

**HUMAN AND ECOLOGICAL RISK SCREENING
TOOL FOR CHEMICAL POLLUTANTS IN
WASTEWATER EFFLUENTS
(HERWE)**

Background document and user manual



HUMAN AND ECOLOGICAL RISK SCREENING TOOL FOR CHEMICAL POLLUTANTS IN WASTEWATER EFFLUENTS

This document is a result of the projects “*Evaluación de riesgo ambiental y económica de la producción de cultivos energéticos en regadío mediante reutilización de aguas residuales de EDAR*¹” (ref. CTM2007-65544/TECNO), and “*Tratamiento y reutilización de aguas residuales para una gestión sostenible*²” (ref. CSD 2006-00044, www.consolider-tragua.com), funded by the Spanish Ministry of Science and Innovation.

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¹ “Environmental and economic evaluation of energy crops irrigated with urban wastewater”.

² “Treatment and reuse of wastewater for a sustainable management”.

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1. Purpose

This document presents a “Human and Environmental Risk Screening Tool for Chemical Pollutants in Wastewater Effluents (HERWE)”. This tool is intended for wastewater treatment plant managers, public authorities and researchers to support decision making by predicting potential impacts on human health and the environment from wastewater effluent discharges. Using this tool is not synonymous of carrying out a Risk Assessment. Although the models on which this tool relies are based on standard Risk Assessment methods, conducting a complete Risk Assessment is a much more complex process. For this reason, the present tool is suitable only for a preliminary screening of potential impacts at the local scale, using a limited dataset. For a deeper understanding of the Risk Assessment framework, please see the European Union’s Technical Guidance Document on Risk Assessment (TGDR) (EC, 2003).

2. Description of the model

2.1. General principles of Risk Assessment

Risk is estimated by HERWE using a stepwise procedure encompassing the common stages in Risk Assessment (EC, 2003):

- Exposure assessment: estimation of the concentrations/doses to which human populations or environmental compartments are or may be exposed.
- Effects assessment, comprising: a) hazard identification: identification of the adverse effects which a substance has an inherent capacity to cause; and b) dose-response assessment: estimation of the relationship between the level of exposure to a substance (dose, concentration) and the incidence and severity of an effect.
- Risk characterisation: estimation of the incidence and severity of the adverse effects likely to occur in a human population or environmental compartment due to actual or predicted exposure to a substance.

2.2. Main features and limitations of the tool

2.2.1. Target substances in wastewater effluents

HERWE is designed for the assessment of organic substances in general. Inorganic substances like metals can in principle be included as well, but it must be borne in mind that the ability of the tool to handle them is limited, due to several factors that are not heeded, such as bioavailability, natural background concentrations, etc. Therefore, if the focus of the assessment is on risks from metal emissions, other tools should be preferably be used. For an overview on the framework of Risk Assessment for metals, see Fairbrother *et al.* (2007). In addition, as opposed to organic substances, octanol-water partition coefficients (Kow) for metals are not meaningful, because metals bind specifically to carbohydrates rather than lipids, except for mercury (Crommentuijn *et al.* 1997). Since the tool uses Kow to estimate many parameters required in the environmental distribution and exposure assessment, this means that metals require additional effort by the user in order to collect experimental values for all these parameters.

The tool focuses on the concentration of individual pollutants in wastewater effluents. There is no limit to the number of substances that can be included in the screening. As for the type of wastewater effluents, there is neither any particular limitation; as long as the concentration of the pollutants is known, any wastewater (urban/industrial, raw/treated) can be subject to the risk screening.

2.2.2. Data input

We can distinguish three types of data needed by HERWE:

- Pollutant concentration in wastewater: the main input required to the user is the concentration of the target substances in the wastewater effluent. These concentrations, expressed in mg L^{-1} , are the starting point for the tool to calculate the final concentrations in the environment.
- Substance-dependent data: in order to estimate the distribution in the environment, as well as the toxicity thresholds, HERWE requires a number of physical-chemical and toxicological parameters to be defined for each target substance.
- Environmental and exposure parameters: these parameters refer to the characteristics of the environment into which pollutants are emitted, the so-called “standard environment” (see section 2.2.8),

and to the conditions for exposure of humans and other species to the pollutants. All these parameters are given default values, although they can be modified by the user if desired.

For a detailed description of data requirements, see chapter 3.

2.2.3. Hazards included

Risks addressed by the tool are those related to toxic effects in the environment and in humans. Concerning the latter, only non-carcinogenic effects are taken into account. The areas of protection, for which risk characterisation ratios are calculated, are the following:

- Soil organisms
- Terrestrial (worm-eating) predators
- Fresh water organisms
- Fresh water sediment-dwelling organisms
- Fresh water (fish-eating) predators
- Sea water organisms
- Sea water sediment-dwelling organisms
- Sea water (fish-eating) predators
- Sea water top predators
- Humans

Several hazards are not yet considered in Risk Assessment. Some examples are global warming, ozone depletion, acidification, eutrophication, depletion of raw materials, effects on materials, calamities and hazardous waste. Other tools, such as Life Cycle Assessment (Guinée et al. 2002), can be used to assess some of these environmental impacts.

2.2.4. Underlying models

HERWE performs most of the calculations based on the methods suggested by the TGDRA. Where alternative methods have been used, these are explicitly stated.

2.2.5. Worst-case approach

The exposure assessment is based on reasonable worst-case results by applying unfavourable, but not unrealistic, standard exposure scenarios and, as much as possible, mean, median or typical parameter values, as suggested in the TGDRA.

2.2.6. Risk screening

The output of the tool is a risk characterisation ratio (RCR) for each substance and area of protection. As it has been stated in section 1, this RCR is not the result of a complete Risk Assessment of a substance, but a preliminary screening of potential risks when this substance is released to the environment by a wastewater treatment plant (WWTP). If the outcome of the risk characterisation indicates that the substance is not of concern ($RCR < 1$), the assessment for that substance can be stopped with regard to the area of protection considered. If, in contrast, the outcome is that the substance is of concern ($RCR > 1$), a refined Risk Assessment should be conducted.

2.2.7. Wastewater effluent scenarios

The tool allows the user to assess three alternative scenarios:

- Discharge of the effluent to an aquatic ecosystem
- Discharge of the effluent to a marine ecosystem
- Reuse of the effluent in agriculture

These scenarios are assessed at the same time by the tool, so that the user is able to obtain the risk characterisation results for all three scenarios in one run. However, the user may be only interested in one or two of them, or just in a particular area of protection in a given scenario, for example the risk to soil organisms when wastewater is reused in agriculture.

In each scenario the number and type of areas of protection may differ, as can be seen in table 1. On the other hand, human health is included in all the scenarios, but the exposure routes considered are different.

Table 1. Areas of protection included in the three scenarios considered.

Discharge of the effluent to an aquatic ecosystem	Discharge of the effluent to a marine ecosystem	Reuse of the effluent in agriculture
<ul style="list-style-type: none"> ▪ Fresh water organisms ▪ Fresh water sediment-dwelling organisms ▪ Fresh water (fish-eating) predators ▪ Humans (exposed to drinking water and Fresh water fish) 	<ul style="list-style-type: none"> ▪ Sea water organisms ▪ Sea water sediment-dwelling organisms ▪ Sea water (fish-eating) predators ▪ Sea water top predators ▪ Humans (exposed to Sea water fish) 	<ul style="list-style-type: none"> ▪ Soil organisms ▪ Terrestrial (worm-eating) predators ▪ Humans (exposed to leaf and root crops, drinking water, milk and meat)

2.2.8. Standard environment

The concentrations of substances released from WWTPs are assessed for a generic local environment. This is not an actual site, but a hypothetical site with predefined, agreed environmental characteristics, the so-called "standard environment" (TGDR, part II, p. 16). These standard environmental conditions can be average values, or reasonable worst-case values, depending on the parameter in question. HERWE uses default values for environmental parameters, as suggested in the TGDR, but they can be adapted for particular situations (e.g. the fraction of organic carbon in soil, or the volume of irrigation water used in agriculture are some examples of parameters for which default values can be changed to make them more representatives of a particular location) if a site-specific assessment is required.

2.2.9. Spatial scale

A complete Risk Assessment usually includes several spatial scales. EUSES (EC, 2004), the software tool for carrying out Risk Assessments according to the TGDR, includes three spatial scales: local, regional and global. A distinction is usually made between substances that are emitted through point sources at specific locations and substances that enter the environment through diffuse releases. According to the TGDR, point source releases have a major impact on the environmental concentration on a local scale, and also contribute to the environmental concentrations on a larger scale. Since a wastewater effluent discharge can be clearly considered as a point source, HERWE has been designed to take into account the local scale only. Therefore the environmental concentrations are estimated in the vicinity of the emission source.

2.2.10. Time scale

Local emissions can either be continuous or discontinuous. Since the activity under study is wastewater treatment, it is assumed that a continuous discharge to the environment occurs. In the case of agricultural reuse, the same is assumed (irrigation is assumed to occur on a daily basis). This means that local concentrations are calculated on the basis of a daily release rate. In principle, degradation and distribution processes are taken into consideration on the local scale. However, because of the relatively small time scale, the ultimate concentration in a compartment is typically governed by only one or two key processes. Only for the soil compartment (being a less dynamic environment) do longer-term averages apply.

2.2.11. Excluded upstream and downstream processes

While a complete Risk Assessment requires the complete life cycle of a substance to be included, HERWE is only concerned with processes taking place downstream of the wastewater treatment plant. As a consequence, upstream processes such as production of the substance, its use by industries or consumers, as well as the wastewater treatment process itself, are disregarded. Treatment of wastewater sludge is also excluded.

2.2.12. “GIGO”

The acronym GIGO, coined by computer scientists, stands for “garbage in, garbage out”. This acronym is used here to call attention to the fact that mathematical models can only produce output data of good quality when the corresponding input data are good too. The user of HERWE needs a sufficient degree of expertise to be able to evaluate the quality of the input data, to make a proper data selection, to understand the assumptions made as well as the inherent limitations of the estimation methods, and, finally, to correctly interpret the results. Even with a perfect model, unreliable results can still be obtained if quality control of input data is neglected or performed in a very rough manner.

2.2.13. Uncertainty

A model can never give an exact representation of reality. This is due to the complexity of reality, and our limited knowledge of it. Furthermore, the data available for a model are often incomplete and contain measurement errors. In risk assessment, we are typically confronted with this situation, as the available data are limited and mechanisms often poorly understood. The values for nearly all parameters are therefore accompanied by a significant amount of uncertainty, not only resulting from limited scientific understanding, but also from natural variability in time and space. Pollutant concentrations in wastewater effluents, as an example, can be measured with reasonable accuracy. Nevertheless, variability in time can be a significant source of uncertainty. Furthermore, differences between locations will result in large spatial variability. As a consequence, a tool like HERWE can only give an approximation of the potential risk of a substance.

2.2.14. Validation

A strict validation of a model like HERWE is not possible. The outcome of this tool is a risk estimate: for example, a PEC/PNEC quotient (quotient of the Predicted Environmental Concentration and the Predicted No-Effect Concentration for an endpoint). These risk estimates are abstractions and cannot be determined in the real world. Nevertheless, an evaluation in a less strict manner should be performed to clarify the degree

of confidence in the final results. Wastewater concentrations can be measured. Nevertheless, exposure, as modelled by this tool is usually not representative of a particular situation, for two reasons: in the absence of specific data, several chemical-specific parameters are set to worst-case values, and the assessment is performed for a worst-case exposure scenario, the so-called “standard environment”. Measured field data will invariably be non-representative for this situation. The concept of a standard scenario clearly plays a crucial role in the assessment and its applicability and appropriateness should be considered in a model validation.

The use of a standard scenario does not mean that HERWE is “not valid”. In fact, its purpose is not to predict actual effects or concentrations occurring in the environment. In fact, the system will provide the user with a conservative estimate for a non-existing standard environment, based on limited data requirements.

2.3. Environmental distribution and exposure assessment

The goal of the exposure assessment is to estimate the predicted environmental concentrations or doses to which organisms in ecosystems and humans will be exposed. In the exposure assessment the calculations proposed by the TGDRA are followed. Nevertheless, one of the scenarios included in HERWE, namely agricultural wastewater reuse, is not included in the TGDRA. For this reason, a set of original equations are suggested in order to take into account this exposure route for terrestrial organisms and humans.

For a detailed understanding of the calculations, the reader is required to consult the TGDRA and EUSES documents.

Not all substances are subject to assessing all the exposure routes. In particular, exposure of benthic organisms through sediments and of predators through secondary poisoning should only be assessed for substances with a high sorption and accumulation capacity.

2.3.1. Predicted environmental concentration in surface water (PEC_{water})

The concentration in surface water is calculated after complete mixing of the effluent. Because of the short time between effluent discharge and exposure, dilution will usually be the dominant process. Therefore, degradation in surface water, volatilisation from the water body and sedimentation are not taken into account as removal processes. A standard dilution factor (10) is used and adsorption to suspended matter is accounted for. PEC in surface water is calculated with eq. 45 in the TGDRA (part II, p. 76), where $C_{\text{local}_{\text{eff}}}$, representing the concentration of the pollutant in wastewater effluent, is not estimated as in the TGDRA, but entered by the user of HERWE. If measured data for $C_{\text{local}_{\text{eff}}}$ are not available, the estimation method by the TGDRA (eq. 33, part II, p. 62) can alternatively be used.

