04E+04				
Metolachlor ESA	3.77E+04				
Imidacloprid	3.63E+04				
Metolachlor OXA	1.18E+04				
S-Metolachlor	2.01E+01				
Bisphenol A	1.48E+01			x	x
PFHxS	1.29E-01	x	x	x	
PFHxA	4.03E-02	x	x	x	
4-Nonylphenol	6.09E-05			x	x
PFOS	2.39E-06	x	x	x	
N-EtFOSAA	5.16E-07				
GenX	1.06E-08	x	x		
PFBA	1.21E-10	x	x	x	
PFOA	1.83E-11	x	x	x	



Graph depicting the prioritisation for human toxicity – ingestion of soil and crops for France. The substances are sorted to show the highest priority on the right. The log-scale of the graph shows the trend of the prioritisation.

Annex L: Minutes of stakeholders' meeting

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Soil and land research funding platform for Europe

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