

A rule-based screening environmental risk assessment tool derived from EUSES

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Abstract

Within the context and scope of the forthcoming European Union chemical regulations (REACH), there is a need to be able to prioritise the chemicals for evaluation. Therefore, a simple, pragmatic and adequately conservative approach for the identification of substances of very low or no immediate concern at an early stage is presented. The fundamental principles and basic concepts are derived from the EU Technical Guidance Document and EUSES, and are translated into an easy-to-use rule-based system. For this development, the effect on risk characterisation ratios (RCRs) of the key environmental parameters in EUSES was quantified (taking into account several standardised chemical release scenarios). Using statistical analysis, ranges were identified for each key parameter, within which the end result of the assessment was not significantly affected. This information was then translated into a lookup table from which environmental risk characterisation ratios can be directly read as a function of a few parameters.

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1. Introduction

Increasing concern that current EU chemicals policy does not provide sufficient protection and that less than 50 high priority substances underwent a risk assessment in the past 10 years (Bodar et al., 2003) led to an EU

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Commission review of the current policy on chemicals. A new system called REACH (Registration, Evaluation, Authorization of Chemicals) has now been proposed (CEC, 2003). The aim of REACH is 'to establish a single coherent system focusing public resources on those substances where, according to experience, the involvement of authorities is indispensable and the added value in terms of provision of safety is substantial'.

Within the context and scope of the forthcoming chemical regulations (REACH), there is a need to be able to perform risk assessments on 30000 chemicals manufactured in or imported into Europe. Currently when the environmental exposure assessment is performed in accordance with the EU Technical Guidance Document (TGD) or via EUSES software requires many data acquisitions and consequently can absorb considerable time and resource allocation. Therefore, there is a need for a pragmatic and adequately conservative (i.e. no false negatives) approach, that shares the same fundamental principles and basic concepts and methodology as the TGD (and EUSES) but allows for a ready identification of substances of very low or no immediate concern. The goal of this paper is to quantify the effect that key environmental parameters in the EUSES model have on risk characterisation ratios (RCRs) of the compartment of concern, taking into account several standardised chemical release scenarios. Further, the paper will describe how this information was used to develop a pragmatic approach in the format of a simple lookup table with RCRs.

2. Methodology

2.1. Key drivers of EUSES risk assessment

2.1.1. Complexity of EUSES model

The fundamental principles and methodology of the EU Technical Guidance Document (TGD) for risk assessment of new and existing substances (EC, 1996b; ECB, 2003b) is implemented in the computer program EUSES (European Union System for the Evaluation of Substances). This was designed to be a decision-support system for the evaluation of the risks of substances to man and the environment. The documentation and program can be obtained from the European Chemicals Bureau, Ispra, Italy (EC, 1996a).

The main outputs of EUSES are local and regional risk characterisation ratios (RCRs) for several environmental compartments (air, surface water, sediment, soil, biota). A RCR is the ratio of the predicted environmental concentration (PEC) and the predicted no effect concentration (PNEC). A substance is potentially of concern when the RCR is larger than 1. The core EUSES model (without the embedded models Simple

Treat, Simple Box and the effect and risk characterisation) requires 466 input parameters, 961 connections between parameters and 132 defaults (Berding et al., 1999). In addition, the number of emission scenarios is large because an emission scenario is determined by a combination of one of the four main categories (MC), one of the 15 industry categories (IC) and one of the 55 use categories (UC). The MCs were intended originally to provide a general impression of the relevance of the exposure during the whole life-cycle of the chemical. In the context of environmental risk assessment, MCs are often used to characterise release scenarios for the estimation of emissions to the environment at individual stages of the life-cycle, i.e. at production, formulation and industrial/professional use. They can therefore be allocated to release fractions, which are used as default values where specific information is lacking. The four MCs are (I) "Use in closed systems", (II) "Use resulting in inclusion into or onto a matrix", (III) "Non-dispersive use" and (IV) "Wide dispersive use" (EC, 1996b; ECB, 2003b). The ICs (Industrial Categories) specify the branch of industry (including personal and domestic use, and use in the public domain) where considerable emissions occur by application of the substance as such, or by the application and use of preparations and products containing the substance. The UC (Use Category) specifies the specific function of the substance.