2.3.2. Predicted environmental concentration in surface water sediment ($PEC_{\text{water sed}}$)

The concentration of pollutant in bulk sediment is derived from the corresponding water body concentration, assuming a thermodynamic partitioning equilibrium (Di Toro et al. 1991). Therefore, PEC_{water} is used in the calculation as shown in eq. 50 of the TGDRA (part II, p. 78).

In HERWE a $\log K_{ow} \geq 3$ is used as trigger criterion for assessment of sediment toxicity (TGDRA, part II, p. 111). In the case of metals, where a $\log K_{ow}$ is not available, this rule does not apply and they are included by default.

2.3.3. Predicted environmental concentration in sea water (PEC_{seawater})

The local concentration in sea water is obtained with eq. 83 in the TGDRA (part II, p. 142). This is basically the same expression used in the calculation of PEC_{water} with the only difference that a different default dilution factor is used, namely 100 instead of 10.

2.3.4. Predicted environmental concentration in sea water sediment ($PEC_{\text{seawater sed}}$)

The concentration of pollutant in bulk marine sediment is derived from the corresponding sea water concentration, assuming a thermodynamic partitioning equilibrium (Di Toro et al. 1991). Therefore, PEC_{seawater} is used in the calculation as shown in eq. 87 of the TGDRA (part II, p. 144).

In HERWE a $\log Kow \geq 3$ is used as trigger criterion for assessment of sediment toxicity (TGDRA, part II, p. 111). In the case of metals, where a $\log Kow$ is not available, this rule does not apply and they are included by default.

2.3.5. Predicted environmental concentration in soil (PEC_{soil})

Exposure assessment for the soil compartment is important with respect to exposure of terrestrial organisms. Furthermore, crops for human consumption are grown on agricultural soils and cattle, producing meat and milk, graze on grasslands. For wastewater effluent irrigation a typical Spanish application rate of $495 \text{ L m}^{-2} \text{ year}^{-1}$ is used as default (National Statistics Institute, 2008).

A simple, one-compartment soil model is used. The top layer of the soil compartment is described, with influx of pollutants from irrigation only, and removal from the box by degradation, volatilisation and leaching. Accumulation of a substance may occur when wastewater is applied over consecutive years. As default scenario, wastewater is assumed to be applied for 10 consecutive years. This is the period of time considered in the TGDRA for sludge application to soil. Nevertheless, the user is allowed to adapt this period of time to his needs.

Since the concentration in soil is not constant in time (it is higher just after irrigation and lower just before the next irrigation event), for exposure of the endpoints, the concentration needs to be averaged over a certain time period. Different averaging times are used for these end-points: for the ecosystem a period of 30 days is used. In order to determine biomagnification effects and indirect exposure to man, an extended period of 180 days is used (see table 11 in TGDRA, part. II, p. 85).

The TGDRA considers only two possible routes for pollutants to enter the soil compartment: aerial deposition and application of wastewater sludge, which are not considered in HERWE. In order to accommodate wastewater irrigation as a route for pollutant exposure, the following equation is used:

$$D_{\text{irr}} = \frac{C_{\text{local}}_{\text{eff}} \text{ APPL}_{\text{water}}}{\text{DEPTH}_{\text{soil}} \text{ RHO}_{\text{soil}}} \quad (1)$$

Where D_{irr} is the substance daily flux to soil through irrigation ($\text{mg kg}_{\text{wwt}}^{-1} \text{ d}^{-1}$), $C_{\text{local}}_{\text{eff}}$ is the concentration in wastewater effluent (mg L^{-1}), $\text{APPL}_{\text{water}}$ is the wastewater irrigation rate ($\text{L m}^{-2} \text{ d}^{-1}$), $\text{DEPTH}_{\text{soil}}$ is the mixing depth of soil (m), and RHO_{soil} is the bulk density of soil ($\text{kg}_{\text{wwt}} \text{ m}^{-3}$). This expression is similar to that used in the TGDRA for calculating the concentration in soil due to sludge application at $t=0$ (eq. 60, part II, p. 83), but here the parameters C_{sludge} and $\text{APPL}_{\text{sludge}}$ of eq. 60 are substituted by $C_{\text{local}}_{\text{eff}}$ and $\text{APPL}_{\text{water}}$, respectively.

The concentration in soil after n years of continuous irrigation is determined with eq. 2, assuming an initial concentration of zero:

$$C_{irr,n} = \frac{D_{irr}}{k} - \frac{D_{irr}}{k} \cdot e^{-365 n k} \quad (2)$$

Where $C_{irr,n}$ is the concentration ($\text{mg kg}_{\text{wwt}}^{-1}$) of pollutant in soil at the beginning of year n, and k is a substance-specific first order rate constant for removal from top soil (d^{-1}). This constant is calculated with eq. 56 in the TGDRA, and includes the following removal processes: volatilisation, leaching to groundwater and biodegradation. The final concentration in soil (PEC_{soil} , in $\text{mg kg}_{\text{wwt}}^{-1}$) is calculated with eq. 3:

$$PEC_{\text{soil}} = \frac{D_{irr}}{k} + \frac{1}{kT} \cdot \left(C_{irr,n} - \frac{D_{irr}}{k} \right) \cdot \left(1 - e^{-kT} \right) \quad (3)$$

Where T is the averaging time (days). Equation 3 is similar to eq. 55 in the TGDRA (part II, p. 81). Three different PECs can be calculated with eq. 3: PEC_{soil} , $PEC_{\text{agr soil}}$ and $PEC_{\text{grassland}}$. PEC_{soil} is used for the exposure of soil organisms, $PEC_{\text{agr soil}}$ is used for exposure of humans through crops and for secondary poisoning of terrestrial predators, and $PEC_{\text{grassland}}$ is used for exposure of humans through animal products (dairy and meat). The values of T and DEPTH_{soil} are different depending on the PEC to be calculated, as can be seen in table 11 of the TGDRA (part. II, p. 85).

2.3.6. Secondary poisoning of aquatic fish-eating predators ($PEC_{\text{water predator}}$)

Starting from the concentration in the environment, the resulting concentration in food of higher organisms is estimated. This exposure concentration is compared to the avian or mammalian toxicity of the chemical as an indication of possible effects on birds and mammals in the environment via the food chain. Secondary poisoning of aquatic fish-eating predators involves the following food chain:

Freshwater → *fish* → *fish-eating predator*

The concentration of pollutant in fish ($PEC_{\text{water predator}}$) is estimated with eq. 76 in the TGDRA (part II, p. 127), based on the concentration in water (PEC_{water}) and the potential bioconcentration and biomagnification of the substance. In HERWE a $\log Kow \geq 3$ is used as trigger criterion for bioaccumulation potential in secondary poisoning (TGDRA, part II, p. 124). In the case of metals, where a log Kow is not available, this rule does not apply and they are included by default.

It must be noted that according to the TGDRA, 50% of the diet of fish-eating predators is assumed to originate at the regional scale and the remaining 50% at the local scale. Since only the latter is included in HERWE, we have to assume that the concentration of the pollutant at the regional scale is zero. The user is allowed to change the percentage of the local scale as a source of food, from 0% to 100%.

2.3.7. Secondary poisoning of marine fish-eating predators ($PEC_{\text{seawater predator}}$)

Secondary poisoning of marine fish-eating predators involves the following food chain:

Seawater → *fish* → *fish-eating predator*

The concentration of pollutant in fish ($PEC_{\text{seawater predator}}$) is estimated with eq. 89 in the TGDRA (part II, p. 159), based on the concentration in water (PEC_{seawater}) and the potential bioconcentration and biomagnification of the substance. In HERWE a $\log Kow \geq 3$ is used as trigger criterion for bioaccumulation

potential in secondary poisoning (TGDR, part II, p. 124). In the case of metals, where a log Kow is not available, this rule does not apply and they are included by default.

It must be noted that according to the TGDR, 50% of the diet of fish-eating predators is assumed to originate at the regional scale and the remaining 50% at the local scale. Since only the latter is included in HERS-WW, we have to assume that the concentration of the pollutant at the regional scale is zero. The user is allowed to change the percentage of the local scale as a source of food, from 0% to 100%.

2.3.8. Secondary poisoning of marine top predators ($PEC_{\text{seawater top predator}}$)

Secondary poisoning of marine fish-eating predators involves the following food chain:

Seawater → fish → fish-eating predator → top-predator

The concentration of pollutant in food of marine top predators is estimated with eq. 90 in the TGDR (part II, p. 159), based on the concentration in water (PEC_{seawater}) and the potential bioconcentration and biomagnification of the substance. In HERWE a log Kow ≥ 3 is used as trigger criterion for bioaccumulation potential in secondary poisoning (TGDR, part II, p. 124). In the case of metals, where a log Kow is not available, this rule does not apply and they are included by default.

It must be noted that according to the TGDR, 90% of the diet of marine top predators is assumed to originate at the regional scale and only the remaining 10% comes from the local scale. Since only the latter is included in HERS-WW, we have to assume that the concentration of the pollutant at the regional scale is zero. The user is allowed to change the percentage of the local scale as a source of food, from 0% to 100%.

2.3.9. Secondary poisoning of terrestrial worm-eating predators ($PEC_{\text{soil predator}}$)

Secondary poisoning of worm-eating birds or mammals involves the following food chain:

Soil → earthworm → worm-eating predator

The PEC in worm-eating predators is calculated by means of eq. 82c in the TGDR (part II, p. 132), using $PEC_{\text{agr soil}}$ and $PEC_{\text{agr soil porewater}}$, i.e. the concentration of pollutant in porewater of agricultural soil, which is in turn calculated by equilibrium partitioning with eq. 67 in the TGDR (part II, p. 85). In HERWE a log Kow ≥ 3 is used as trigger criterion for bioaccumulation potential in secondary poisoning (TGDR, part II, p. 124). In the case of metals, where a log Kow is not available, this rule does not apply and they are included by default.

It must be noted that according to the TGDR, 50% of the diet of worm-eating predators is assumed to originate at the regional scale and the remaining 50% at the local scale. Since only the latter is included in HERWE, we have to assume that the concentration of the pollutant at the regional scale is zero. The user is allowed to change the percentage of the local scale as a source of food, from 0% to 100%.

2.3.10. Human exposure through food and drinking water (PHD_{water} , PHD_{seawater} , PHD_{soil})

The routes for human exposure are different according to the scenario considered:

- Discharge to aquatic environment (figure 1): in this scenario humans are exposed to the pollutant by means of drinking water and fish, the latter being assumed to be entirely originated from rivers/lakes.
- Discharge to marine environment (figure 2): in this scenario the only exposure route is contaminated fish, which is assumed to be entirely caught in sea water.

- Reuse in agriculture (figure 3): this scenario involves exposure through leaf and root crops, meat and dairy from animals grazing in contaminated grassland, and drinking water which is assumed to be originated from groundwater.

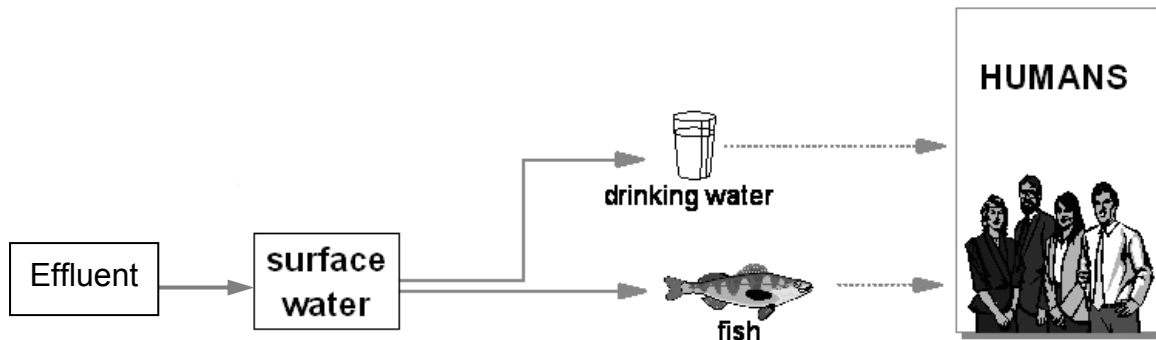


Figure 1. Exposure routes included in the aquatic discharge scenario. Source: adapted from EC, 2004.

