Courtesy translation

INDICATORS AND ASSESSMENT RULES OF CHEMSELECT

November 2024

Frank Hintsch IT Consulting

Imprint :

ÖKOPOL GmbH
Institut für Ökologie und Politik

Nernstweg 32–34
D – 22765 Hamburg

www.oekopol.de
info@oekopol.de
++ 49-40-39 100 2 0

Authors: Antonia Reihlen, Dirk Bunke

Table of content

Abbreviations

Aquat.	Aquatic
Art. Proc.	Article processing
CLP	Regulation on the Classification, Labelling and Packaging of Chemicals
CMR	Carcinogenic, Mutagenic and Reprotoxic substances
Cons	Consumer
CRM	Critical Raw Materials
ED	Endocrine disruptor
EDC	Endocrine Disrupting Chemical
ED List	Endocrine Disruptor List
EMKG	Simple concept of measures for hazardous substances (Einfaches Maßnahmenkonzept Gefahrstoffe)
env	Environment
EP	Exposure potential
EU	European Union
Form	Formulation
GWP	Global warming potential
hh	Human Health
H-Satz	H statement according to the CLP regulation
Inhal	Inhalation
LRTP	Long Range Transport Potential
ODS	Ozone Depleting Substance
OECD	Organisation for Economic Cooperation and Development
PBT/vPvB	Persistent, bioaccumulative and toxic substance / very persistent and very bioaccumulative substance
PC	Physico-chemical
PFAS	Per- and polyfluorinated alkyl substances
PMT/vPvM	Persistent, mobile and toxic substances / very persistent and very mobile substances
POP	Persistent Organic Pollutants
REACH	Regulation on the registration, evaluation, authorisation and restriction of chemicals

SIN – List	Substitute It Now – List
SSbD	Safe and Sustainable by Design
SVHC	Substances of Very High Concern
TRGS	Technical Rules for Hazardous Substances (Technische Regeln Gefahrstoffe)
UN	United Nations

Summary

ChemSelect is an online application that can be used to assess and compare the sustainability of substances and mixtures based on various criteria. ChemSelect was developed especially for small and medium sized companies using chemicals (formulators and end users) and is designed to provide a simple and quick assessment that is possible even with limited resources and competences. In many cases, the results of sustainability comparisons are clear and allow more sustainable chemicals to be selected. In other cases, further assessments are necessary.

This document explains the concept behind the ChemSelect online application. The main and sub-criteria and their respective indicators for determining the sustainability of substances and mixtures are described and justified. The concept also describes how the ChemSelect online application summarises individual assessment results, how it deals with data gaps and how the sustainability rankings are determined when comparing either several substances or several mixtures with each other.

The ChemSelect online application is based on the German Environment Agency's Guideline for Sustainable Chemicals and a former version of the SubSelect programme and expands these with some assessment parameters. ChemSelect is available both online and as a download.

The ChemSelect assessment concept is explained below. It is based on 10 main criteria, each of which has specific sub-criteria.

Entry on lists of problematic substances

If chemicals are included on regulatory lists, e.g. the POP Convention or the authorisation list of REACH (Annex XIV), there is an official assessment that a substance has particularly problematic properties. The main criterion “Mentioned on lists of problematic substances” has no sub-criterion. Substances on the following lists are rated red: Stockholm Convention on Persistent Organic Pollutants, Kyoto Protocol, Montreal Protocol, REACH Candidate List, List of Carcinogens, Mutagens and Reproductive Toxins (CMR List) from the Classification and Labelling Regulation (CLP) and the Technical Rules for Hazardous Substances 905 (TRGS 905). Substances that are on the SIN list or the list of “groups of structurally related substances“ are labelled yellow, as no assessment by authorities has yet been concluded but there are indications of very severe hazards.

Mixtures containing substances which are included on a list of hazardous substances are also rated red, regardless of the concentration of the substance.

Physical-chemical hazards

The classification of substances and mixtures is used to assess the main criterion “physical-chemical hazards”. There are no sub-criteria. The indicators for this criterion are based on the indicators suggested in the Easy-to-use workplace control scheme for Hazardous Substances (EMKG) by the German Federal Office for Workers Safety and Health. The EUH phrases are also considered here. The physical-chemical hazards for mixtures are entered and evaluated based on the classification of the mixture.

Human toxicity

The main criterion “human toxicity” has 4 sub-criteria: Carcinogenicity, mutagenicity and reproductive toxicity (CMR); endocrine disruption for human health (EDC hh); adverse effects in contact with skin and eyes; and other adverse effects. The evaluation of the sub-criteria is mainly based on the H statement entered. For the endocrine effect, it is also possible to include further

information (lists, literature) in the assessment. The indicators for the evaluation are based on the indicators of the EMKG. EUH phrases are available in the selection.

The result of the human toxicity criteria of mixtures is first derived from the classification of the mixture. The result is then checked on the basis of the toxicity of the ingredients: If the mixture contains a (suspected) CMR substance or EDCs hh in concentrations above 0.1%, the initial assessment result is overwritten with a more stringent assessment of the individual substances, if necessary.

Environmental toxicity

The main criterion “environmental toxicity” has 4 sub-criteria: Persistence, bioaccumulation and toxicity / high persistence and high bioaccumulation (PBT/vPvB); persistence, mobility and toxicity / high persistence and high mobility (PMT/vPvM); aquatic toxicity and endocrine disrupting effects for the environment (EDC env). The evaluation of the criteria is based on the prioritisation of environmental pollutants by the EU Commission in accordance with the Chemicals Strategy for Sustainability. Substances for which the existence of such properties is only suspected are rated as yellow. On the one hand, the indicators are based on the H statement. On the other hand, further information (lists, literature) can be used for the criteria PBT/vPvB, PMT/vPvM and endocrine disruption, as no classifications with H-statements are yet available for these properties.

As with human toxicity, the environmental toxicity of mixtures is initially assessed on the basis of the classification of the mixture. The result is then checked for regarding the content of substances with PBT/vPvB, PMT/vPvM and EDC env properties: If the mixture contains at least one such substance above 0.1%, the assessment of the mixture is overwritten with a more stringent assessment of the individual substances.

Exposure potential

The exposure potential is characterised on the basis of the main criteria “Occupational exposure potential”, “Consumer exposure potential" and “Environmental exposure potential”. The main criterion “Occupational exposure potential” has two sub-criteria corresponding to the relevant exposure routes (skin and inhalation). The main criterion “Consumer exposure potential” has three sub-criteria covering the dermal, oral and inhalation routes. The main criterion “Exposure potential environment” is divided into the three environmental media water, soil and air.