It can be concluded that EUSES is a highly complex model. Running this model appropriately requires a significant amount of substance-specific data as well as a thorough understanding of release and emissions scenarios. As such, in practice the EUSES model is only useable for priority substances (for which a large and complete data set is available), and can only be handled by experienced risk assessors.

2.1.2. Key drivers of EUSES model

Some input parameters in EUSES have a more important contribution to the RCRs than others. Thus in attempting to simplify the exposure assessment these key drivers need to be identified. In literature, some sensitivity analysis on EUSES has already been performed to identify these key parameters.

In Jager et al. (1997, 1998, 2000), tonnage and the release fraction (based on the release scenario) were identified as important input parameters for the exposure assessment of the aquatic compartment (water and sediment), the sewage treatment plant and the atmospheric exposure. Biodegradability can be important in almost every compartment. The organic carbon–water partition coefficient (K_{oc}) and the bioconcentration factor (BCF) are important in respectively the terrestrial compartment and the fish and worm eating predators. Both K_{oc} and BCF are highly correlated with the octanol–water partitioning coefficient (K_{ow}) (Schrapp and Opperhuizen, 1990).

Table 1
Parameters of the production and wide dispersive use scenario

Local	Point source or production scenario	Wide dispersive or private use scenario	Unit
Local direct emission to air	6.85E–3	0	kg/d
Local emission to wastewater	266.8E–3	0.542E–3	kg/d
Number of days for emission	365	365	d
Fraction to air	0.025	0	[-]
Fraction to wastewater	0.974	0.99	[-]
Fraction to industrial soil	0.001	0.01	[-]
Fraction of the main local source ^a	1	0.002	[-]

^a Conversion factor from regional to local emission.

Berding (2000) carried out a local sensitivity analysis on the estimation of regional background concentrations for a number of substances. It was not possible to link classes of substances with particular physico-chemical and biodegradation properties to sensitivities of input parameters. Nevertheless, some correlations between model parameters and sensitivities could be established (Berding, 2000). The lower the degradation rate in a compartment, the higher the sensitivity to the physico-chemical data. The sewage treatment plant model plays only a minor part in calculating regional background concentrations. A sensitivity analysis on the local PEC, which is always higher and therefore more relevant than the regional PEC, was not performed.

Further, volatility is a critical parameter for the exposure assessment in case of highly volatile substances (as these substances will eventually end up in the atmospheric compartment rather than the aquatic or terrestrial).

Consequently, the key parameters for an environmental risk assessment are: on the exposure side: tonnage, release scenario, biodegradability, lipophilicity (octanol/water partitioning) and volatility; and on the effects side: ecotoxicity. Release scenario and biodegradability are specified in EUSES as categorical (respectively nominal and ordinal) parameters. All other key parameters are continuous variables.

2.2. Effect of key parameters on EUSES output

2.2.1. Release scenarios

In EUSES (and the TGD), a large number of release scenarios are defined (A/B Tables in the TGD, dealing with emissions at different life cycle stages, depending on a chemical's industry and use category). Essentially, these scenarios can be reduced to two distinct release options: point source and wide dispersive release. All release scenarios are effectively linear combinations of these 2 basic options, with a different weighting of the two (EC, 1996b; ECB, 2003b).

In this exercise, the two options for release were production (point source emission assuming 100% release) and wide dispersive use (private use, based on the

TGD detergent scenario IC5/UC9). The parameters of the two scenarios can be found in Table 1.

The release fractions presented in Table 1 can be overly conservative especially for particular uses such as intermediate chemicals for which emissions are extremely low. The release scenarios could therefore be more refined based on the Main Category (MC). In order to determine a conservative and representative release fraction for each MC, a quantification of all possible release fractions (defined in the A tables of the TGD) is needed. In Verdonck et al. (2003), an attempt was made to characterise the probability distribution of release fractions per MC. However, no information about the frequency of occurrence of specific scenarios (industry and use categories, tonnage, classes of physico-chemical properties) in the overall chemical universe was available. It was concluded that an extensive database of chemicals and their use scenarios would be needed to successfully conduct this analysis.