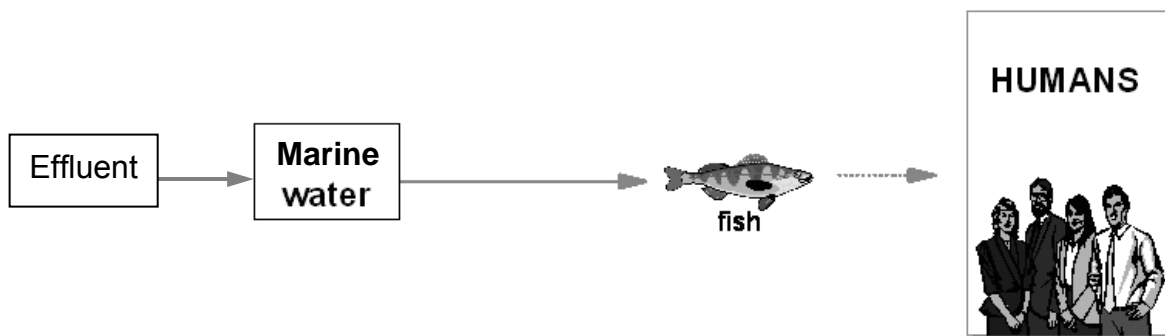


Figure 2. Exposure routes included in the marine discharge scenario. Source: adapted from EC, 2004

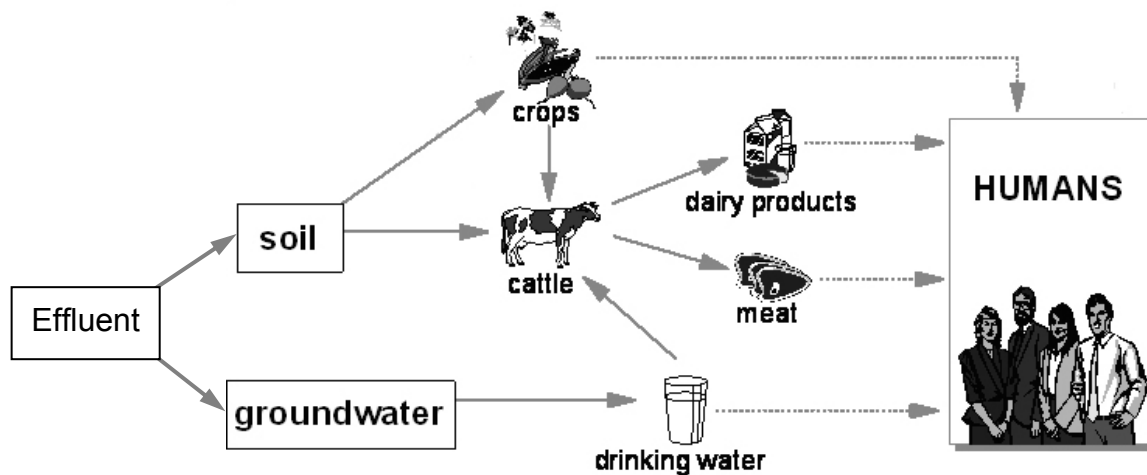


Figure 3. Exposure routes included in the agricultural reuse scenario. Source: adapted from EC, 2004

As it can be seen in the figures, the source of drinking water and fish is different in each scenario. Concerning fish, it is only considered in the scenarios where pollutants are discharged to either surface or sea water. In the agricultural reuse scenario, the model does not include connections between the compartment affected, agricultural soil, and the surface and sea water compartments. For this reason, fish is

excluded from the reuse scenario. As for drinking water, in the sea water scenario it is excluded since it is assumed that water used in drinking water production plants is taken from freshwater bodies. With regard to the aquatic discharge and reuse scenarios, drinking water is assumed to be originated entirely in the compartments affected by these scenarios. In the aquatic discharge scenario this corresponds to surface water, while in the reuse scenario the model only includes the connection from soil to groundwater, but not to surface water. For this reason, the reuse scenario considers that all water abstracted for drinking comes from groundwater resources.

It can also be seen that there is no exposure from the air compartment. First of all, this is due to the fact that the pollutants being assessed are not emitted to the atmosphere but to the hydrosphere or soil. The model at the local scale does not include volatilisation from water or soil as a potential exposure route, and it is thus excluded. For highly volatile substances this is a clear limitation of HERWE. In order to take this route into account, a more complex model should be used, such as a level III fugacity model (Mackay et al. 1992). This kind of model is implemented in the EUSES software (EC, 2004), in order to evaluate distribution of the pollutants at the regional scale. A stand-alone level III model can be downloaded at the Canadian Centre for Environmental Modelling and Chemistry web site³.

In HERWE, assessment of human exposure via the environment is carried out according to the methods described in the EUSES 2.0 background report (EC, 2004) in section III.5.2. It comprises the following steps:

- Assessing the concentrations in intake media (food and drinking water), as done in section III.5.2.1 to III.5.2.4.
- Assessing the intake rate of each medium using a standard consumption pattern, namely that shown in table III-89 of EC (2004)
- Combining the concentrations in the media with the intake of each medium, as done in eqs. 206 to 209 of EC (2004).

The outcome of these calculations is a so-called predicted human dose (PHD), which will be different in each scenario, due to the different exposure routes considered.

Owing to the considerable uncertainties accompanying the methodology, it serves primarily for screening purposes. The concentration of a substance in food is estimated from its concentration in water, soil and its bioconcentration or bioaccumulation behaviour. The estimation of most bioconcentration factors (BCF) or bioaccumulation factors (BAF) is highly dependent on K_{ow} . These estimations are therefore only valid for organic, non-ionised or non-dissociating chemicals. Metals can also be evaluated if experimental BCFs are known.

The local assessment of HERWE involves that all food products are derived from the vicinity of the discharge point source. Clearly, the local situation represents a worst case. People do not consume 100% of their food products from the immediate vicinity of a point source. Therefore, the local assessment represents a situation which does not exist in reality. In the light of the above limitations, it is clear that a generic indirect-exposure assessment, as required in this framework, can only be used to indicate potential problems. The assessment should be seen as a helpful tool for decision-making and not as a prediction of human exposure actually occurring at some place or time.

³ <http://www.trentu.ca/academic/aminss/envmodel/models/VBL3.html>

2.4. Effects Assessment

Effects assessment concerns the hazard identification and dose-response assessment of toxicological and ecotoxicological data. In ecotoxicological effects assessment, Predicted No-Effect Concentrations (PNECs) are derived from experimental toxicity data using assessment factors. In human toxicological effects assessment, a human reference dose is derived from the available data.

2.4.1. Aquatic toxicity ($PNEC_{water}$)

The following ecotoxicity end-points can be used, in order of preference, for aquatic organisms:

- PNEC: there are PNEC values available for many pollutants. It is preferred to use existing PNEC values in order to avoid the use of assessment factors.
- NOEC: long-term NOECs for (typically) fish, Daphnia, and algae can be used along with assessment factors to obtain a PNEC.
- LC50/EC50: in the absence of NOECs, acute endpoints like LC50 or EC50 for (typically) fish, Daphnia, and algae can be used along with assessment factors to obtain a PNEC.

It is common for emerging pollutants to lack experimental toxicological data. In such a case, reliable quantitative structure-activity relationships (QSAR) estimates for fish, Daphnia and algal toxicity are available for chemicals with a non-specific mode of action. These estimates can be used in the effects assessment to estimate a PNEC.

Assessment factors in HERWE can be entered manually. Otherwise, the tool is prepared to apply default assessment factors, according to table 16 in the TGDRA (part II, p. 101).

2.4.2. Aquatic sediment toxicity ($PNEC_{sed}$)

Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms. To avoid extensive testing of chemicals a log Kow of ≥ 3 can be used as a trigger value for sediment effects assessment.

Toxicity data for sediment-dwelling organisms is scarce. In the absence of any ecotoxicological data for sediment-dwelling organisms, according to the TGDRA the PNEC may provisionally be calculated using the equilibrium-partitioning method. This method which is regarded as a "screening approach" uses the PNEC for aquatic organisms and the sediment-water partition coefficient (eq. 70 in part II, p. 113). In the partitioning method, it is assumed that:

- Sediment-dwelling organisms and water-column organisms are equally sensitive to the chemical.
- Concentration in sediment, interstitial water and benthic organisms are in thermodynamic equilibrium: the concentration in any of these phases can be predicted using the appropriate partition coefficients.
- Sediment-water partition coefficients can either be measured or derived on the basis of a generic partition method from separately measurable characteristics of the sediment and the properties of the chemical.

Regardless of whether the partition coefficient in sediment is measured or estimated, the following remark should be noted for the calculation of the PNEC using the equilibrium-partitioning method. The approach considers uptake via the water phase only, but uptake may also occur via ingestion of sediment. This may become important, especially for adsorbing chemicals. Thus, for these compounds the total uptake may be underestimated. There is evidence from studies in soil (Belfroid et al. 1995) that the proportion of the total

dose remains low for chemicals with a log Kow up to 5. The possible underestimation of exposure is considered acceptable when using the equilibrium-partitioning method for chemicals with a log Kow between 3 and 5. For compounds with a log Kow greater than 5 or with a corresponding adsorption or binding behaviour, the equilibrium method is used in a modified form, according to the TGDR: in order to take uptake via ingestion of sediment into account, the PEC/PNEC ratio in sediment is increased by a factor of 10 in risk characterisation for these compounds. This correction is not performed with heavy metals, due to the lack of Kow data.

According to the TGDR, when only acute toxicity data are available (at least for one species), PNEC is calculated on the basis of both the most sensitive species for which data are available using an assessment factor of 1000, and the equilibrium partitioning method. The lowest $PNEC_{sed}$ is used in risk characterisation.

Finally, when long-term toxicity test data are available for benthic organisms the $PNEC_{sed}$ must be calculated using assessment factors for long-term tests and this result should prevail in the risk assessment (See table 19 in section 3.5.4 of the TGDR (part II, p. 114).

Assessment factors in HERWE can be entered manually. Otherwise, the tool is prepared to apply default assessment factors according to what has been mentioned above.

2.4.3. Sea water toxicity ($PNEC_{seawater}$)

The greater diversity of taxa in the marine environment, compared to freshwaters, will produce a broader distribution of species sensitivity. In those cases where only data for freshwater or saltwater algae, crustaceans and fish are available a higher assessment factor should be applied than that for the derivation of $PNEC_{water}$ for freshwaters. This higher assessment factor reflects the greater uncertainty in the extrapolation. Where data is available for additional marine taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a data set can be lowered. The assessment factors for $PNEC_{seawater}$ used in HERWE are those in table 25 of the TGDR (part II, p. 149). The user of HERWE can enter specific assessment factors, or let the tool apply the default assessment factors from table 25.

2.4.4. Sea water sediment toxicity ($PNEC_{seawater\ sed}$)

Marine sediment effects assessment is necessary for substances that are known to be persistent in marine waters, and may accumulate in sediments over time. To avoid extensive testing of chemicals a log Kow ≥ 3 can be used as a trigger value for sediment effects assessment.

The assessment of effects in seawater sediments is similar to that for aquatic sediments. In the absence of experimental toxicity data, the equilibrium partitioning method is used, according to eq. 88 in the TGDR (part II, p. 153). When experimental data is available, the same procedures described for $PNEC_{sed}$ apply.

2.4.5. Soil toxicity ($PNEC_{soil}$)

For most chemicals, the number of toxicity data on soil organisms will be limited. To compensate for this lack of toxicity data, the equilibrium-partitioning method is therefore used, following the approach used for sediment. For some substances, however, it is possible to obtain acute toxicity data estimations for earthworms using QSARs (see section 3.3).

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, is influenced by these soil properties. This means that results from different test soils cannot be compared directly. If possible data should be normalised using relationships describing the bioavailability of chemicals in soils (see eq. 71 in the TGDRA, part II, p. 116).

According to the TGDRA, three situations can be distinguished for deriving a PNEC for soil:

- If no toxicity data are available for soil organisms, the equilibrium-partitioning method is applied to identify a potential risk to soil organisms (eq. 72 in the TGDRA, part II, p. 117). This method is regarded as a 'screening approach' and has been already explained for sediment.
- If toxicity data are available for a producer (plant), a consumer and/or a decomposer (microorganism, earthworm), the PNEC is calculated using assessment factors. The assessment factors are presented in table 20 of the TGDRA (part II, p. 118).
- If only one test result with soil-dwelling organisms is available, the risk assessment is performed both on the basis of this test, using assessment factors, and on the basis of the equilibrium-partition method. From these two PNECs, the lowest is chosen for risk characterisation.

Assessment factors in HERWE can be entered manually. Otherwise, the tool is prepared to apply default assessment factors according to table 20 in the TGDRA.

As with sediment, the equilibrium-partitioning method for soil assumes that the bioavailability and therefore toxicity of chemicals to soil organisms is determined only by the concentration in the pore water of the soil. Further effects that chemicals adsorbed to soil particles may have on soil organisms via ingestion are not considered in this approach. In order to compensate for this limitation, the same approach is used as for the derivation of the PNEC of sediment: in order to take uptake via ingestion of soil into account, the PEC/PNEC ratio in soil is increased by a factor of 10 for compounds with a log Kow > 5 in the risk characterisation.

2.4.6. Secondary poisoning (PNEC_{oral})

If secondary poisoning is to be avoided, the concentration of chemicals in food for predators should be below the No-Observed-Effect Concentration (NOEC) in a (sub)chronic dietary toxicity test with animals representative of fish-eating birds or mammals. The NOEC is considered as a maximum concentration in food which will not lead to adverse effects after ingestion of this food. Only toxicity studies reporting on dietary and oral exposure are relevant, as the pathway for secondary poisoning refers exclusively to uptake through the food chain. The results of these tests may be expressed as a concentration in the food (NOEC in mg/kg) or a dose (NOAEL in mg/kg body weight/day) causing no effect. For the assessment of secondary poisoning, the results must be expressed as the concentration in food (mg/kg food). In the absence of a NOEC, the NOAEL for mammals and birds is converted to a concentration in food by means of equations 77 and 78 in the TGDRA (part II, p. 128). Acute lethal doses (LD50, rat, bird) are not suitable for extrapolation to chronic toxicity, as these tests are not dietary tests. Acute-effect concentrations (LC50, 5 day avian dietary studies) are acceptable for extrapolation because these are dietary studies.