To determine the exposure potential, a formula is used which takes into account the emission from the application, the mobility of the substance, its application quantity, concentration and frequency (only work and consumer), and the degradability (only environment). Factors are defined for each of these exposure-influencing parameters, which are included in the calculation. The emission potential from the application is determined on the basis of a rough use scenario.

The exposure potential is first categorised for each life cycle step and exposure pathway for humans and the environment. The resulting values (which are not exposure levels!) are then summarised into sub-criteria that describe the exposure potential per exposure pathway (i.e. a total of 8 sub-criteria). In a further aggregation step, the colour of the main criteria are formed.

The procedure in no way corresponds to a scientific exposure assessment, but is merely an approximation with the final statement as to whether there are exposure situations in the life cycle that are critical (red), significant (yellow) or if no relevant exposure potentials exist (green). The exposure potential is not used as part of a risk assessment, i.e. is not combined with a substance’s hazard at this point.

Mixtures are assessed on the basis of the results of the ingredients they contain. This requires an additional aggregation step for determining the exposure potential. Substances with different functions can have slightly different life cycles (in a paint, the solvent is not contained in an article at the end, but the pigments are). This is taken into account in the assessment.

Effects on climate and ozone

The main criterion “climate and ozone-depleting effect” is divided into the sub-criteria “Intrinsic global warming potential”, “CO2 emissions during production” and “Ozone-depletion”. For the two climate impact criteria, the assessment is based on the CO2 equivalent values. Due to the wide range of Global Warming Potentials (GWP), the distinction between the three categories (red/yellow/green) is naturally relatively coarse. This also applies to the ozone depletion potential, which is determined using information from substance lists and H statements as well as self-entered values. The definition of the indicators is based on the expert assessment of the project team.

The evaluation of mixtures is based on the evaluation of the individual substances. The scores for the respective sub-criteria and the main criterion are derive using average values.

Resource consumption

The main criterion “Resource consumption” has three sub-criteria: “Water consumption”, “Energy consumption” and “Consumption of raw materials”. For water and energy consumption, the respective quantity per kg of material produced needs to be entered by the user. The indicators for the traffic light colours were derived from a comparison of values from databases for various substances. In ChemSelect, users are provided with so-called comparison lists that contain various substances and substance groups and their consumption data. This means that if data is missing for the substance being assessed, “similar” substances can be searched for and used as a guiding value.

The evaluation of mixtures is based on the evaluations of the individual substances. The scores for the respective sub-criteria and the main criterion are averaged.

Potential for circular economy

The main criterion “Circularity” has two sub-criteria: “Potential for recovery” and “Potential to contaminate secondary materials”. As ChemSelect is intended to be used globally, this criterion must be assessable independent of the existing waste treatment infrastructure and also take into account that ChemSelect users may have little knowledge of the end products containing “their” chemicals and their disposal routes.

The central distinctions in this criterion are whether a substance/mixture becomes waste as such or as part of an article. In the first case, the assessment is linked to the quantity of recyclates used. This is information that users should be aware of. In the second case, the assessment is closely linked to the materials in/on which the substances are contained. The indicators have been derived based on expert judgement of the project team.

Mixtures are assessed with regard to recovery as a whole and with regard to the contamination of secondary materials based on their ingredients. The indicators should be reviewed in 10 years, as a lot of change is also taking place globally in this area.

Responsibility of the supplier

The main criterion “Supplier responsibility” is determined on the basis of three sub-criteria, which relate to the areas of occupational health and safety, environmental protection and social commitment. These criteria therefore only indirectly relate to chemicals and represent a (small) part

of the social dimension of sustainability. Indicators were chosen for this criterion that can probably also be researched or enquired about by the users of ChemSelect.

Substitutability

The query of the main criterion “Substitutability” has a different status in ChemSelect than the other evaluation criteria: The evaluation only follows if the substance has a high priority for substitution. The criterion "substitutability" is intended to provide an indication of how “easily” substitution is possible and can therefore contribute to prioritisation if a user has identified several problematic substances or mixtures.

If it is determined in the first sub-criterion “Availability of alternatives” that there are alternatives to the substance/mixture, no further assessment of substitutability is required. Otherwise, an assessment of the complexity of the use and whether there has been a regulatory discussion about the substance (in a mixture) for some time will indicate the likelihood with which alternatives are available.

Evaluation concept

The ChemSelect assessment should be simple and reliable. For this reason, it was necessary to find parameters that are understandable and can be determined by the ChemSelect users, and to link them in such a way that sustainability is not overestimated. For the criteria relating to the toxicity of substances and mixtures in particular, an approach was chosen that ensures that the (environmental) toxicity cannot be “overwritten” or “diluted” in the final results by other aspects of sustainability.

In principle, an assessment is made for each sub-criterion using defined indicators for red, yellow and green. The colours are also assigned a value for the calculations, and to support the colour-blind in seeing the results: red = 5, yellow = 3 and green = 1. The lower the value, the better a substance or mixture performs in the sustainability assessment.

If information is missing, the colour pink (between red and yellow) is assigned, which has a value of 4. If a criterion has not yet been processed (no entry in the tool), it is marked grey, but for the calculations the same value as for pink is used, i.e. 4. In some cases, certain aspects are not relevant for a substance (e.g. persistence for inorganic substances). In these cases, a bright blue colour is assigned, which means that the criterion is not taken into account in the assessment.

When aggregating the evaluation results of the sub-criteria to main criteria for substances, two principles are applied:

- For criteria relating to hazard (toxicity, environmental toxicity, lists), the sub-criterion with the worst rating determines the rating of the main criterion. This principle is called “precedence of red”.
- For the other criteria, the main criterion is derived on the basis of the mean values of the sub-criteria, which is compared to a value ranges allocated to the three colours: 1-1.67 = green, 1.67 - 3.3 = yellow, 3.3 to 4.14 = pink and > 4.14 = red.

If there is no evaluation with the colour pink or grey, the sub-criteria are evaluated with red if above the value of 3.3. For main criteria with only one sub-criterion, the rating for the sub-criterion and the main criterion is the same.

A similar procedure is used for the evaluation of mixtures. The principle of precedence of red is used for the aggregation of the results of the ingredients for the mixture as a whole when it comes to main criteria relating to the safety of chemicals. For the other criteria, mean values are calculated.

The three main criteria for exposure have their own logic of aggregation because an additional level of complexity is added by the fact that several substances are contained in one mixture in different concentrations. Details are provided in Chapter 2.5.