2.2.2. Parameters with linear effect

The effect of tonnage and ecotoxicity on RCR is easily predictable because the tonnage is linearly related to the RCR and the PNEC is inversely related to the RCR. If, for example, tonnage is doubled, RCR is also doubled. Similarly, if the predicted no effects concentration (PNEC) is decreased twofold, the RCR will be doubled. As the effect of these parameters is highly transparent, it was not further assessed in this paper. The PNEC for the aquatic compartment was set to 1 µg/l. PNECs for other compartments were calculated based on the partition distribution theory as described in the TGD. In this way, the PEC was always compared to its proper PNEC for each compartment.

2.2.3. Parameters with non-linear effect

The lipophilicity (expressed in the octanol/water partitioning coefficient or in short K_{ow}) is a continuous variable, ranging for the log transformed value from less than 0 (highly hydrophilic) to larger than 6–7 (highly hydrophobic). $\log K_{ow}$ has a continuous effect on the RCR except for a step-increase in the RCR where

$\log K_{ow}$ equals 5 due to specific correction factors in the EUSES model that are activated if $\log K_{ow}$ is larger than or equal to 5 (EC, 1996b; ECB, 2003b).

Volatility (expressed as the air/water partition coefficient (K_{aw}) or dimensionless Henry's Law Constant (H)) is a continuous variable that ranges from very low (close to 0) to very high (order of magnitude $10E+6$). The effect of H on the RCR is especially meaningful when the environmental compartment of concern is changed due to H. Henry's law constant is equal to the ratio of the vapour pressure and the water solubility (SOL). In the EUSES model the Vapour Pressure (VP) is used instead of the Henry's law constant.

The dependence of the water solubility (SOL) on the octanol–water partition coefficient ($\log K_{ow}$) was taken into account by using the QSAR of Hansch et al. (1968) to calculate solubility from K_{ow} :

$$\log(\text{SOL}) = -1.214 * \log K_{ow} + 0.85$$

where SOL is the water solubility in mol/l.

This way, unrealistic combinations of $\log K_{ow}$ and SOL were avoided.

For biodegradability, four standard options are available in EUSES: non-biodegradable, ultimately (inherently) biodegradable, readily biodegradable failing the 10-day window, and readily biodegradable. The effect of these four options was examined, and a first screening indicated that only two options really needed to be considered: readily biodegradable and non-biodegradable. The other two options are intermediates of these two extremes, with results closest to the 'non-biodegradable' option.

2.2.4. Other (fixed) EUSES input parameters

The properties of the hypothetical substance 'hypotheticum' (as described in the publications on the SimpleTreat model, Struijs et al., 1991) were used. The EUSES default parameters were used as much as possible. The physico-chemical properties of hypotheticum, can be found in Table 2.

Table 2
Physico-chemical properties of hypotheticum

Physico-chemical properties	Symbol	Value	Unit
Melting point		-35	°C
Molecular weight		200	g/mol
Octanol–water	$\log K_{ow}$	Variable	[-]
Water solubility	SOL	Dep on K_{ow}	mg/l
Vapour pressure	VP	Variable	Pa
Predicted no effect concentration (aquatic) ^a	PNEC	0.000001	kg/m ³

^a PNECs for other compartments are calculated according to the partition distribution theory.

3. Response analysis

3.1. Response plots

Based on the identification of the EUSES key parameters, it was decided to investigate the effect of two release scenarios (wide dispersive use and point source), two biodegradation options (readily and non-biodegradable), the continuum of $\log K_{ow}$ and the continuum of $\log VP$ on the RCR_{max} . RCR_{max} is the maximum local RCR found for either the aquatic, the terrestrial or the sediment compartment, i.e. the compartment of most concern.

Response plots are three-dimensional displays of a response variable (RCR_{max} in this case) on the regular grids of the explanatory variables ($\log K_{ow}$ and VP in this case). A Monte Carlo type of analysis was used to create response plots. Uniform distributions were assumed for $\log K_{ow}$ and $\log VP$ with their respective ranges 0–7 and -2 to 6. Independent random samples are then taken from each distribution in several runs (using the efficient sampling algorithm Latin Hypercube (McKay, 1988)). In each run, RCR_{max} is calculated using the EUSES model. The water solubility is also varied based on $\log K_{ow}$ as described above. After many runs, enough data is gathered to construct the response plots.

The result of these four scenarios is represented as a series of three-dimensional plots, representing the RCR_{max} (for a given tonnage, ecotoxicity, release scenario and biodegradability) in one axis as a function of $\log K_{ow}$ and $\log VP$ in the remaining axis in so-called response plots.