PNEC_{oral} is calculated using eq. 79 in the TGDRA (part II, p. 129), by applying the corresponding assessment factors in table 23 of the same document (part II, p. 130). In HERWE it is possible to apply user-defined assessment factors, or otherwise let the tool choose the most appropriate among those from table 23. This PNEC_{oral} is used in the risk characterisation to predict risks for all kinds of predators: terrestrial worm-eating predators, aquatic fish-eating predators, marine fish-eating predators and marine top predators.

2.4.7. Human reference dose (HRD)

Only non-carcinogenic effects of substances are included in HERWE. The HRD is used in the tool as a human toxicity threshold that should not be exceeded. The HRD can be set by the user by means of the following data, in order of preference:

- Acceptable daily intake (ADI) values or Reference Dose (RfD) values. These values represent the maximum oral intake values for which long-term adverse effects are not expected. They are the result of extensive toxicological testing with animals, and assessment factors are already included to account for different kinds of uncertainty.
- When the above values are not available, NOAEL or LOAEL values from oral exposure in mammals can be used. In this case, an assessment factor must be applied to account for uncertainty related to inter-species variability, human variation in sensitivity, etc. In order to derive a HRD from NOAEL, an assessment factor of 100 is used (Falk-Filipsson et al. 2007), while from LOAEL to HRD an additional factor of 3 is used (ECETOC, 2003), leading to an assessment factor of 300.
- In the absence of a NOAEL or LOAEL, which is a very likely situation for emerging pollutants, acute toxicity data in mammals (LD50 oral) can be used to derive a preliminary HRD, as shown by Layton et al. (1987). When LD50 from a mammal is used an assessment factor of 10^5 is applied.

Again, the assessment factors mentioned above are those applied by default by HERWE, but the user can choose to use his specific factors if desired.

2.5. Risk Characterisation

After exposure and effects assessment, the Risk Characterisation Ratios (RCR) are derived for all end-points, environmental and human. RCRs are derived by comparing exposure levels to suitable (no)-effect levels. For the environmental areas of protection, the RCR is the ratio of PEC to PNEC, while for the human end-points in the TGDRA the so-called Margin Of Safety (MOS) is used. Nevertheless, in HERWE it has been decided to use for characterisation of human risks a similar expression as that used for the environment, i.e. the ratio of PHD to HRD. In all the RCRs a value ≤ 1 means that there is no risk at the local scale associated to the corresponding substance and area of protection, whereas a value above 1 involves a potential risk. Since several substances occurring in the wastewater effluent can be assessed at the same time, only when the RCRs for all substances are ≤ 1 can may the effluent be considered safe (for the assessed substances).

The following RCRs are included in the HERST-WW tool in the scenario for discharge of wastewater to the aquatic environment:

- $RCR_{\text{water}} = PEC_{\text{water}} / PNEC_{\text{water}}$
- $RCR_{\text{sed}} = PEC_{\text{sed}} / PNEC_{\text{sed}}$
- $RCR_{\text{water predator}} = PEC_{\text{water predator}} / PNEC_{\text{oral}}$
- $RCR_{\text{water human}} = PHD_{\text{water}} / HRD$

In the scenario for discharge of wastewater to the marine environment:

- $RCR_{\text{seawater}} = PEC_{\text{seawater}} / PNEC_{\text{seawater}}$
- $RCR_{\text{seawater sed}} = PEC_{\text{seawater sed}} / PNEC_{\text{seawater sed}}$
- $RCR_{\text{seawater predator}} = PEC_{\text{seawater predator}} / PNEC_{\text{oral}}$

- $R_{CR_{\text{seawater top predator}}} = P_{EC_{\text{seawater top predator}}} / P_{NEC_{\text{oral}}}$
- $R_{CR_{\text{seawater human}}} = P_{HD_{\text{seawater}}} / HRD$

And in the scenario for agricultural wastewater reuse:

- $R_{CR_{\text{soil}}} = P_{EC_{\text{soil}}} / P_{NEC_{\text{soil}}}$
- $R_{CR_{\text{soil predator}}} = P_{EC_{\text{soil predator}}} / P_{NEC_{\text{oral}}}$
- $R_{CR_{\text{soil human}}} = P_{HD_{\text{soil}}} / HRD$

3. How to use the spreadsheet

HERWE is programmed in Microsoft® Excel 2003. Therefore, the user must have basic knowledge on how to work with this program. The tool is organized in seven sheets:

- Cover: this sheet only introduces the tool.
- Data input: this is the only sheet where the user must introduce data, in particular those related to the substance. In addition, it is also possible to change the values for environmental and exposure parameters.
- ERS calculations: in this sheet the exposure and effects assessment calculations for the environment are carried out. Do not modify any cell in this sheet.
- HRS calculations: in this sheet the exposure and effects assessment calculations for humans are carried out. Do not modify any cell in this sheet.
- RCR-aquatic discharge: in this sheet the risk characterisation ratios are shown for the scenario involving discharge of the effluent to surface water. Do not modify any cell in this sheet.
- RCR-marine discharge: in this sheet the risk characterisation ratios are shown for the scenario involving discharge of the effluent to sea water. Do not modify any cell in this sheet.
- RCR-reuse: in this sheet the risk characterisation ratios are shown for the scenario involving agricultural reuse of the effluent. Do not modify any cell in this sheet.

3.1. Entering data

The spreadsheet is organised for every assessed substance to use one row, and the total number of substances that can be assessed at the same time is 300⁴. As stated above, the user needs to introduce all the necessary data in the 'Data input' sheet, in the green rows. In the columns the different fields are specified. Most of the fields have an empty cell in the right side to be filled with comments, references, etc.

First of all write the name of the substance in column A, and if desired, the CAS registry number in column B. In column C the concentration of the substance in the effluent is introduced, in mg L⁻¹ ⁵. This concentration can be either the result of chemical analysis or an estimate. HERWE is not able to handle uncertainty information such as standard deviations. In the following sections, instructions are given on how to introduce the necessary data and performing the risk screening.

3.1.1. Substance-dependent physical-chemical properties and environmental distribution parameters

From columns C to AL the fields correspond to physical-chemical properties, and some parameters to estimate the fate of the substance in the environment. A list of all these parameters, with their units and definitions, is given in table 2. The user of HERWE might not be interested in obtaining all the RCRs available. This is very important due to the fact that the most time-consuming task when using this tool is collecting the necessary data. Therefore, in this section we try to answer the question of which parameters

⁴ In principle this number should be more than enough. Nevertheless, if the user knows how to work with Excel, this number can be easily increased, just by copying down in new rows the format and formulas of the currently available rows.

⁵ Some useful conversion factors: 1 mg = 10³ µg = 10⁶ ng = 10⁹ pg.

must be filled in, and which can be left blank, for each RCR. This is done in table 3, where the requirements for each RCR are displayed.

Concerning the RCRs for secondary poisoning and sediment toxicity, it must be borne in mind that only substances with a log Kow ≥ 3 are candidates for risk screening.

Table 2. Substance-dependent physical-chemical properties and environmental distribution parameters.

Parameter	Units	Comments
Physical-chemical properties and biodegradability		
<i>Clocal_{eff}</i>	mg·L ⁻¹	Concentration of pollutant in wastewater effluent
<i>log K_{ow}</i>	L·kg ⁻¹	Logarithm of the octanol-water partition coefficient
<i>log K_{oc}</i>	L·kg ⁻¹	Logarithm of the partition coefficient organic carbon-water
<i>Henry's Law Constant</i>	Pa·m ³ ·mol ⁻¹	Henry's Law Constant
<i>Vapour Pressure</i>	Pa	Vapour pressure
<i>pKa</i>	-	Acid/base dissociation constant, if any
<i>Biodegradability</i>	-	If the substance is known to fall in one of the following groups, it can be selected from the drop-down menu: Readily biodegradable, Readily, but failing 10-d window, Inherently biodegradable, Not biodegradable. This parameter is used to obtain a half-life in soil, according to table 8 in the TGDRA (part II, p. 56). Important note: It is not necessary to fill in this field if a specific value is entered for DT50 <i>bio_{soil}</i>
<i>DT50 _{bio_{water}}</i>	d	Half-life for aerobic biodegradation of substance in water. This parameter is used for estimation of purification factors in drinking water production (see table III-88 in the EUSES background report (EC, 2004)
<i>DT50 _{bio_{soil}}</i>	d	Half-life for aerobic biodegradation of substance in soil
Environmental distribution and biotransfer parameters		
<i>K_{p_{susp}}</i>	L·kg ⁻¹	Partition coefficient solid-water in suspended matter. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>K_{p_{soil}}</i>	L·kg ⁻¹	Partition coefficient solid-water in soil. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BCF_{fish}</i>	L·kg _{wet fish} ⁻¹	Bioconcentration factor for fish on wet weight basis. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BMF_{fish}</i>	L·kg _{wet fish} ⁻¹	Biomagnification factor in fish. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BCF_{earthworm}</i>	L·kg _{wet earthworm} ⁻¹	Bioconcentration factor for earthworm on wet weight basis. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BCF_{root-soil}</i>	kg _{wwt} ·kg _{wwt} ⁻¹	Bioconcentration factor in plant roots relative to contaminant soil concentration. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BCF_{leaf-soil}</i>	kg _{wwt} ·kg _{wwt} ⁻¹	Bioconcentration factor in plant leaves relative to contaminant soil concentration. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BAF_{milk}</i>	d·kg ⁻¹	Biotransfer factor for milk. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in
<i>BAF_{meat}</i>	d·kg ⁻¹	Biotransfer factor for meat. For organic substances, it is optional to fill in this parameter, since it can be estimated by the model from Kow. For metals this field must be filled in

Table 3. Summary of substance-dependent physical-chemical properties and environmental fate parameters required for each RCR.

RCR_{water}, RCR_{sed}, RCR_{seawater}, RCR_{seawater sed}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances)
	Environmental distribution and biotransfer parameters	None for organic substances. Kp _{susp} for metals
RCR_{water predator}, RCR_{seawater predator}, RCR_{seawater top predator}, RCR_{seawater human}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances)
	Environmental distribution and biotransfer parameters	None for organic substances. Kp _{susp} , BCF _{fish} and BMF _{fish} for metals
RCR_{water human}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances), DT50 _{bio_{water}}
	Environmental distribution and biotransfer parameters	None for organic substances. Kp _{susp} , BCF _{fish} and BMF _{fish} for metals
RCR_{soil}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances), DT50 _{bio_{soil}}
	Environmental distribution and biotransfer parameters	None for organic substances. Kp _{soil} for metals
RCR_{soil predator}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances), DT50 _{bio_{soil}}
	Environmental distribution and biotransfer parameters	None for organic substances. Kp _{susp} , Kp _{soil} , and BCF _{worm} for metals
RCR_{soil human}	Physical-chemical properties and biodegradability	Clocal _{eff} , log Kow, log Koc, Henry's Law Constant, Vapour Pressure, pKa (only for dissociating substances), DT50 _{bio_{water}} , DT50 _{bio_{soil}}
	Environmental distribution and biotransfer parameters	None for organic substances, Kp _{susp} , Kp _{soil} , BCF _{fish} , BMF _{fish} , BCF _{root-soil} , BCF _{leaf-soil} , BAF _{milk} , and BAF _{meat} for metals

3.1.2. Toxicological data

Collecting and choosing the appropriate toxicological data and assessment factors for the calculation of toxicity thresholds is the most complicated part of risk screening with HERWE, for this reason, it is strongly recommended to be familiar with the handling of toxicological data and read carefully the TGDR.

Toxicological data are introduced in HERWE in the 'Data input' sheet, from column AM to column DN. The list of parameters with their units and definitions is displayed in table 4. All fields have an empty cell to be filled with comments, references, etc. In many fields the tool requires the user to choose the kind of data being entered, by means of a drop-down menu in the next cell, as shown in figure 4. In the particular case of toxicological data for predators, the user may be required to choose values from two drop down menus, one in column CT, related to the type of toxicological endpoint, and the other one in column CV, related to the concerned species.

Table 4. Substance-dependent parameters in HERST-WW.