Ranking in comparisons

In addition to creating a sustainability profile, ChemSelect allows comparing up to 5 substances or mixtures with each other. In addition to showing the sustainability profiles next to each other, ranks are derived that indicate the relative performance of the chemicals in that specific comparison. When evaluating substances, the ranks result from the mean values of the main criteria. When comparing mixtures, the concentration of the substances is included in the ranking and the evaluation results of the individual substances are weighted as a result. For example, users can compare a mixture to be replaced with four alternative products and see which one performs best for the various criteria. No single rank is provided by ChemSelect.

Description of the results

The evaluation results are presented as tables in which both the main and sub-criteria are shown with their evaluation result (colour) and, in the case of comparisons, the ranks. This creates a high level of transparency about the sub-results and allows users to check and determine which of the criteria should be given which weight in their decision-making processes. It also makes it possible to identify optimisation potentials, in particular regarding exposures, where improvements could be implemented with measures other than substitution.

To ensure that the assessment results can also be communicated within the company, it is possible to summarise the results. A total of 5 evaluation aspects are described in the summary:

- The mentioning of substances (in mixtures) on lists of problematic substances;
- Risk indications resulting from a combination of the human and environmental toxicity results with the relevant exposure potentials and
- A summary of the further adverse environmental impacts (climate impact, ozone depletion, resource consumption and circularity).

The supplier's responsibility as well as the physical-chemical properties are not taken into account in this summary, because they are considered as of lower overall importance in decision making.

Compatibility of ChemSelect

ChemSelect is an application-orientated tool to support (small and medium-sized) companies that want to improve their chemicals management by selecting more sustainable chemicals. Where possible, the criteria and indicators are based on existing assessment systems. Where no corresponding systems are in place, an expert assessment from the project team was used. The data and knowledge base for some parameters will continue to develop over time (e.g. information on substances and their impact on the climate or the possibilities for recycling materials) and should be reviewed after 10 years, for example.

The evaluation concept and the indicators for ChemSelect were discussed with experts from the German authorities and companies, and adapted according to the results of the discussions. ChemSelect was also tested and validated during its various development phases. When developing the assessment method and parameters, care was taken to ensure compatibility with the Safe and Sustainable by Design (SSbD) concept at EU level.

This document provides basic information about the assessment logics and the indicators applied in ChemSelect. A complete German version is available on UBA's website.

1 Overview of the assessment

1.1 Assessment aspects

The sustainability of substances and mixtures is assessed by ChemSelect based on several main criteria. These can consist of one or more sub-criteria. Table 1 gives an overview of the criteria.

Table 1: Overview of assessment areas and their main criteria and sub-criteria

Assessment aspect	Main criterion	Sub-criterion
Intrinsic safety of substances	Mentioned on lists of problematic substances	Mentioned on lists of problematic substances
	Physical-chemical properties	Physical-chemical properties
	Human toxicity	Carcinogenic, mutagenic and reprotoxic effects (CMR) Disruption of the hormone system (ED hh) Harmful effects on skin and eye Further harmful effects
	Environmental toxicity	Aquatic toxicity Persistent, bioaccumulative and toxic substances / very persistent, very bioaccumulative substances and long range transport potential (PBT/vPvB and LRTP) Persistent, mobile and toxic substances / very persistent, very mobile substances (PMT/vPvM) Disruption of the hormone system (ED env)
Exposure	Exposure potential worker Exposure potential consumer Exposure potential environment	Exposure potential worker, dermal Exposure potential worker, inhalation Exposure potential consumer, dermal Exposure potential consumer, oral Exposure potential consumer, inhalation Exposure potential environment, water Exposure potential environment, air Exposure potential environment, soil
Harmful effects along the lifecycle	Climate and ozone depletion	Intrinsic global warming potential CO2 emissions during production Depletion of the ozone layer
	Resource use	Water consumption Energy consumption Consumption of raw materials
	Circularity	Potential of recovery Potential to contaminate secondary materials
	Supplier responsibility	Responsibility for workers Responsibility for the environment Responsibility for the social environment

The assessment of the substitution potential is not included in the sustainability assessment, but is a support for prioritizing the need for action if several substances need to be substituted. The evaluation logic for substitutability is also described below.

1.2 Identification of assessment colours

1.2.1 Substances

1.2.1.1 Sub-criteria

The result of the assessment is presented as one of the traffic light colours

- Red for the least sustainable result,
- Green for the most sustainable and
- Yellow for a result in between.

Each sub-criterion is assessed individually using indicators. The indicators define when a substance is "more sustainable" (green), "less sustainable" (yellow) or "not sustainable" (red) for a sub-criterion. The indicators can be numerical or qualitative (e.g. "substance is included on a list of problematic substances").

In addition, three additional cases or colours are possible in the evaluation:

- The colour grey is assigned if a criterion has not (yet) been edited or the user decides not to edit a criterion.
- The colour pink is assigned if a ChemSelect user has not found any useful information for the evaluation. The lack of data may be due actually missing data or it not being accessible.
- The colour light blue is assigned if a sub-criterion is not relevant, e.g. because a life cycle step does not occur.

1.2.1.2 Main criteria

The rating colour of a main criterion results from the ratings of its sub-criteria. The meaning of the colours is the same for the main and sub-criteria. If a sub-criterion is rated light blue, it is generally not taken into account in the aggregation, i.e. the colour of the main criterion then depends on the colours of the other sub-criteria. If all sub-criteria of a main criterion are light blue, the main criterion is rated as "not relevant" (i.e. also light blue).

There are three approaches for deriving a main criterion's colour from the colours of the sub-criteria:

- For "mentioning on problem substance lists", "physico-chemical properties", "human toxicity" and "environmental toxicity": The "precedence of red principle" (see text box on the next page) is applied because toxic effects cannot and should not be offset by any other aspect. ChemSelect gives priority to intrinsic safety of chemicals.
- For "climate change and ozone depletion", "resource consumption", "circularity" and "supplier responsibility": The "averaging principle" (see text box on the next page) is used because one aspect can compensate another. E.g. if a lot of water ("red") but little energy ("green") is used to produce a substance, the overall resource consumption is rated "yellow".
- For "exposure potential" (workers, consumers, environment): a mixture of the two approaches is used in order to reduce complexity.

Principle „precedence of red“

Precedence of red means a “worst case” assessment, which is, however, put into perspective by the transparent presentation of the results. The rating colour for a main criterion is determined by the following questions, which must be asked and answered in the order given here:

Checks sub-criteria	Colour main criterion
1 or more sub-criteria are red?	Red
All sub-criteria = green?	Green
Max. 1 sub-criterion pink or grey?[1]	This sub-criterion is ignored; next step
Min. 2 sub-criteria pink and/or grey?	≥ 1= pink → pink; all grey → grey
All other cases	Yellow

As soon as one check is answered with “yes”, the further checks can be omitted.