Next, based on the shape of the response plots, the continuum of combinations of $\log K_{ow}$ and VP was divided into a limited number of fields in the parameter space, within which distinctive groups of the RCR_{max} occur. This division was the basis for the creation of the RCR_{max} lookup table.

The EUSES program is a so-called 'closed software' making it impossible to perform an automatic Monte Carlo or sensitivity analysis (Berding, 2000) as the EUSES software needs to be controlled in order to automatically assign different values for $\log K_{ow}$ and $\log VP$. For this, an unofficial spreadsheet version of EUSES was made available by RIVM for this research (RIVM, 2003)¹. This EUSES spreadsheet was benchmarked against the official EUSES program, and was found to be a sufficiently accurate surrogate. The @RISK package (Palisade, 2002) was used for the Monte Carlo analysis in Microsoft Excel. The sampled inputs together with the simulated output (RCR_{max}) are stored and after

¹ RIVM does not take responsibility on the performance of the unofficial EUSES spreadsheet.

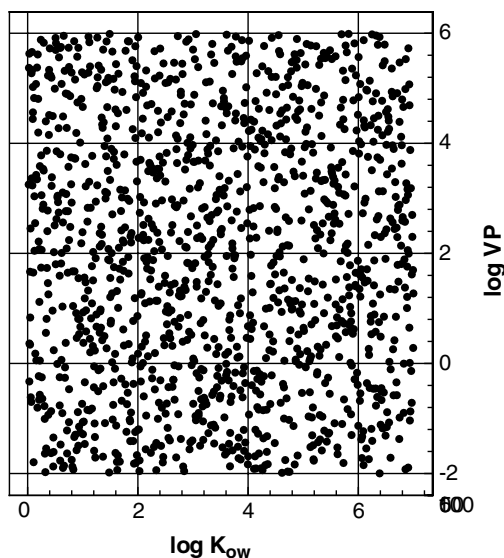


Fig. 1. Thousand sampled points in the $\log K_{ow}$ – $\log VP$ space.

the simulations those data were introduced in Tecplot (Dundas Software, 2001) to obtain a three-dimensional view of the results. The number of Monte Carlo simulations was set at 1000. Fig. 1 shows 1000 combinations of $\log K_{ow}$ and $\log VP$ are sufficient to be randomly distributed over the parameter space of $\log K_{ow}$ and $\log VP$ while totally covering the range for all scenarios.

In Fig. 2, the effect of $\log K_{ow}$ and $\log VP$ on the RCR_{max} is illustrated. On the basis of those figures a division is made in 4 distinct groups of the RCR_{max} . For $\log K_{ow}$, two distinct groups can clearly be discriminated: $\log K_{ow}$ larger and smaller than 5. For $\log VP$, two groups can also be distinguished: $\log VP$ larger and smaller than 0, as for $\log VP$ larger than 0, the RCR_{max} decreases significantly.

3.2. RCR lookup table

For each defined class of $\log K_{ow}$, $\log VP$, release scenario and biodegradability, a distribution of RCR_{max} values was found. The maximum, 95th percentile and median were calculated for each class. The RCR_{max} summary statistics for two release scenarios (production and private use), two biodegradability classes (readily and non-biodegradable), two classes of $\log VP$ and two classes of $\log K_{ow}$ can be found in Table 3. Note that the RCR_{max} values of the private use scenario differ approximately a factor of 0.002 compared to the RCR_{max} values of the production scenario. This corresponds with the different fractions of the main local source (respectively 0.002 and 1).

The RCR_{max} s in the lookup table were determined with a tonnage of 1 tonne/year and a PNEC of 1 $\mu\text{g/l}$.