Parameter	Units	Comments
PNEC _{water}	mg·L ⁻¹	Predicted no-effect concentration in freshwater
Endpoint in fish	mg·L ⁻¹	Ecotoxicity endpoint in freshwater fish species (EC50/LC50, NOEC/NOEL)
Endpoint in daphnid	mg·L ⁻¹	Ecotoxicity endpoint in freshwater daphnid species (EC50/LC50, NOEC/NOEL, PNEC)
Endpoint in algae	mg·L ⁻¹	Ecotoxicity endpoint in freshwater algae species (EC50/LC50, NOEC/NOEL, PNEC)
PNEC _{sed}	mg·kg ⁻¹	Predicted no-effect concentration in freshwater sediments
Endpoint in freshwater sediment-dwelling organism	mg·kg ⁻¹	Ecotoxicity endpoint in a freshwater sediment-dwelling species (EC50/LC50, NOEC/NOEL). Up to three values can be entered
PNEC _{seawater sed}	mg·kg ⁻¹	Predicted no-effect concentration in sea water sediments
Endpoint in marine sediment-dwelling organism	mg·kg ⁻¹	Ecotoxicity endpoint in a marine sediment-dwelling species (EC50/LC50, NOEC/NOEL). Up to two values can be entered
PNEC _{soil}	mg·kg ⁻¹	Predicted no-effect concentration in soil
Endpoint in soil organism	mg·kg ⁻¹	Ecotoxicity endpoint in a soil species (EC50/LC50, NOEC/NOEL). Up to three values can be entered
PNEC _{seawater}	mg·kg ⁻¹	Predicted no-effect concentration in sea water
Endpoint in marine organism	mg·L ⁻¹	Ecotoxicity endpoint in a sea water species (EC50/LC50, NOEC/NOEL). Up to five values can be entered
Endpoint in mammalian/bird	kg·kg _{food} ⁻¹ or kg·kg bw·d ⁻¹	Ecotoxicity endpoint in predators: mammals and birds (NOEC in bird, chronic, NOEC in mammal, 28 days, NOEC in mammal, 90 days, NOEC in mammal, chronic, LC50 in bird, 5 days, NOAEL in bird, NOAEL in mammal, 28 days, NOAEL in mammal, 90 days, NOAEL in mammal, chronic, PNEC _{oral}). If a NOAEL for mammals is entered, the user is required to enter the particular species in the test: <i>Canis domesticus</i> (dog), <i>Macaca sp.</i> (macaque), <i>Microtus spp.</i> (vole), <i>Mus musculus</i> (mouse), <i>Oryctolagus cuniculus</i> (European rabbit), <i>Rattus norvegicus</i> (>6 weeks) (common rat), <i>Rattus norvegicus</i> (≤6 weeks) (common rat). If a NOAEL value for birds is entered, NOEC for birds is estimated using a conversion for <i>Gallus domesticus</i>
Endpoint in humans, oral	kg·kg bw ⁻¹ ·d ⁻¹	Oral toxicity endpoint in humans (LD50, LOAEL, NOAEL, ADI/RfD)
Assessment factor for PNEC _{water}	-	User-defined assessment factor to derive a PNEC for the aquatic compartment
Assessment factor for PNEC _{sed}	-	User-defined assessment factor to derive a PNEC for the aquatic sediment compartment
Assessment factor for PNEC _{soil}	-	User-defined assessment factor to derive a PNEC for the soil compartment
Assessment factor for PNEC _{seawater}	-	User-defined assessment factor to derive a PNEC for the sea water compartment
Assessment factor for PNEC _{seawater sed}	-	User-defined assessment factor to derive a PNEC for the sea water sediments compartment
Assessment factor for PNEC _{oral}	-	User-defined assessment factor to derive a PNEC for predators
Assessment factor for HRD	-	User-defined assessment factor to derive a HRD

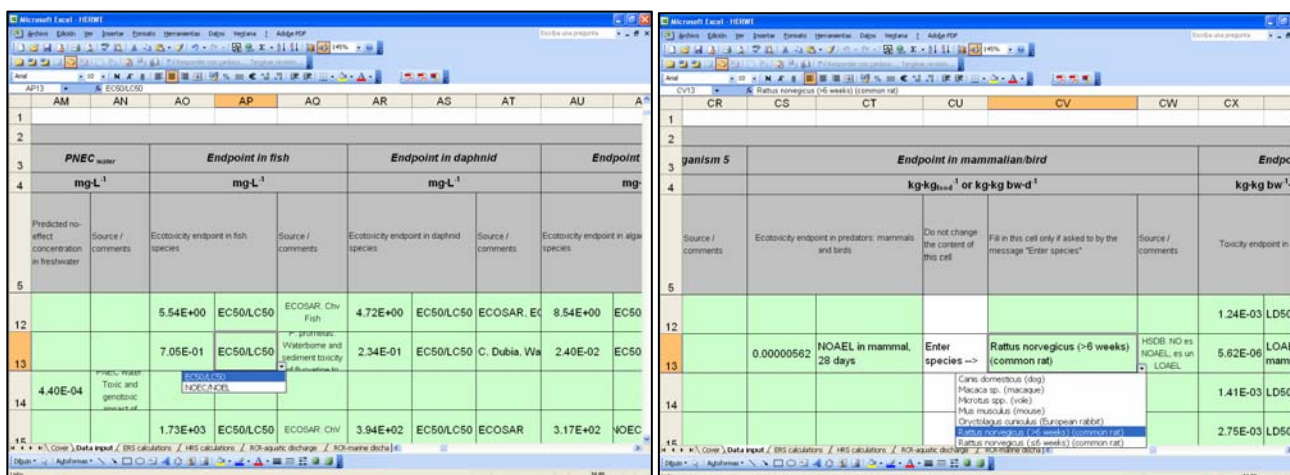


Figure 4. Drop-down menus in HERWE.

PNEC and HRD can be defined in HERWE in several ways. They are listed below, in order of preference:

1. When a PNEC for an ecotoxicity endpoint or an ADI/RfD for human toxicity is available, the user should use it. For water, sediments, sea water, sea water sediments and soil there is a specific column for entering PNEC values. For secondary poisoning and humans, the value has to be labelled as PNEC or ADI/RfD in the corresponding drop-down menus. When a PNEC or ADI/RfD is entered, HERWE will use it without any further change.
2. When the conditions in point 1 are not met, the next preferred option is to enter the toxicity value and the assessment factor, both chosen by the user after judgement of the available information, in terms of quantity and quality. In this case, the user introduces the toxicity value in one of the columns available for that endpoint, for example, in either column AO, AR, or AU if the endpoint is aquatic ecotoxicity. It does not matter neither which of these columns are chosen, nor if the type of toxicity value entered is labelled with the drop-down menu. If the user enters more than one value, the lowest one will be chosen by the tool for the calculation. The user-defined assessment factor must be entered in the appropriate column from DA to DN.
3. When the conditions in point 2 are not met, the user can enter all the available data for the substance, and depending on the amount of values entered and their quality (acute toxicity, long-term toxicity, etc.), the tool will automatically apply an assessment factor, based on the general rules set in the TGDR. For this to take place, the user must enter as many toxicity values as possible: in some endpoints, such as human toxicity, only one value is allowed, while in others up to five values are allowed. In addition, in some endpoints, like seawater toxicity, not only the values from marine organisms can be used, but also those from aquatic organisms (see table 5 for the required data for each RCR). If the user has more values than can be entered, those of highest quality should be entered. It must be borne in mind that the tool will choose for the calculation the lowest value entered, even if it is not the best one in terms of quality⁶. This automatic system for application of assessment factors, although useful, is far from being satisfactory, so it can not be guaranteed that the assessment factor chosen is the most appropriate. For

⁶ For example, in aquatic ecotoxicity, if a LC50 for fish is 5 mg L⁻¹, and a NOEC for Daphnia is 6 mg L⁻¹, the value for LC50 will be used. However, this is not a typical case, since usually NOECs are lower than LC50.

this reason, it is strongly recommended for the user to rely on the procedures explained in points 1 and 2.

4. When there is no toxicity data at all available, the calculation of PNEC or HRD is not possible, except for ecotoxicity in sediments and soil. In these cases, if the user does not enter any specific toxicological data, PNEC will be calculated based on equilibrium partitioning, provided that the data for the equilibrium partitioning calculation is available.

The user of HERWE might not be interested in obtaining PNECs for all the RCRs. In table 5, the specific requirements for each RCR are displayed.

Table 5. Summary of toxicological data required for each RCR.

RCR	Required data
RCR _{water}	<p>Several options are available to obtain PNEC_{water}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for aquatic organisms is available, it must be entered in column AM, and it will be used as such. ▪ In the absence of a PNEC, the user can calculate it with a user-defined assessment factor, which can be entered if desired in column DA. In this case the user must enter a toxicity value in either columns AO, AR or AU. If more than one value is entered, the lowest one will be used. ▪ If the user wants HERWE to apply an assessment factor, the available toxicity data (NOEC/NOEL, EC50/LC50) must be entered in columns AO, AR or AU. At least one toxicity value for either fish, daphnid or algae must be entered. If more than one value is entered, the lowest one will be used for calculating PNEC. PNEC will be calculated applying an assessment factors from table 16 of the TGDRA (part II, p. 101). The assessment factor chosen by HERWE can be seen in column AQ of the 'ERS calculations' sheet.
RCR _{sed}	<p>Several options are available to obtain a PNEC_{sed}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for sediment-dwelling organisms is available, it must be entered in either column AX, and it will be used as such. ▪ In the absence of a PNEC, the user can calculate it with a user-defined assessment factor, which can be entered if desired in column DC. In this case the user must enter a toxicity value in either columns AZ, BC, or BF. If more than one value is entered, the lowest one will be used. ▪ If the user wants HERWE to apply an assessment factor, the available toxicity data (NOEC/NOEL, EC50/LC50) must be entered in columns AZ, BC, or BF. If more than one value is entered, the lowest one will be used for calculating PNEC. PNEC will be calculated applying an assessment factor from table 19 of the TGDRA (part II, p. 114). The assessment factor chosen by HERWE can be seen in column BA of the 'ERS calculations' sheet. In the case that the only toxicity data entered corresponds to acute toxicity tests (EC50/LC50), then the tool will also calculate PNEC_{sed} by equilibrium partitioning from PNEC_{water} (see RCR_{water} in this table for the required data for PNEC_{water}). The tool will compare the PNEC_{sed} values from acute sediment toxicity and from equilibrium partitioning, and the lowest one will be chosen. ▪ In the absence of any toxicity test data for sediment-dwelling organisms, PNEC_{sed} will be calculated by equilibrium partitioning from PNEC_{water} (see RCR_{water} in this table for the required data for PNEC_{water}).

<p>RCR_{water predator}, RCR_{seawater predator}, RCR_{seawater top predator}, RCR_{soil predator}</p>	<p>Several options are available to obtain a PNEC_{oral}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for birds/mammals is available, it must be entered in column CS, and it will be used as such. ▪ In the absence of a PNEC, the user can calculate it with a user-defined assessment factor, which must be entered in column DK. In this case the user must enter the chosen toxicity value for birds or mammals in column CS. ▪ If the user wants HERWE to apply an assessment factor, then if there is long-term toxicity test data (NOEC) for bird/mammal, the lowest value found must be entered in column CS. If long-term toxicity test data is available in the form of NOAEL, the tool is able to convert NOAEL to NOEC. In this case the user is called to choose from a drop-down menu in column CV the species to which the NOAEL refers. PNEC_{oral} will be calculated using an assessment factor from table 23 of the TGDRA (part II, p. 130). The assessment factor chosen by the tool can be seen in columns CK/CL of the 'ERS calculations' sheet. If more than one NOEC is available, or NOEC values are available for both birds and mammals, the one resulting in the lowest PNEC must be chosen. ▪ If long-term toxicity test data are not available, acute-effect concentrations (LC50) expressed as mg kg_{food}⁻¹ can be used if available*. the lowest value found must be entered in column CS. PNEC_{oral} will be calculated using an assessment factor from table 23 of the TGDRA (part II, p. 130). The assessment factor chosen by the tool can be seen in columns CK/CL of the 'ERS calculations' sheet. <p>*Acute lethal doses LD50 in rats, birds, etc., are not acceptable here.</p>
<p>RCR_{soil human}, RCR_{seawater human}, RCR_{soil human}</p>	<p>Several options are available to obtain a HRD:</p> <ul style="list-style-type: none"> ▪ If an oral ADI or RfD is available, it must be entered in column CX, and it will be used as HRD. ▪ In the absence of ADI/RfD, the user can calculate HRD with a user-defined assessment factor, which must be entered in column DM, along with a toxicity value in column CX. ▪ If the user wants HERWE to apply an assessment factor, if there is long-term toxicity test data (NOAEL) in mammals, the lowest value found must be entered in column CX. HRD will be calculated using the default assessment factor (100) as discussed in section 2.4.7. In the absence of a NOAEL, if there is long-term toxicity test data expressed as LOAEL in mammals, the lowest value found must be entered in column CX. HRD will be calculated using the default assessment factor (300) as discussed in section 2.4.7. If no LOAEL is available, if there is an acute lethal dose in mammals, the lowest value found must be entered in column CN. HRD will be calculated using the default assessment factor (10⁵) as discussed in section 2.4.7. The assessment factor chosen by the tool can be seen in column AU in the 'HRS calculations' sheet.
<p>RCR_{seawater}</p>	<p>Several options are available to obtain PNEC_{seawater}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for sea water organisms is available, it must be entered in column CB, and it will be used as such. ▪ In the absence of a PNEC, the user can calculate it with a user-defined assessment factor, which can be entered in column DG. In this case the user must enter a toxicity value in either columns CD, CG, CJ, CM or CP. If more than one value is entered, the lowest one will be used. ▪ If the user wants HERWE to apply an assessment factor, if there is long-term toxicity test data available (NOEC/NOEL) for sea water organisms, up to five values can be entered in columns CD, CG, CJ, CM and CP. In addition, if there is long-term toxicity test data available (NOEC/NOEL) for fresh water organisms, up to three values can be entered in columns AO, AR an AU. Depending on the number of fresh water and sea water toxicity data entered, the tool will apply an assessment factor from table 25 of the TGDRA (part II, p. 149). This assessment factor can be seen in columns BS/BT of the 'ERS calculations' sheet. ▪ In the absence of long-term toxicity data, if there is acute toxicity data (EC50/LC50) from sea water species, up to five values can be entered in columns CD, CG, CJ, CM and CP. In addition, if there is acute toxicity data from fresh water organisms, up to three values can be entered in columns AO, AR an AU. Depending on the number of fresh water and sea water toxicity data entered, the tool will apply an assessment factor from table 25 of the TGDRA (part II, p. 149). As stated above, this assessment factor can be seen in columns BS/BT of the 'ERS calculations' sheet.