Principle of averaging

A value is allocated to the three traffic light colours as well as in the case of lack of information:

Colour	Value
Green	1
Yellow	3
Pink/grey	4
Red	5

The values of the sub-criteria are added and divided by the number of sub-criteria. For the result the following rule applies:

Average value	Colour main criterion
< 1,67	Green
1,67-3,3	Yellow
> 3,3 – 4,14	Pink
> 4,14	Red

If no pink is assigned to any sub-criterion in the assessment, also the main criterion cannot turn pink. In this case the following value ranges are used to determine the main criterion’s colour rating.

Average	Colour main criterion
< 1,67	Green
1,67-3,3	Yellow
> 3,3	Red

1.2.2 Mixtures

The same criteria and evaluation principles are used to evaluate the mixtures as for the substances. There are two cases for evaluating the sub-criteria:

a) Assessment of the mixture as a whole or
b) Evaluation based on the ratings of the ingredients.

If the mixture is evaluated as a whole, the same indicators and the same procedures are used as for the substance evaluation. If the evaluation is based on the results of the ingredients, the individual results of the ingredients are aggregated for a sub-criterion. This is done either:

- Based on the principle of “precedence of red” (see text box above),
- Or using Formula 1 (see below).

The assessment colour of a sub-criterion in a mixture is determined as weighted average, calculate from the values of the colours (red = 5, pink/grey = 4, yellow = 3, green = 1). The value of each

[1] Here, it is accepted that for 25% of the criteria it is unknown how the assessment actually is. This principle of a threshold of negligibility of 25% is also applied in the assessment of mixtures, when results of various substances in a mixture are aggregated.

component is multiplied by the concentration of the substance in the mixture and the sum is divided by the number of ingredients. Sub-criteria rated bright blue are ignored in the evaluation.

Equation 1: Calculation of the values for a sub-criterion of a mixture (weighted average)

$$\frac{(\sum Conc_{red} * 5 + \sum Conc_{pink/grey} * 4 + \sum Conc_{yellow} * 3 + \sum Conc_{green} * 1)}{\sum Conc_{all\ colours}}$$

The assessment colour of the sub-criterion of the mixture is determined based on these weighted averages.

- Green: Average < 1,67
- Yellow: Average between 1,65 and 3,3
- Red: Average > 3,3.

The following table provides an overview of which approach is used for which main criteria and how the results are aggregated in the case of evaluation based on the ingredients.

Table 2: Approach for the assessment of the main criteria in the mixture

Main criterion	Assessment approach	Aggregation sub-criteria
Substance lists	Based on ingredients	Precedence of red
PC-properties	For the mixture as a whole	According to indicators
Human toxicity	Classification of mixture and based on ingredients	Precedence of red
Environmental toxicity	Classification of mixture and based on ingredients	Precedence of red
Exposure potential	Based on ingredients	C.f. separate chapter
Climate and ozone	Based on ingredients	Weighted average
Resource consumption	Based on ingredients	Weighted average
Circularity	Based on ingredients	Weighted average
Supplier responsibility	For the mixture as a whole	According to indicators
Substitution potential	For the mixture as a whole	According to indicators

Mixtures are initially evaluated for human and environmental toxicity based on their classification. However, the results of the sub-criteria “CMR”, “PBT/vPvB”, “PMT/vPvM” and “EDC (hh/env)” can be overwritten if the mixture contains substances with these properties in concentrations > 0.1%. This can be the case if the mixture has not been classified correctly, or e.g. not the substance classification but other information (e.g. scientific literature) was considered for the evaluation.

1.3 Ranking of sustainability when comparing chemicals

In addition to creating sustainability profiles, ChemSelect offers the opportunity to compare several substances and mixtures with each other. For this purpose, ChemSelect determines a ranking of the evaluated substances or mixtures for all sub- and main criteria. The chemical with the lowest rank (1) is the most sustainable for the sub- or main criterion under consideration. The chemical with the highest rank (maximum 5, since a total of 5 substances or mixtures can be compared with each

other) is the one that is the least sustainable for the corresponding criterion. The ranks are relative and only apply to the specific set of substances/mixtures included in the comparison.

1.3.1 Ranking of substances

For all criteria except the exposure potentials, the ranks are determined as follows:

Sub-criteria

To determine the ranks, the evaluation colours are translated into numerical values, which also represent the ranks of the sub-criteria for the substances: Green = 1; Yellow = 3 and Red = 5. Sub-criteria rated pink receive the value and rank 4. Sub-criteria rated grey or light blue are not taken into account in the ranking of the sub-criteria.

Main criteria

To determine the ranks of the main criteria for substances, the procedure is as follows:

For the human and environmental toxicity criteria, the ranking is based on the “precedence of red” principle, i.e. the substance with the highest number of red sub-criteria receives the worst rank, and the substance with the fewest red criteria receives the best rank. This check is then continued for the criteria rated yellow. Finally, rank 1 is awarded for all main criteria that only have sub-criteria rated green.

For all other criteria

1) The mean value of the ranks of the sub-criteria of a main criterion is formed.
2) The ranks are assigned according to the size of the mean values. The lowest average receives rank 1, the second lowest receives rank 2, etc. The highest average receives the highest rank (least sustainable).

In the sustainability comparison, the traffic light colours of the main and sub-criteria are shown in addition to the ranks.

1.3.2 Ranks for mixtures

1.3.2.1 Main criteria Lists, Human Toxicity and Environmental Toxicity

Sub-criteria

If several mixtures are compared with each other, the rankings for the sub-criteria of main criteria, which are evaluated based on the individual substances, are determined as follows:

1) The results of the sub-criteria for each substance in each mixture are determined
2) All sub-criteria = green --> rank 1
3) The sum of the concentrations of all substances with a red rating are added up per mixture
4) The mixture with the highest concentration of substances rated red gets the last (least sustainable) rank. The one with the second highest concentration the second last etc.
5) Then all mixtures that do not contain any substances with a red rating but substances with a pink rating are compared and proceed as follows:
    a) If the sum of the concentrations of the substances rated pink is <25%, they are not considered (-->Step 6; test yellow).

b) If the sum of the concentrations of the substances rated pink is ≥ 25%, the mixture with the highest concentration of pink gets the highest, not yet assigned, rank, and the one with the second-highest concentration gets the "worst" (highest) rank etc.