But since the RCR is linearly related to tonnage and ecotoxicity, the RCR_{max} s from the lookup table can easily be adjusted to other tonnages and $PNEC_{aquatic}$ s by using the following simple transformation rule:

$$RCR_{max, \text{tonnage}, PNEC} = \frac{RCR_{max, \text{lookuptable}} \cdot 1 \mu\text{g/l}}{1 \text{ tonne/year}} \cdot \frac{\text{tonnage (tonne/year)}}{PNEC (\mu\text{g/l})}$$

3.3. Example

An example is given for the substance acrylaldehyde (CAS No. 107-02-8). Substance specific information on acrylaldehyde was downloaded from the EU Risk Assessment Report at the ECB website (2003a) and can be found in Table 4. The information needed for application of the lookup table is also listed. The RCR_{max} from the lookup table is 2.12 (95th percentile is taken). Transforming this RCR_{max} to a tonnage of 100000 tonnes/year and $PNEC_{aquatic}$ of 0.1 $\mu\text{g/l}$ gives an RCR_{max} of 2120000. This indicates that further (more detailed) risk assessment is required. The example demonstrates that only a limited amount of information and only the simple lookup table and formula is needed to calculate a worst case risk characterisation ratio.

4. Preliminary validation

A preliminary validation was performed in order to explore the conservativeness of the developed lookup table. The approach was applied on 41 chemicals which were identified by the authorities as a priority for a detailed and comprehensive risk assessment. The data used were extracted from the current draft and finished EU Risk Assessment Reports (RAR) on these chemicals (downloaded from ECB, 2003a). The outcome was then compared with the risk assessment outcome based on the full EUSES assessment. The RARs indicated that all chemicals had a RCR_{max} larger than one. The screener, based on the proposed lookup table (95th percentiles were used) indicated a potential concern for all chemicals and therefore required further assessment for all chemicals.

As such, the preliminary validation exercise has demonstrated that the substances that were selected as priority chemicals within the EU existing substances work, would also trigger further risk assessments when applying the lookup table approach. This indicates there may be a low risk of false negatives.

Clearly, a more extended validation study is needed based on a more diverse database of chemicals (with representatives from all main, industry and use categories and with different physico-chemical and biodegradation