<p>RCR_{seawater sed}</p>	<p>Several options are available to obtain a PNEC_{seawater sed}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for marine sediment-dwelling organisms is available, it must be entered in either column BI, and it will be used as such. ▪ In the absence of a PNEC, the user can calculate it with a user-defined assessment factor, which must be entered in column DI. In this case the user must enter a toxicity value in either column BK or BN. If more than one value is entered, the lowest one will be used. ▪ If the user wants HERWE to apply an assessment factor, if there is long-term toxicity test data available (NOEC/NOEL) for marine sediment organisms, up to two values can be entered in columns BK and BN. In addition, if there is long-term toxicity test data available (NOEC/NOEL) for fresh water sediment organisms, up to three values can be entered in columns AZ, BC or BF. Depending on the number of freshwater and seawater toxicity data entered, the tool will apply an assessment factor from table 26 and 27 of the TGDRA (part II, pp. 154-155). This assessment factor can be seen in columns CC/CD of the 'ERS calculations' sheet. ▪ If long-term toxicity test data is not available, but acute toxicity data is available (EC50/LC50) for fresh water and/or sea water sediment organisms, then those acute toxicity data for seawater sediment organisms must be entered, up to two values in columns BK and BN. If available, up to three acute toxicity values for fresh water sediment organisms can be entered in columns AZ, BC or BF. If more than one value is entered in these five columns, the lowest one will be used. Depending on the number and type of freshwater and seawater sediment toxicity data entered, the tool will apply an assessment factor from table 26 and 27 of the TGDRA (part II, pp. 154-155). This assessment factor can be seen in columns CC/CD of the 'ERS calculations' sheet. In addition, PNEC_{seawater sed} will be calculated by equilibrium partitioning from PNEC_{seawater} (see RCR_{seawater} for the required data for PNEC_{seawater}). The tool will compare the two PNEC_{sed seawater} values from acute toxicity and equilibrium partitioning and the lowest one will be chosen. ▪ In the absence of any toxicity test data for sediment-dwelling organisms, PNEC_{seawater sed} will be calculated by equilibrium partitioning from PNEC_{seawater} (see RCR_{seawater} for the required data for PNEC_{seawater}).
<p>RCR_{soil}</p>	<p>Several options are available to obtain PNEC_{soil}:</p> <ul style="list-style-type: none"> ▪ If a PNEC value for soil organisms is available, it must be entered in column BQ and it will be used as such. ▪ In the absence of a PNEC, if the user wants to define PNEC from a specific soil toxicity value and an assessment factor, enter the soil toxicity value in either column BS, BV or BY and the assessment factor in column DE. If more than one soil toxicity value is entered, the lowest one will be chosen by the tool for the calculation. ▪ If the user wants HERWE to apply a default assessment factor for soil, as in table 20 of the TGDRA, then the following actions are needed: if there is long-term toxicity test data available (NOEC/NOEL) for soil organisms, enter the available values in columns BS, BV and BY, and the tool will automatically calculate PNEC_{soil}. In the case that a single NOEC/NOEL value for soil is entered, PNEC_{soil} will be calculated from both the NOEC value and also from PNEC_{water} using the equilibrium partitioning method (see RCR_{water} in this table for the required data for PNEC_{water}). The lowest PNEC_{soil} from the two calculations will be chosen by the tool. In the absence of long-term soil toxicity data, if there is acute toxicity test data available (EC50/LC50) for soil organisms, enter the available values in columns BS, BV and BY, and the tool will automatically calculate PNEC_{soil}. In the case that a single NOEC/NOEL value for soil is entered, PNEC_{soil} will be calculated from both the NOEC value and also from PNEC_{water} using the equilibrium partitioning method (see RCR_{water} for the required data for PNEC_{water}). The lowest PNEC_{soil} from the two calculations will be chosen by the tool. The assessment factors used by the tool can be seen in column BJ of the 'ERS calculations' sheet. ▪ In the absence of any toxicity test data for soil organisms, PNEC_{soil} will be calculated by equilibrium partitioning from PNEC_{water} (see RCR_{water} for the required data for PNEC_{water}).

3.1.3. Substance-independent parameters

Environmental parameters defining the “standard environment” and parameters defining the exposure scenario for humans and predators have default values (table 6), which can be accepted as such or changed by the user to make them more representative of a given location or exposure scenario.

Table 6. Environmental and exposure parameters used in HERST-WW.

Parameter	Units	Value	Comments
$SUSP_{water}$	$mg \cdot L^{-1}$	15	Concentration of suspended matter in surface water
Foc_{susp}	$kg_{oc} \cdot kg_{solid}^{-1}$	0.1	Weight fraction of organic carbon in suspended solids
$Fsolid_{susp}$	$m_{solid}^3 \cdot m_{susp}^{-3}$	0.1	Volume fraction of solids in suspended solids
RHO_{solid}	$kg \cdot m^{-3}$	2500	Density of solids
$Fwater_{susp}$	$m_{water}^3 \cdot m_{susp}^{-3}$	0.9	Volume fraction of water in suspended solids
RHO_{water}	$kg \cdot m^{-3}$	1000	Density of water
TEMP	$^{\circ}K$	285	Temperature at the air-water interface
R	$Pa \cdot m^3 \cdot mol^{-1} \cdot K^{-1}$	8.314	Gas constant
$kasl_{air}$	$m \cdot d^{-1}$	120	Partial mass transfer coefficient at air side of the air-soil interface
$kasl_{soilair}$	$m \cdot d^{-1}$	0.48	Partial mass transfer coefficient at soil air-side at the air-soil interface
$kasl_{soilwater}$	$m \cdot d^{-1}$	0.000048	Partial mass transfer coefficient at soil water-side at the air-soil interface
$DEPTH_{soil}$	m	0.2	Mixing depth of soil and agricultural soil
$DEPTH_{grassland}$	m	0.1	Mixing depth of grassland
$Fair_{soil}$	$m_{air}^3 \cdot m_{soil}^{-3}$	0.2	Volume fraction air in soil
$Fwater_{soil}$	$m_{water}^3 \cdot m_{soil}^{-3}$	0.2	Volume fraction water in soil
$Fsolid_{soil}$	$m_{solid}^3 \cdot m_{soil}^{-3}$	0.6	Volume fraction solids in soil
Foc_{soil}	$kg_{oc} \cdot kg_{solid}^{-1}$	0.02	Weight fraction of organic carbon in soil solids
$Finf_{soil}$	-	0.25	Fraction of rain water that infiltrates into soil
$RAIN_{rate}$	$m \cdot d^{-1}$	0.00192	Rate of wet precipitation (700 mm/year)
RHO_{air}	$kg \cdot m^{-3}$	1.3	Density of air
$APPL_{irr.water}$	$L \cdot m^{-2} \cdot d^{-1}$	1.36	Irrigation application rate, terrestrial ecosystem and agricultural soil
T_{soil}	d	30	Averaging time, terrestrial ecosystem
$T_{agr.soil / grassland}$	d	180	Averaging time, agricultural soil and grassland
F_{gut}	$kg_{dwt} \cdot kg_{wwt}^{-1}$	0.1	Fraction of gut loading in worm
$RHO_{earthworm}$	$kg_{wwt} \cdot L^{-1}$	1	Density of earthworms in wet weight
$Fwater_{plant}$	$m^3 \cdot m^{-3}$	0.65	Volume fraction of water in plant tissue
$Flipid_{plant}$	$m^3 \cdot m^{-3}$	0.01	Volume fraction of lipids in plant tissue
b	-	0.95	Correction exponent for differences between plant lipids and octanol
RHO_{plant}	$kg_{wwt} \cdot m^{-3}$	700	Bulk density of plant tissue
$Fair_{plant}$	$m^3 \cdot m^{-3}$	0.3	Volume fraction of air in plant tissue
$AREA_{plant}$	m^2	5	Leaf surface area
q_{plant}	$m \cdot d^{-1}$	86.4	Conductance ($0.001 m \cdot s^{-1}$)
V_{leaf}	m^3	0.002	Shoot volume
k_{metab}_{plant}	d^{-1}	0	Pseudo-first order rate constant for metabolism in plant
k_{photo}_{plant}	d^{-1}	0	Pseudo-first order rate constant for photodegradation in plant
$kgrowth_{plant}$	d^{-1}	0.035	Growth-rate constant for dilution by plant growth
Q_{transp}	$m^3 \cdot d^{-1}$	0.001	Transpiration stream in plants
IH_{leaf}	$kg \cdot d^{-1}$	1.2	Daily intake of leaf crops (including fruits and cereals)
IH_{root}	$kg \cdot d^{-1}$	0.384	Daily intake of root crops
IH_{milk}	$kg \cdot d^{-1}$	0.561	Daily intake of dairy products
IH_{meat}	$kg \cdot d^{-1}$	0.301	Daily intake of meat
IH_{fish}	$kg \cdot d^{-1}$	0.115	Daily intake of fish
IH_{drw}	$m^3 \cdot d^{-1}$	0.002	Daily intake of drinking water
BW	kg	70	Body weight of adult
$T_{irr.water}$	years	10	Period in which arable soil is irrigated with wastewater
$ICdwt_{grass}$	$kg_{dwt} \cdot d^{-1}$	16.9	Daily intake for cattle of grass in dry weight
$ICdwt_{soil}$	$kg_{dwt} \cdot d^{-1}$	0.41	Daily intake for cattle of soil in dry weight
$CONV_{grass}$	$kg_{wwt} \cdot kg_{dwt}^{-1}$	4	Conversion dry weight to wet weight grass
$DILUTION_{aquatic}$	-	10	Dilution factor in the aquatic compartment
$DILUTION_{aquatic}$	-	100	Dilution factor in the marine compartment
% local diet _{predators}	-	0.5	Percentage of predator diet coming from the local scale
% local diet _{top predators}	-	0.1	Percentage of top predator diet coming from the local scale

Sources: TGDRA and EC (2004), except $APPL_{irr.water}$ taken from the Spanish National Statistics Institute (2008).

3.2. Results

When all the necessary data have been filled in, the user can go to the RCR sheets, where the following information is shown, for each area of protection:

- Substance: in column A the name of the substances being assessed will appear.
- Exposure level (PEC, PHD): the predicted environmental concentration or the dose for humans is shown. If the initial concentration in the effluent was zero, or there is no substance being assessed in that row, PEC and PHD are zero.
- Effects level (PNEC, HRD): the calculated ecotoxicological or human toxicity threshold is shown. If the user has not introduced enough data for calculating PNEC/HRD, or if there is no substance being assessed in that row the message “insufficient information” will appear.
- RCR: the risk characterisation ratio is calculated, using the values from exposure and effects. The numerical value of RCR appears in blue, eventually with a message in the next column, in red lettering. This message can take the following values: “insufficient data” if there is no substance being assessed in that row, “>0.1” if the resulting RCR is above 0.1 but under 1, and “>1” if the RCR is above 1. In sediment toxicity and secondary poisoning, the message “log Kow ≤ 3” will appear if the value for Kow is ≤ 1000 for that substance, meaning that it is not a candidate for risk screening in these areas of protection.

3.3. Useful data sources

Data collection is the most-resource consuming task when using HERWE, and also a critical one, since the quantity and quality of the input data will affect the quality of the results. The user may have experience in Risk Assessment and on data collection for substances, but it can also be the case that the user has a different background and lacks the experience in data collection. As a consequence this section offers a review (which does not attempt to be extensive) of useful sources of the kind of data required by the tool.

- Scientific literature databases (Scopus: www.scopus.com; Sciencedirect: www.sciencedirect.com; American Chemical Society Publications: <http://pubs.acs.org>): scientific literature is always a primary source for information on many topics, especially experimental data concerning many parameters, such as physical-chemical properties, fate in the environment and toxicology.
- Chemidplus Advanced (<http://chem.sis.nlm.nih.gov/chemidplus>): this is a very useful online database for chemicals. Includes data on physical-chemical properties and results of acute toxicology tests in animals.
- Hazardous Substances Data Bank (<http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>): another useful resource for physical-chemical properties, fate in the environment, toxicity and ecotoxicity. The amount of information available depends on how much published data for that substance are available.
- FOOTPRINT Pesticide Properties Database (<http://www.eu-footprint.org/ppdb.html>): a very complete online database focusing on pesticides.
- European System chemical Substances Information System (ESIS) (<http://ecb.jrc.ec.europa.eu/esis/>): ESIS can be a useful source for many substances. Datasheets from the International Uniform Chemical Information Database (IUCLID) can be found, and sometimes complete Risk Assessment reports.
- Integrated Risk Information System (IRIS) (<http://cfpub.epa.gov/ncea/iris/index.cfm>): this is an electronic database containing information on human health effects (non-carcinogenic and carcinogenic) from

environmental pollutants. The main data provided by this database is the reference dose (RfD) and/or reference concentration (RfC) for each chemical.