6) All mixtures with yellow as strictest rating are compared following the same procedure: the concentrations of all yellow-rated substances are summed up. The lowest sum gets the lowest still available rank, the second lowest concentration gets the second best, etc.

Sub-criteria evaluated as light blue or grey are not considered in ranking.

Main criteria

The ranks of the main criteria are derived from the averages of the ranks of the sub-criteria. Rank 1 is allocated to the most sustainable (i.e. the mixture with the lowest average) and the highest rank to the least sustainable mixture (i.e. the one with the highest average value). The comparison of sustainability presents the colours of the main and the sub-criteria in addition to the ranks.

1.3.2.2 Climate damage and ozone depletion, resource consumption and circularity

Sub-criteria

The numeric value of the colours assigned in the assessment of sub-criteria per ingredient is used for these criteria (red = 5, pink/grey = 4, yellow = 3 and green = 1). The concentration of all mixture components with the same colour are added up and multiplied with the value of that a colour. The sum of all values (category value) is used to identify the ranks: the higher the category value, the less sustainable is the mixture. Substances in the mixture, of which a sub-criterion is evaluated as light blue are not considered in the ranking. The following numeric ranges are defined to derive the assessment colour for the sub-criteria for the mixture:

- Average < 1,67 = green
- Average 1,67 ≤ 3,3 → yellow
- Average 3,3 ≤ 4,14 → pink
- Average ≥ 4,14 → red

If there is no assessment resulting in the colour pink, the sub-criteria are evaluated as red starting from the value of 3.3.

Main criteria

The ranks of the main criteria are derived based on the average value of the ranks of the sub-criteria. The lowest rank is assigned to the most sustainable product. The assessment colours are also shown in the sustainability comparison.

As the ranks result from averaging the sub-criteria and depend on the concentration of substances, it is possible that a main criterion evaluated as yellow gets a higher rank (i.e. is less sustainable) than one that is evaluated with the colour red.

1.3.2.3 PC properties, responsibility of the supplier and substitution potential

For the main criteria “PC properties” and “responsibility of the supplier” the indicators defined for substances are directly used also for the mixture.

The ranks in the sustainability comparison correspond to the value of the assessment colour: there are the ranks 5 (red), 4 (pink), 3 (yellow) and 1 (green). If two mixtures have the same colour, they also get the same rank. The following table shows the approaches to derive the ranks.

Table 3: Approaches to derive ranks for mixtures

Main criterion	Deriving assessment colour	Rank for sub-criterion of mixture	Rank main criterion
Substance lists	Component-based, precedence of red	Rank acc. to ∑ concentrations of substances evaluated red/pink/yellow/green (precedence of red)	Precedence of red
PC properties	Mixture as such	Based on colour	As sub-criterion
Human toxicity	Component-based, precedence of red	Rank acc. to ∑ concentrations of substances evaluated red/pink/yellow/green (precedence of red)	Precedence of red[2]
Environmental toxicity	Component-based, precedence of red	Rank acc. to ∑ concentrations of substances evaluated red/pink/yellow/green (precedence of red)	Precedence of red[2]
Exposure potential	Component-based	Ranks based on average of exposure results	Average of ranks of sub-criteria
Climate and ozone depletion	Component-based	Sum of concentrations • „red substances" * 5 • „pink/grey substances" * 4 • „yellow substances"* 3 • „green substances" *1 Rank acc.to increasing sums	Average of ranks of sub-criteria
Resource consumption	Component-based	Sum of concentrations • „red substances" * 5 • „pink/grey substances" * 4 • „yellow substances"* 3 • „green substances" *1 Rank acc.to increasing sums	Average of ranks of sub-criteria
Circularity	Component-based	Sum of concentrations • „red substances" * 5 • „pink/grey substances" * 4 • „yellow substances"* 3 • „green substances" *1 Rank acc.to increasing sums	Average of ranks of sub-criteria
Supplier responsibility	For mixture as such	Based on colour	Average of ranks of sub-criteria
Substitution potential	For mixture as such	Based on colour	Average of ranks of sub-criteria

1.4 Presentation of results

The sustainability profile is presented in detail and in tabular form. In the sustainability comparison, both the ranks and the assessment colours are shown. From the presentation of the profile, it is possible to create a summary with a reduced number of criteria:

[2] The mixture with the highest number of sub-criteria evaluated as red gets the worst rank.

- **Aspect „specific concern“:** The substance or substances in the mixture are included on a substance list.
- **Aspect „Indication of risk for health or the environment “:** The information on environmental / health toxicity is combined with the results of the assessment of exposure potentials.

Table 4: Indication of risk for workers

Exposure potential Hazard	Min. 1 expo potential = red	Min. 1 expo potential = yellow	All expo potentials = green	All expo potentials grey
CMR, ED hh (list)	Red	Red	Red [3]	Red
Human toxicity red	Red	Yellow	Yellow	Pink
Human toxicity yellow	Yellow	Yellow	Green	Pink
Human toxicity green	Green	Green	Green	Green

Table 5: Indication of risk for consumers

Exposure potential Hazard	Min. 1 expo potential = red	Min. 1 expo potential = yellow	All expo potentials = green	All expo potentials grey
CMR, ED hh, PBT/vPvB, or PMT/vPvM[4] (lists)	Red	Red	Red [5]	Red
Human toxicity red	Red	Yellow	Yellow	Pink
Human toxicity yellow	Yellow	Yellow	Green	Pink
Human toxicity green	Green	Green	Green	Green

Table 6: Indication of risk for the environment

Exposure potential Hazard	Min. 1 expo potential = red	Min. 1 expo potential = yellow	All expo potentials = green	All expo potentials grey
PBT/vPvB, ED env or PMT/vPvM (list)	Red	Red	Red [6]	Red
Environmental tox red	Red	Yellow	Yellow	Pink
Env. tox yellow	Yellow	Yellow	Green	Pink
Env. tox green	Green	Green	Green	Green

Aspect „Effects in the lifecycle“: From the criteria climate, resource consumption and circularity, an average is calculated.

The physical-chemical properties and the responsibility of the supplier are not included in the assessment summary, as they are considered of lower relevance than the other criteria.

[3] For SVHCs any exposure is considered problematic and therefore evaluated as red.

[4] Other than for workers PBT/vPvB and PMT/vPvM are considered red for consumers as exposure is possible/likely via the environment.

[5] As any exposure is considered problematic for SVHCs, this is evaluated red.

[6] As for SVHCs any exposure is considered problematic, this combination is also evaluated as red.