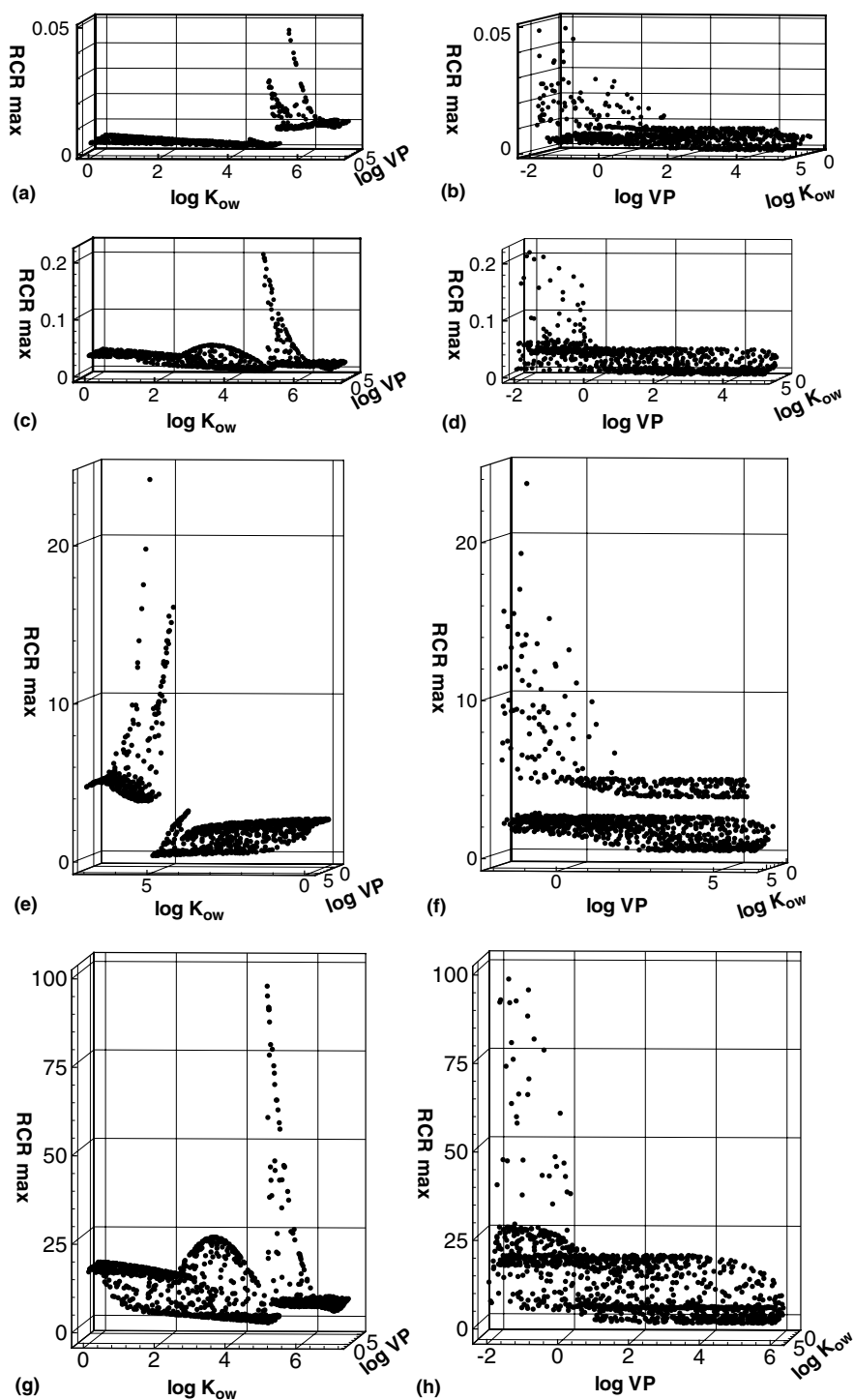


Fig. 2. Three-dimensional view of $\log K_{ow}$, $\log VP$ and RCR_{max} (tonnage = 1 tonne/year, PNEC = 10 $\mu\text{g/l}$). (a,b) Private use, readily biodegradable; (c,d) private use, non-biodegradable; (e,f) production use, readily biodegradable; (g,h) production use, non-biodegradable.

properties) in order to further assess both absence of false negatives and the limited occurrence of false posi-

tives. In particular, the database should also contain chemicals of no concern, with RCR_{max} smaller than

Table 3
RCR_{max} lookup table (median – 95th percentile – maximum) (based on 1000 shots, tonnage = 1 tonne/year, PNEC = 1 µg/l)

log <i>K</i> _{ow}	log VP	Production scenario		Private use scenario	
		Readily biodegradable	Non-biodegradable	Readily biodegradable	Non-biodegradable
0 → 5	–2 → 0	2.01 – 2.24 – 2.67	16.80 – 26.04 – 26.73	0.0040 – 0.0043 – 0.0050	0.034 – 0.052 – 0.054
	0 → 6	1.51 – 2.12 – 2.19	6.29 – 16.82 – 21.53	0.0034 – 0.0043 – 0.0050	0.019 – 0.034 – 0.046
5 → 7	–2 → 0	9.15 – 15.46 – 23.61	16.81 – 91.14 – 97.66	0.0177 – 0.0384 – 0.0488	0.048 – 0.181 – 0.215
	0 → 6	4.68 – 5.61 – 13.05	6.00 – 7.71 – 45.69	0.0096 – 0.0150 – 0.0276	0.011 – 0.017 – 0.061

Table 4
Key parameters of acrylaldehyde

Key parameter	Description/value	Lookup table information
Tonnage [tonne/year]	20000–100000	100000
Release scenario	Chemical industry: used in syntheses	Production scenario
Biodegradability	Readily biodegradable	Readily biodegradable
Log(octanol/water partitioning)	–1.1	0–5
Log(vapour pressure [Pa])	4.5	0–6
Ecotoxicity (PNEC _{aquatic} [µg/l])	0.1	0.1

one, in order to check whether the lookup table is not overly conservative (and identifies a need for further assessment for essentially all chemicals). The availability of such database will also enable the determination of conservative and representative release fractions for each main category in order to further refine the lookup table.

5. Conclusions

An easy-to-use, pragmatic and adequately conservative rule-based approach for the de-selection of substances of very low or no immediate environmental concern at an early stage was developed based on the principles and basic concepts from the EU Technical Guidance Document and EUSES. A simple lookup table gives environmental risk characterisation ratios (RCRs) for two groups of standardised chemical release scenarios, two biodegradability groups and two octanol–water partition coefficient and two vapour pressure groups. A simple transformation rule can then be used to calculate the RCR for specific tonnages and ecotoxicities (predicted no effect concentrations). The development of the rule-based screener and a preliminary validation, demonstrating its objectives, also indicated the need for an extensive and representative list of chemicals to further improve and validate the tool.

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