- Summary of Evaluations Performed by the Joint FAO/WHO Expert Committee on Food Additives (<http://jecfa.ilsa.org/>): this database summarizes the evaluations performed by JECFA since 1956 of food additives contaminants and residues of veterinary drugs in food. ADI values can be found here.
- ECOTOX Database (<http://cfpub.epa.gov/ecotox/>): this an extensive database with aquatic and terrestrial ecotoxicological data for chemical pollutants.
- Environmental Quality Standards (EQS) datasheets for priority substances under the Water Framework Directive (http://ec.europa.eu/environment/water/water-dangersub/other_doc.htm): datasheets for 35 chemical pollutants affected by the Water Framework Directive can be found in this public library. These datasheets include many data on physical-chemical properties, environmental fate, and toxicology for these priority pollutants.
- EPI Suite (<http://www.epa.gov/oppt/exposure/pubs/episuite.htm>): the Estimation Program Interface Suite (EPI Suite) is a very useful tool, allowing the user to estimate many parameters based on quantitative structure-activity relationships (QSARs). It is a easy-to-use software that must be downloaded from the USEPA website and installed in the computer. The parameters that can be estimated with EPI Suite, in the absence of experimental data, are: Kow, boiling point, melting point, vapour pressure, water solubility, Henry's Law constant, octanol-air partitioning coefficient, biodegradability, particle/gas partition coefficient, atmospheric oxidation rate with hydroxyl radicals and Koc, among others.
- ECOSAR (<http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>): the Ecological Structure Activity Relationships (ECOSAR) is a similar tool to EPI Suite, but focuses on ecotoxicity. Estimated ecotoxicity values on several aquatic organisms (fish, daphnid, algae) and sometimes also for terrestrial organisms (earthworm) can be obtained with this tool.

4. Practical example

After a detailed description of the tool, an example of application is shown here for two organic substances: galaxolide and fluoxetine, two common pollutants in wastewater effluents. Galaxolide is a synthetic fragrance used in domestic cleaning products, whereas fluoxetine is a pharmaceutical. These substances are intended to be examples of a case of most data available (galaxolide) and a case of many data gaps (fluoxetine). The example is shown for assessing the three alternative scenarios included in HERWE: discharge to aquatic environment, discharge to marine environment, and wastewater reuse.

4.1. Data input

In the following table, the physical-chemical properties and half-lives in water and soil of both substances is shown. As can be seen, for fluoxetine most of the parameters are estimated with EPI Suite.

Table 6. Physical-chemical properties and biodegradability of galaxolide and fluoxetine.

Parameter	Units	Galaxolide	Source	Fluoxetine	Source
CAS number	-	1222-05-5		54910-89-3	
Clocal _{eff}	mg·L ⁻¹	8.3E-03	Experimental data from a Spanish WWTP effluent after secondary treatment	7.7E-05	Experimental data from a Spanish WWTP effluent after secondary treatment
log Kow	L·kg ⁻¹	5.7	Balk and Ford (1999a)	4.05	EPI Suite
log Koc	L·kg ⁻¹	4.8	Balk and Ford (1999a)	5.32	EPI Suite
Henry's Law Constant	Pa·m ³ ·mol ⁻¹	12.5	Balk and Ford (1999a)	0.027	EPI Suite
Vapour Pressure	Pa	0.0682	Balk and Ford (1999a)	3.4E-03	EPI Suite
pKa	-	-		10.05	Ploemen et al. (2004)
DT50 _{bio_{water}}	d	150	HERA Project (2004)	60	Estimated from EPI Suite data (see text)
DT50 _{bio_{soil}}	d	180	Balk and Ford (1999a)	120	Estimated from EPI Suite data (see text)

A common situation is to lack data on biodegradability in water and soil. In that case, EPI Suite can be used to estimate half-lives. They can be indirectly estimated as it is done by the level III fugacity model included in this program⁷. This model uses the results from the estimation program BIOWIN3, included in EPI Suite, to provide an indication of a chemical's environmental biodegradation rate in relative terms such as hours, hours to days, days, days to weeks, etc. These terms represent the approximate amount of time needed for degradation to be "complete". This output is converted to a half-life using a set of conversion factors. These conversion factors consider that 6 half-lives constitute "complete" degradation of a chemical substance, assuming first-order kinetics. It is generally believed that the biodegradation rate for a chemical in soil is, on average, one-half (1/2) that in water. EPI Suite, therefore, assigns the half-life in soil to be twice that estimated for water. The resulting conversion factors for water and soil are provided in table 7. Note that the maximum value returned by this model is 180 days for water and 360 days for soil, even though the half-life of recalcitrant molecules in the environment is likely to be substantially longer. As a consequence, this can be considered only as a rough estimation, to be used only in cases where no experimental data are available.

⁷ See the Fugacity Model Help in EPI Suite.

Table 7. Procedure for estimation of half-lives in water and soil from BIOWIN 3 results.

BIOWIN3 results	Half-life in water (d)	Half-life in soil (d)
Hours	0.17	0.34
Hours to Days	1.25	2.5
Days	2.33	4.66
Days to Weeks	8.67	17.2
Weeks	15	30
Weeks to Months	37.5	75
Months	60	120
Recalcitrant	180	360

The data from table 6 has to be entered in the columns A to S of the 'Data input' sheet. The column O can be left blank, since we have entered DT50 values in water and soil. Concerning columns U to AK, they can also be left blank, since filling them in is only mandatory when metals are assessed. For organic substances, all these parameters are indirectly estimated using, e.g. log Kow. However if experimental data for the parameters in columns U to AK are found, they can be entered, and the tool will rely on them instead of on the estimated ones.

In table 8 the toxicological data used in the assessment is shown. Since both chemicals have a log Kow above 3, they are candidates for secondary poisoning and risk for sediments. As it can be seen in the table, in the case of galaxolide we have been able to find PNEC values for surface water, soil, aquatic sediments and predators, but not for sea water and sea water sediments. For sea water, when no toxicity data from sea water organisms are available, it is possible to calculate $PNEC_{seawater}$ using toxicity data from aquatic organisms (see table 5). This is the reason why we have collected data from fish, daphnid and algae: we will not use them for calculating $PNEC_{water}$ (because we already have it), but $PNEC_{seawater}$. For sea water sediments we do not have any data either. However, as it can be seen in table 5, $PNEC_{seawater\ sed}$ can be calculated from $PNEC_{seawater}$ by means of equilibrium partitioning. PNEC values must be entered in the corresponding columns. In the case of $PNEC_{oral}$ it is very important to label the value as "PNEC" in the drop-down menu next to the cell where the value is entered. For $PNEC_{water}$, $PNEC_{soil}$, $PNEC_{sed}$, and $PNEC_{oral}$, there is no need to define assessment factors. For $PNEC_{seawater}$ we let the tool choose an assessment factor, which can be seen in columns BS/BT of the 'ERS calculations' sheet. The assessment factor chosen for 3 aquatic NOECs is 100, and it is applied to the lowest value, namely the one for fish, leading to a $PNEC_{seawater}$ of $6.8E-04\text{ mg L}^{-1}$, as it can be seen in column BU of the 'ERS calculations' sheet. For $PNEC_{seawater\ sed}$, the tool will perform the calculation by equilibrium partitioning from $PNEC_{seawater}$, thus no assessment factor is needed. As for human toxicity, we don't have a HRD but a NOAEL in mammals, therefore an assessment factor must be used. We don't define one but let the tool apply one. When we label the value as NOAEL mammal in the drop-down menu of column CY, the default assessment factor for NOAEL values (100) is chosen. The assessment factor and the final HRD can be seen in columns AU and AV, respectively, of the 'HRS calculations' sheet.

Table 8. Toxicological data used for galaxolide and fluoxetine.

Parameter	Units	Galaxolide	Source	Fluoxetine	Source
PNEC _{water}	mg·L ⁻¹	3.5E-03	Balk and Ford (1999b)		
PNEC _{seawater}	mg·L ⁻¹				
PNEC _{soil}	mg·kg ⁻¹	0.32	Balk and Ford (1999b)		
PNEC _{sed}	mg·kg ⁻¹	11	Balk and Ford (1999b)		
PNEC _{sed seawater}	mg·kg ⁻¹				
Endpoint in fish	mg·L ⁻¹	0.068	NOEC in <i>Pimephales promelas</i> , Balk and Ford (1999b)	0.705	EC50 in <i>Pimephales promelas</i> , Brooks et al. (2003)
Endpoint in daphnid	mg·L ⁻¹	0.111	NOEC in <i>Daphnia magna</i> , Balk and Ford (1999b)	0.234	EC50 in <i>Ceriodaphnia dubia</i> , Brooks et al. (2003)
Endpoint in algae	mg·L ⁻¹	0.201	NOEC in <i>Pseudokirchneriella subcapitata</i> , Balk and Ford (1999b)	0.024	EC50 in <i>Pseudokirchneriella subcapitata</i> , Brooks et al. (2003)
Endpoint in freshwater sediment-dwelling organism	mg·kg ⁻¹				
Endpoint in marine sediment-dwelling organism	mg·kg ⁻¹				
Endpoint in soil organism	mg·kg ⁻¹				
Endpoint in marine organism	mg·L ⁻¹				
Endpoint in mammalian/bird	kg·kg _{food} ⁻¹ or kg·kg _{bw} ⁻¹ ·d ⁻¹	3.33E-06	PNEC _{oral} , Hera Project (2004)	5.62	LOAEL in mammal, from HSDB
Endpoint in humans, oral	kg·kg _{bw} ⁻¹ ·d ⁻¹	5.0E-05	NOAEL in mammal, Hera Project (2004)	5.62	LOAEL in mammal, from HSDB
Assessment factor for PNEC _{water}	-				
Assessment factor for PNEC _{sed}	-				
Assessment factor for PNEC _{soil}	-				
Assessment factor for PNEC _{seawater}	-				
Assessment factor for PNEC _{sed seawater}	-				
Assessment factor for PNEC _{oral}	-				
Assessment factor for HRD	-				

For fluoxetine it can be seen in table 8 that we have only been able to find acute toxicity data for aquatic organisms and a LOAEL for mammals. The latter will be used for calculating PNEC_{oral} and HRD, whereas the values for aquatic organisms will be used first to calculate PNEC_{water} and PNEC_{seawater}. As it can be seen in table 5, in the absence of specific data for soil and sediments, PNEC_{soil} and PNEC_{sed} can be calculated from PNEC_{water} by equilibrium partitioning. Finally, PNEC_{seawater sed} can also be calculated from PNEC_{seawater} using the equilibrium partitioning method. For the calculation of PNEC_{water} we let the tool choose an assessment factor. In order to do this, we introduce the available data in columns AO, AR and AU, and label them all as "EC50/LC50" in the corresponding drop-down menus. If we now go to the 'ERS calculations' sheet, columns AQ and AR, we can see the assessment factor chosen (1000) and the final PNEC_{water}

obtained, $2.4\text{E-}05 \text{ mg L}^{-1}$. As we can see, when several values are available (fish, daphnid, algae), the tool always chooses the lowest one, in this case the one for algae. In columns BS/BT and BU of the same sheet we can see the assessment factor (10000) and final value for $\text{PNEC}_{\text{seawater}}$, namely $2.4\text{E-}06 \text{ mg L}^{-1}$. Again, the lowest value available (algae) has been used in the calculation. Once $\text{PNEC}_{\text{water}}$ and $\text{PNEC}_{\text{seawater}}$ are calculated, all the PNECs for soil and sediments are automatically calculated by equilibrium partitioning. Concerning $\text{PNEC}_{\text{oral}}$, we will use the LOAEL and let the tool choose an assessment factor. In order to do this, we enter the LOAEL in column CS of the 'Data input' sheet. In the drop-down menu of column CT there is no LOAEL option, so we choose NOAEL instead. Since the calculation of $\text{PNEC}_{\text{oral}}$ needs a NOEC, we will be asked in column CU to enter the test species in column CV, in this case "Rattus norvegicus (>6 weeks) (common rat)" is chosen. In columns CK/CL and CM of the 'ERS calculations' sheet, the assessment factor used (300) and the calculated $\text{PNEC}_{\text{oral}}$ ($3.7\text{E-}07 \text{ mg kg}_{\text{food}}^{-1}$) can be seen, respectively. Finally, HRD has to be calculated using the LOAEL in mammals. Again we let the tool apply an assessment factor. We enter the value in column CX of the 'Data input' sheet and label it as "LOAEL mammal" in the drop-down menu of column CY. The default assessment factor for LOAEL values (300) is chosen. The assessment factor and the final HRD can be seen in columns AU and AV, respectively, in the 'HRS calculations' sheet.

4.2. Results

At this point we are ready to look at the results of the risk characterisation stage. Since we are interested in the three discharge scenarios, the results of the three RCR sheets must be looked for. In tables 9 to 11 the RCRs for galaxolide and fluoxetine are summarised, as displayed in the spreadsheet.

Table 9. Risk characterisation results for galaxolide and fluoxetine in the aquatic discharge scenario.

Parameter name	Ecotoxicological risk for aquatic organisms through surface water			Ecotoxicological risk for benthic organisms through aquatic sediments			Ecotoxicological risk for aquatic fish-eating predators through secondary poisoning			Human toxicological risk through food and water intake		
Parameter name	PEC_{water}	$PNEC_{water}$	RCR_{water}	PEC_{sed}	$PNEC_{sed}$	RCR_{sed}	$PEC_{water predator}$	$PNEC_{oral}$	$RCR_{water predator}$	PHD_{water}	HRD	$RCR_{water human}$
Parameter units	mg·L ⁻¹	mg·L ⁻¹	-	mg·kg ⁻¹	mg·kg ⁻¹	-	mg·kg ⁻¹ _{wet fish}	mg·kg ⁻¹ _{food}	-	kg·kg ⁻¹ _{bwt d}	kg·kg ⁻¹ _{bwt d}	-
Parameter definition	Predicted environmental concentration in surface water	Predicted no effect concentration in surface water	Risk characterisation ratio for aquatic organisms in the surface water compartment	Predicted environmental concentration in sediment	Predicted no effect concentration in freshwater sediment	Risk characterisation ratio for aquatic organisms in the aquatic sediments	Predicted environmental concentration in freshwater fish on wet weight basis	Predicted no effect concentration in food for fish-eating predators	Risk characterisation ratio for predators via the terrestrial food chain	Total daily intake via aquatic fish and drinking water	Maximum human reference dose	Risk characterisation for human consumption of crops
Fluoxetine	5.9E-06	2.4E-05	2.4E-01 > 0.1	2.6E-02	1.1E-01	2.4E-01 > 0.1	1.6E-03	3.7E-01	4.3E-03	5.4E-12	1.9E-08	2.9E-04
Galaxolide	7.8E-04	6.8E-03	1.2E-01 > 0.1	6.5E-01	1.1E+01	5.9E-02	8.1E+01	1.0E+02	8.1E-01 > 0.1	2.7E-07	5.0E-07	5.3E-01 > 0.1

Table 10. Risk characterisation results for galaxolide and fluoxetine in the sea water discharge scenario.