The criterion substitution potential can be assessed in addition. It provides and assumption on whether substitution could be easily done or rather difficult.

1.5 Classification of substances and related uncertainties ran

For several main criteria, the hazard statements (H statements) of the legal classification according to the EU CLP regulation are used. The H statements are internationally harmonized by the Globally Harmonized System for the classification of substances and mixtures (GHS). The placers on the market of substances and mixtures must determine which H statements are applicable to them. In addition, authorities at EU level can agree on a harmonized classification for a substance. The classification is published by the European Chemicals Agency's (ECHA's) Classification and Labelling Inventory. The classification must be communicated with the safety data sheet (REACH Annex 2).

Companies handling substances and mixtures should be familiar with H statements, as they provide crucial safety information. H statements are also a reference point for deriving risk management measures, e.g. according to the German "Simple Concept of Measures" (EMKG)[7], which was developed by the Federal Institute for Occupational Safety and Health. H statements enable a quick assessment of problematic substance properties and are therefore used as indicators in ChemSelect.

Classifications is always based on the "existing" data. However, for many (most) substances, studies and test results necessary for a complete classification for all possible endpoints are missing. Therefore, a substance may not classified either because test results do show that the property does not exist but also because there is not enough data to assess the classification. In the second case, the lack of classification does not mean that there is a lack of hazard, but only that it is unknown.

ChemSelect cannot close this gap in hazard identification and communication. The assessment of the dangerous properties as "green" (= not dangerous) is therefore "based on the current state of knowledge" and subject to new data that may change this assessment.

Another difficulty in using the classifications is that different manufacturers may classify a substance differently. This means that the H-statements for one substances are not always identical. This can be due to different purities of the substance, which may affect their hazard, indeed, as well as due to the use of different data which seemingly results in different hazards, but most likely one of the classifiers used invalid information. Again, it is not up to ChemSelect or its users to decide on the right classification.

ChemSelect refers to the classifications available in ECHA's databases, which show the H statements that have been assigned by the authorities (harmonized classification), those that come from registration dossiers (a certain quality assurance is required here) and those that come from individual manufacturers. In this way, ChemSelect users can choose the information with the highest quality or make a comparison with the information in their safety data sheet.

It cannot be ruled out that existing classifications for substances are incomplete or incorrect. These uncertainties can only be resolved through a complex evaluation of other existing scientific information on the substance or through additional analyses. It is unlikely that companies will make this additional effort. In other evaluation systems (e.g. GreenScreen), the H statements are also the main basis for evaluation for many criteria.

[7] The EMKG is a Control-Banding-Tool and proposes the adequate measures for handling hazardous substances in the workplace. It supports the risk assessment at the workplace.

Individual existing classifications are regularly reviewed and, if necessary, changed by the European authorities as part of the Adaptation on Technical Progress (ATP). This and the places where the changes are documented are indicated in a help text in ChemSelect.

2 Main criteria and sub-criteria

In the following sections the indicators of the sub-criteria are provided. For in-depth information on the reasons for indicators and how the values are processed, please refer to the German version of the concept of ChemSelect.

2.1 Mentioning on lists of problematic substances

Table 7: Lists that are considered for the criterion

Nr	List	Geography	Comments
1	Stockholm Convention on Persistent Organic Pollutants - POPs	Global	POPs annexes plus POP candidates
2	Kyoto-Protocol, greenhouse gases	Global	
3	Montreal Protocol, ozone depleting substances – ODPs	Global	
4	REACH candidate list	EU	
5	SIN-List	EU	
6	List of carcinogenic, mutagenic and reprotoxic substances (CMR list) of the classification and labelling regulation (CLP) and the technical rules on hazardous substances 905 (TRGS 905)	Global (CLP) + EU	Safety net for critical classifications
7	Groups of structurally similar substances	Global (e.g. OECD PFAS[8])	Prevent regrettable substitution

Indicators

- Red: Substance is on at least one regulatory list (POPs, SVHC etc.).
- Yellow: Substance is on SIN list or is assumed to have similarly hazardous properties as one of the substances on the regulatory lists.
- Green: Substance is not listed.

2.2 Physical chemical properties

Table 8: Indicators on physical chemical properties

RED	YELLOW	GREEN
H200, 201, 202, 203, 205, 220, 221, 222,228,230,231,240, 241, 242, 250, 251,260, 261, 270, 271, EUH014, EUH019, EUH044	H204, 222, 223, 224, 225, 226, 228, 229, 251, 252,272, 280, 281, 290, EUH018, EUH206, EUH209, EUH209A, EUH211, EUH212, EUH029, EUH031, EUH032, EUH066, EUH070, EUH071	No H statement for PC hazards

[8] Per- and polyfluorinated alkyl substances / chloro paraffines / bisphenols / phthalates / brominated flame retardants

2.3 Human toxicity

2.3.1 Sub-criterion 1: carcinogenic, mutagenic and reprotoxic effects

Table 9: Indicators for carcinogenic, mutagenic and reprotoxic effects

RED	YELLOW	GREEN
H340, 350, 350i, 360, 360D, 360DF, 360F, 360FD, 360Fd, EUH201, EUH201A, EUH207	H341, 351, 361, 361d, 361f, 361fd, 362	None of these H statements

For mixtures, it is assessed if any ingredient in concentrations above 0.1% has one of the properties evaluated as red. If this is the case, the assessment is dominated by this result, i.e. the classification of the mixture is overwritten by the evaluation of the substance.

2.3.2 Sub-criterion 2: Disruption of the human hormone system

- EU ED List: https://edlists.org/about-this-site
- REACH candidate list: https://echa.europa.eu/de/candidate-list-table
- TEDX-Colborn-List: https://endocrinedisruption.org/interactive-tools/tedx-list-of-potential-endocrine-disruptors/search-the-tedx-list
- SIN-List: https://sinlist.chemsec.org/

Table 10: Indicators for endocrine disruptors for human health

RED	YELLOW	GREEN
EUH 380, EUH 381 / EDC hh on the candidate list or	On TEDX Colborn-List or SIN-List Or EUH201, EUH201A, EUH207	Not listed, no indication of EDC properties for hh or env and
In list 1 of EU ED List (EDC hh or without specification)	In list 2 or 3 of EU ED list (EDC hh or not specified).	Not on EU EU-ED list as EDC hh or without specification or as EDC env
ECHA ED EG assessed as "EDC hh" or without specification.	Other indications of hormone effects	Not evaluated as ED hh or ED env by ECHA ED EG

For mixtures, it is assessed if any ingredient in concentrations above 0.1% has one of the properties evaluated as red. If this is the case, the assessment is dominated by this result, i.e. the classification of the mixture is overwritten by the evaluation of the substance.

2.3.3 Sub-criterion 3: Damage for skin and eye

Table 11: Indicators damage for skin and eyes

RED	YELLOW	GREEN
H310	H311,312, H314 ,315, 317, 318, 319, EUH202, EUH203, EUH204, EUH205, EUH208, EUH070	No classification or EUH066

2.3.4 Sub-criterion 4: Further health damage

Table 12: Indicators for further health damage

RED	YELLOW	GREEN
H300, 330, 370, 372, EUH032, EUH201, EUH201A, EUH207	H301, 302, 304, 314, 331, 332, 334, 370,371, 373 EUH029, EUH031, EUH203, EUH204, EUH208, EUH071	No classification or H335, H336

2.4 Environmental toxicity

2.4.1 Sub-criterion 1: Aquatic toxicity

Table 13: Indicators for aquatic toxicity

RED	YELLOW	GREEN
H400, 410, 420, EUH201, EUH201A, EUH207 Acute aquat. Tox (LC 50) <10,0 mg/l Chronic aquat. Tox (NOEC) <1,0 mg/l	H411, 412 and 413 Acute aquat. tox (LC 50) 10,0 – 100,0 mg/l Chronic aquat. tox (NOEC) 1,0 – 10,0 mg/l	No H statement starting with a 4 Acute aquat. tox (LC 50) > 100,0 mg/l Chronic aquat. tox (NOEC) >10,0 mg/l

2.4.2 Sub-criterion 2: PBT/vPvB and long-range transport

Table 14: Indicators for PBT/vPvB and long-range transport

RED	YELLOW	GREEN
Half-life air > 2 day or LRT demonstrated with models	Half-life air 1-2 days or Indication of LRT from models or literature	Half-life air < 1 day or No indication of LRT from modelling or literature.
or	Or	and
EUH440, EU H441 or On candidate list as PBT/vPvB-	Indication of PBT/vPvB properties- according to ECHA brief profile or from literature or Indications that thresholds for P, B and T or vP and vB are exceeded acc. To CLP (modelled), for B: logKow ≥4	No classification as EUH 440 or. EUH 441 and no indication of these properties or Finalised assessment by authorities concludes no PBT/vPvB

For mixtures, it is assessed if any ingredient in concentrations above 0.1% has one of the properties evaluated as red. If this is the case, the assessment is dominated by this result, i.e. the classification of the mixture is overwritten by the evaluation of the substance.

2.4.3 Sub-criterion 3: PMT/vPvM

Table 15: Indicators for PMT/vPvM

RED	YELLOW	GREEN
EUH 450 or EUH451 or Candidate list PMT/vPvM-	Listed as potential PMT/vPvM Stoff in lists or literature with potential exceedance of thresholds for P, M, T in CLP or Indication that CLP thresholds for P, M and T or vP and vM are exceeded	No classification with EU H450 or EU H451 and no indication that these properties exist or finalised authority assessment concluding no PMT/vPvM

For mixtures, it is assessed if any ingredient in concentrations above 0.1% has one of the properties evaluated as red. If this is the case, the assessment is dominated by this result, i.e. the classification of the mixture is overwritten by the evaluation of the substance.

2.4.4 Sub-criterion 4: Endocrine disruption for the environment

Table 16: Indicators on endocrine disruption in the environment

RED	YELLOW	GREEN
EUH 430, EUH 431 or EDC env on candidate list or In EU ED-List number I (EDC env or not specified or EDC env by ECHA ED EG or no specification	In TEDX Colborn-List or SIN List or In EU ED List No II or III (env, hh or not specified) or Other indications on ED properties or EUH201, EUH201, EUH207	Not classified EUH 430 or 431 and Not on EDC-List as EDC and Not on EU ED list or Assessed by ECHA ED EG as not ED

For mixtures, it is assessed if any ingredient in concentrations above 0.1% has one of the properties evaluated as red. If this is the case, the assessment is dominated by this result, i.e. the classification of the mixture is overwritten by the evaluation of the substance.