Parameter name	Ecotoxicological risk for marine organisms through sea water			Ecotoxicological risk for benthic organisms through marine sediments			Ecotoxicological risk for marine fish-eating predators through secondary poisoning			Ecotoxicological risk for marine top predators through secondary poisoning			Human toxicological risk through food and water intake		
Parameter name	$PEC_{seawater}$	$PNEC_{seawater}$	$RCR_{seawater}$	$PEC_{seawater\ sed}$	$PNEC_{seawater\ sed}$	$RCR_{seawater\ sed}$	$PEC_{seawater\ predator}$	$PNEC_{oral}$	$RCR_{seawater\ predator}$	$PEC_{seawater\ top\ predator}$	$PNEC_{oral}$	$RCR_{seawater\ top\ predator}$	$PHD_{seawater}$	HRD	$RCR_{seawater\ human}$
Parameter units	mg·L ⁻¹	mg·L ⁻¹	-	mg·kg ⁻¹	mg·kg ⁻¹	-	mg·kg ⁻¹ _{wet fish}	mg·kg ⁻¹ _{food}	-	mg·kg ⁻¹ _{wet fish}	mg·kg ⁻¹ _{food}	-	kg·kg ⁻¹ _{bwt} ⁻¹ _d	kg·kg ⁻¹ _{bwt} ⁻¹ _d	-
Parameter definition	Predicted environmental concentration in seawater	Predicted no effect concentration in seawater	Risk characterisation ratio for aquatic organisms in the surface water compartment	Predicted environmental concentration in marine sediment	Predicted no effect concentration in marine sediment	Risk characterisation ratio for marine organisms in the aquatic sediments	Predicted environmental concentration in freshwater fish on wet weight basis	Predicted no effect concentration in food for fish-eating predators	Risk characterisation ratio for predators via the terrestrial food chain	Predicted environmental concentration in marine top predators food on wet weight basis	Predicted no effect concentration in marine top predators food on wet weight basis	Risk characterisation ratio for predators via the terrestrial food chain	Total daily intake if wastewater is discharged to seawater	Maximum human reference dose	Risk characterisation for human consumption of crops
Fluoxetine	5.9E-07	2.4E-06	2.4E-01 > 0.1	2.6E-03	1.1E-02	2.4E-01 > 0.1	1.6E-04	3.7E-01	4.3E-04	1.6E-05	3.7E-01	4.3E-05	5.3E-13	1.9E-08	2.8E-05
Galaxolide	7.8E-05	6.8E-04	1.2E-01 > 0.1	6.5E-02	5.6E-02	1.2E+00 > 1	8.1E+00	1.0E+02	8.1E-02	8.1E+00	1.0E+02	8.1E-02	2.7E-08	5.0E-07	5.3E-02

Table 11. Risk characterisation results for galaxolide and fluoxetine in the agricultural wastewater reuse scenario.

Parameter name	Ecotoxicological risk for soil organisms through soil			Ecotoxicological risk for terrestrial predators through secondary poisoning			Human toxicological risk through food and water intake		
Parameter name	PEC_{soil}	$PNEC_{soil}$	RCR_{soil}	$PEC_{soil\ predator}$	$PNEC_{oral}$	$RCR_{soil\ predator}$	PHD_{soil}	HRD	$RCR_{soil\ human}$
Parameter units	$mg \cdot kg^{-1}$	$mg \cdot kg^{-1}$	-	$mg \cdot kg_{wet}^{-1}$ earthworm	$mg \cdot kg_{food}^{-1}$	-	$kg \cdot kg_{bwt}^{-1} \cdot d^{-1}$	$kg \cdot kg_{bwt}^{-1} \cdot d^{-1}$	-
Parameter definition	Predicted environmental concentration in soil	Predicted no effect concentration in soil	Risk characterisation ratio for soil organisms in the soil compartment	Concentration in earthworm on wet weight basis	Predicted no effect concentration in food for earthworm-eating predators	Risk characterisation ratio for predators via the terrestrial food chain	Total daily intake via crops, meat, milk, and water	Maximum human reference dose	Risk characterisation for human consumption of crops
Fluoxetine	5.3E-05	8.8E-02	6.1E-04	3.6E-06	3.7E-01	9.6E-06	8.8E-15	1.9E-08	4.7E-07
Galaxolide	8.6E-03	3.2E-01	2.7E-01	5.5E-02	1.0E+02	5.5E-04	4.0E-10	5.0E-07	8.1E-04

In tables 9 to 11, the results of risk characterisation are shown. For each RCR, the following information is shown: the PEC or PHD, the PNEC or HRD, and the RCR. In addition, when the RCR is above 1 a message appears, as well as when RCR is above 0.1, even when the latter involves a low risk.

The results for the assessed substances can be summarised as follows:

- In the freshwater discharge scenario there are no risks from galaxolide and fluoxetine.
- In the sea water discharge scenario there is a potential risk from galaxolide to marine sediment-dwelling organisms ($RCR_{\text{seawater sed}} = 1.2$).
- In the agricultural wastewater reuse scenario, there are no risks from galaxolide and fluoxetine.

As a consequence, there are no risks at the local scale for the concentration of fluoxetine in the wastewater effluent, in any of the three scenarios. In the case of galaxolide, a potential risk has been identified for marine sediment-dwelling organisms. This should be interpreted with caution, since there were no specific toxicity data available for marine sediment organisms, and the PNEC is calculated on the basis of freshwater sediment organisms.

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Abbreviations and acronyms

% local diet _{predators}	Percentage of predator diet coming from the local scale
% local diet _{top predators}	Percentage of top predator diet coming from the local scale
ADI	Acceptable daily intake
APPL _{irr.water}	Irrigation application rate, terrestrial ecosystem and agricultural soil
AREA _{plant}	Leaf surface area
b	Correction exponent for differences between plant lipids and octanol
BAF _{meat}	Biotransfer factor for meat
BAF _{milk}	Biotransfer factor for milk
BCF _{earthworm}	Bioconcentration factor for earthworm
BCF _{fish}	Bioconcentration factor for fish
BCF _{leaf-soil}	Bioconcentration factor in plant leaves relative to contaminant soil concentration
BCF _{root-soil}	Bioconcentration factor in plant roots relative to contaminant soil concentration
BMF _{fish}	Biomagnification factor in fish
BW	Body weight of adult
C _{local,eff}	Concentration of pollutant in wastewater effluent
CONV _{grass}	Conversion dry weight to wet weight grass
DEPTH _{grassland}	Mixing depth of grassland
DEPTH _{soil}	Mixing depth of soil and agricultural soil
DILUTION _{aquatic}	Dilution factor in the aquatic compartment
DILUTION _{aquatic}	Dilution factor in the marine compartment
DT50 _{bio,soil}	Half-life for aerobic biodegradation of substance in soil
DT50 _{bio,water}	Half-life for aerobic biodegradation of substance in water
EC50	Concentration entailing effects on 50% of the population
F _{air,plant}	Volume fraction of air in plant tissue
F _{air,soil}	Volume fraction air in soil
F _{gut}	Fraction of gut loading in worm
F _{inf,soil}	Fraction of rain water that infiltrates into soil
F _{lipid,plant}	Volume fraction of lipids in plant tissue
F _{oc,soil}	Weight fraction of organic carbon in soil solids
F _{oc,susp}	Weight fraction of organic carbon in suspended solids
F _{solid,soil}	Volume fraction solids in soil
F _{solid,susp}	Volume fraction of solids in suspended solids
F _{water,plant}	Volume fraction of water in plant tissue
F _{water,soil}	Volume fraction water in soil
F _{water,susp}	Volume fraction of water in suspended solids
GIGO	Garbage in, garbage out
g _{plant}	Conductance (0.001 m·s ⁻¹)
HRD	Human reference dose
IC _{dwt,grass}	Daily intake for cattle of grass in dry weight
IC _{dwt,soil}	Daily intake for cattle of soil in dry weight

IH_{drw}	Daily intake of drinking water
IH_{fish}	Daily intake of fish
IH_{leaf}	Daily intake of leaf crops (including fruits and cereals)
IH_{meat}	Daily intake of meat
IH_{milk}	Daily intake of dairy products
IH_{root}	Daily intake of root crops (including fruits and cereals)
$kasl_{air}$	Partial mass transfer coefficient at air side of the air-soil interface
$kasl_{soilair}$	Partial mass transfer coefficient at soil air-side at the air-soil interface
$kasl_{soilwater}$	Partial mass transfer coefficient at soil water-side at the air-soil interface
$kgrowth_{plant}$	Growth-rate constant for dilution by plant growth
$kmetab_{plant}$	Pseudo-first order rate constant for metabolism in plant
$kphoto_{plant}$	Pseudo-first order rate constant for photodegradation in plant
Kp_{soil}	Partition coefficient solid-water in soil
Kp_{susp}	Partition coefficient solid-water in suspended matter.
LC50	Concentration killing 50% of the population
LOAEL	Lowest observed adverse effects level
log Koc	Logarithm of the partition coefficient organic carbon-water
log Kow	Logarithm of the octanol-water partition coefficient
NOEC	No observed effect concentration
NOEL	No observed effect level
$PEC_{agr\ soil}$	Predicted environmental concentration in agricultural soil
$PEC_{agr\ soil,\ porewater}$	Predicted environmental concentration in pore water of agricultural soil
$PEC_{grassland}$	Predicted environmental concentration in grassland
$PEC_{seawater\ predator}$	Predicted environmental concentration in sea water predator's food
$PEC_{seawater\ sed}$	Predicted environmental concentration in sea water sediments
$PEC_{seawater\ top\ predator}$	Predicted environmental concentration in sea water top predator's food
$PEC_{seawater}$	Predicted environmental concentration in sea water
PEC_{sed}	Predicted environmental concentration in fresh water sediments
PEC_{soil}	Predicted environmental concentration in soil
$PEC_{soil\ predator}$	Predicted environmental concentration in terrestrial predator's food
$PEC_{water\ predator}$	Predicted environmental concentration in fresh water predator's food
PEC_{water}	Predicted environmental concentration in fresh water
$PHD_{seawater}$	Predicted human dose in the sea water discharge scenario
PHD_{soil}	Predicted human dose in the agricultural water reuse scenario
PHD_{water}	Predicted human dose in the fresh water discharge scenario
pKa	Acid/base dissociation constant, if any
$PNEC_{oral}$	Predicted no-effect concentration in predators (mammals/birds)
$PNEC_{seawater\ sed}$	Predicted no-effect concentration in sea water sediments
$PNEC_{seawater}$	Predicted no-effect concentration in sea water
$PNEC_{sed}$	Predicted no-effect concentration in sediments
$PNEC_{soil}$	Predicted no-effect concentration in soil
$PNEC_{water}$	Predicted no-effect concentration in fresh water

QSAR	Quantitative structure-activity relationship
Qtransp	Transpiration stream in plants
R	Gas constant
RAIN _{rate}	Rate of wet precipitation
RCR _{seawater human}	Risk characterisation ratio for humans in the sea water discharge scenario
RCR _{seawater predator}	Risk characterisation ratio for sea water predators
RCR _{seawater sed}	Risk characterisation ratio for sea water sediments
RCR _{seawater top predator}	Risk characterisation ratio for sea water top predators
RCR _{seawater}	Risk characterisation ratio for sea water
RCR _{sed}	Risk characterisation ratio for fresh water sediments
RCR _{soil human}	Risk characterisation ratio for humans in the water reuse scenario
RCR _{soil predator}	Risk characterisation ratio for soil predators
RCR _{soil}	Risk characterisation ratio for soil
RCR _{water}	Risk characterisation ratio for fresh water
RCR _{water human}	Risk characterisation ratio for humans in the fresh water discharge scenario
RCR _{water predator}	Risk characterisation ratio for fresh water predators
RfD	Reference dose
RHO _{air}	Density of air
RHO _{earthworm}	Density of earthworms in wet weight
RHO _{plant}	Bulk density of plant tissue
RHO _{solid}	Density of solids
RHO _{water}	Density of water
SUSP _{water}	Concentration of suspended matter in surface water
T _{agr.soil / grassland}	Averaging time, agricultural soil and grassland
TEMP	Temperature at the air-water interface
TGDRA	Technical Guidance Document on Risk Assessment
T _{irr. water}	Period in which arable soil is irrigated with wastewater
T _{soil}	Averaging time, terrestrial ecosystem
V _{leaf}	Shoot volume
WWTP	Wastewater treatment plant