2.5 Exposure potentials (Worker, consumer, environment)

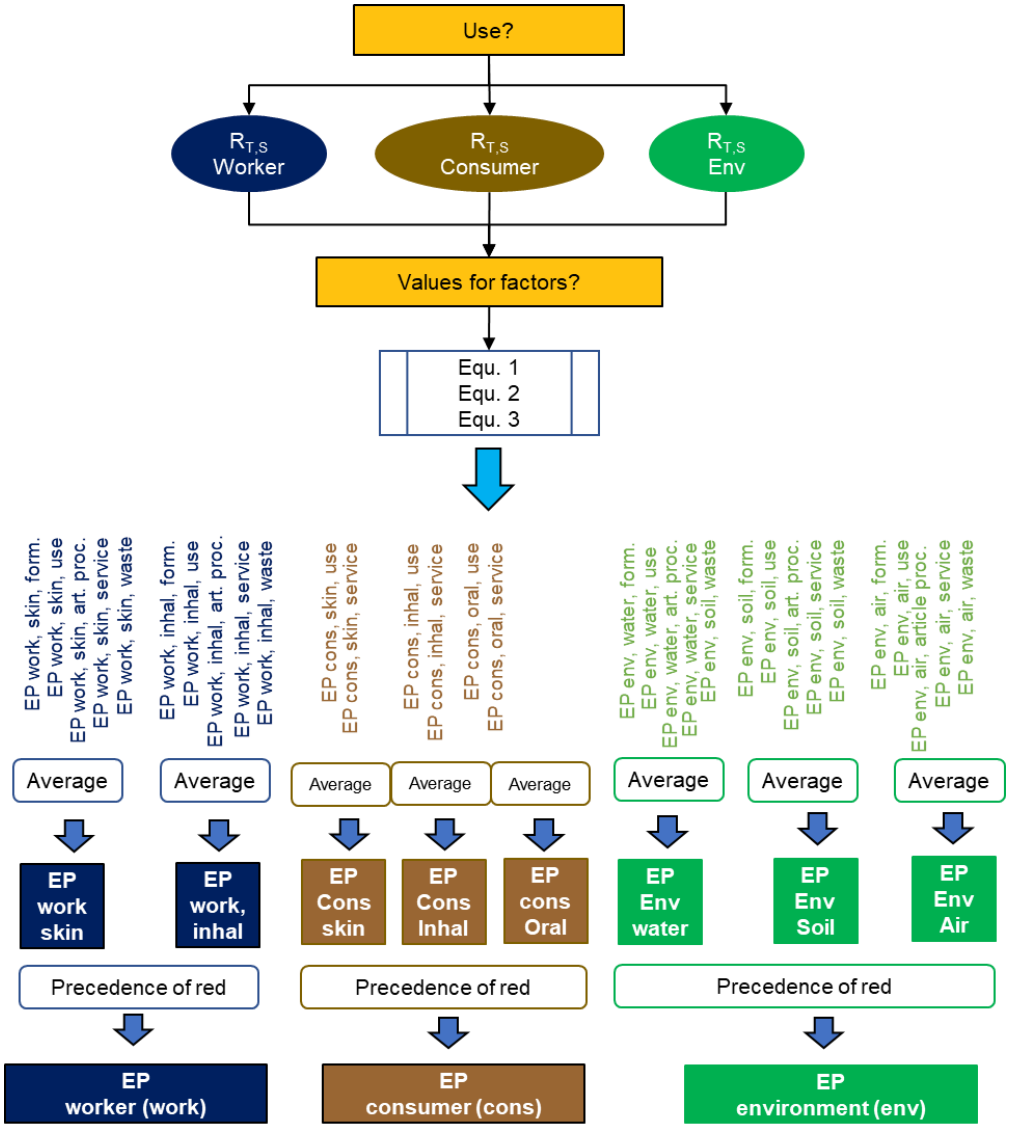
2.5.1 Introduction

ChemSelect roughly assesses whether there are critical exposures along the lifecycle. It is not a risk assessment at workplaces and does not estimate any exposure levels. It also does not consider the hazards of a substance; however, the mobility is considered in the assessment.

2.5.2 Systematics of main and sub-criteria for the exposure potential

The next figure shows how the main criteria are derived from the results of the sub-criteria.

Figure 1: Scheme for the assessment of the main criteria regarding the exposure potential



R = Release potential; T= Subject of protection and exposure route (Target), S = Step in life cycle; EP = Exposure potential; work = worker, cons = consumer, env = environment, inhal = Inhalation; Form. = Formulation; use = application of mixture, incl. when included in articles, art. proc. = processing of articles, service = service life of articles,

2.5.2.1 Equations to calculate a value for the exposure potential

The exposure potential per lifecycle step, target and exposure route is calculated according to the following equation, which includes the following variables for substances

- Use scenario
- Mobility: water solubility, vapour pressure, dustiness
- Concentration in mixture/article (worker and consumer)
- Use amount (worker, environment)
- Degradability (Environment)
- Duration of use (Worker)

The formula is adapted for the various lifecycle steps depending on whether or not the factors are relevant for the exposure potential.

Equation to calculate the exposure potential

$$EP_{T,S} = R_{T,S} * F_{mob} * F_{conc,S} * F_M * F_T$$

2.5.2.2 F_{mob} = Mobility

Table 17: Factor F_{mob}

Property	F_{mob} = 1,75	F_{mob} = 1	F_{mob} = 0,25
Water solubility (env, water)	> 10 mg/l	10 – 0,001 mg/l	< 0,001 mg /l
Vapour pressure (env, air)	0,0005 - 0,5		solid Vp < 0,0005 or > 0,5
Vapour pressure (env, soil)	Solid	Boiling point ≥ 50°C or Vp ≤ 25 kPa	Gases and/or boiling point < 50°C; Vp > 25 kPa
Vapour pressure (work)	> 25 kPa; gases and/or boiling point < 50°C	0,5 – 25 kPa and/or 50 < boiling point ≤ 150°C	< 0,5 kPa and/or boiling point > 150°C
Vapour pressure (consumer)	> 0,1 kPa	0,1 kPa – 0,0005 kPa	< 0,0005 kPa
Dustiness	Fine powders (e.g. TiO2); during use, dust clouds arise that settle only after several minutes	Granular powders, dust that settles quickly	Liquids, non-dusting solids (pellets, waxes)

2.5.2.3 F_{conc} = Concentration in the respective life cycle step

Table 18: Factor F_{conc}

Use of the substance …	F_{conc} = 1,5	F_{conc} = 1	F_{conc} = 0,5
As such in formulation	n.r.	100%	n.r.
In mixture (with or without integration into article)	> 25%	5-25%	< 5%
In article (processing, service life, waste)	> 50%; 100%	10 – 50%	< 10%

2.5.2.4 F_M = use amount

Table 19: Factor F_M for workers

Relevant for lifecycle stage	1,25	1	0,75
Formulation / use of substance or mixture	1-999t or m^3	1-999kg or l	1-999g or ml

Table 20: Factor F_M for consumers

Relevant for lifecycle stage	1,5	1	0,5
Use of substance/mixture	1-999kg or l	1-999g or ml	1-999mg or µl

2.5.2.5 Environment

Table 21: Factor F_M for the environment

Relevant for lifecycle stage	F_M= 1,5	F_M=1	F_M=0,5
Formulation of mixtures, use of substances and mixtures no integration in articles	> 100t/a	10 – 100 t/a	< 10 t/a
Manufacturing of articles, service life and waste treatment	> 10t/a	1–10 t/a	< 1 t/a

2.5.2.6 F_T = additional factors

Table 22: F_T for workers

	F_T = 0,5
Use of mixtures	Use < 15 Min or use < 1/Monat

Table 23: F_T for consumers

	F_T = 1,5	1	0,5
Frequency of product use	Regularly / daily; article in direct living environment (house, car)	Infrequent use	Rare use (< twice per year), article outside, contained

For the environment, the factor is applied for water and soil.

- 0,5 if “ready degradable“
- 1 if “inherently degradable”
- 1,5 if “not degradable“

For the air F_T is 0,5 for all substances, except if persistent or ozone depleting, which are always 1,5.

2.5.3 Identification of assessment colour

1. Identification of value per lifecycle step, target and exposure route
2. Identification of percentage of that value of the maximum value that is achievable
3. Calculation of the average value of all shares → average across the lifecycle
4. Colour sub-criterion: identification according to the average percentage based on the scale of < 33 = green; 33-66 yellow and > 66 red
5. Identification of colour of main criterion via precedence of red principle.

2.5.4 Ranking for substances

Ranks for sub-criteria are derived by comparing the averages of the percentages of the maximum values. Ranks for main criteria are identified by comparing the averages of the ranks of the sub-criteria.

2.5.5 Ranking for mixtures

The exposure potential for mixtures is identified based on the exposure potentials of the components. Also here, the share of the maximum value is calculated. An additional aggregation step is needed for mixtures: The aggregation is performed via averaging of the values for the ingredients at the level of exposure potentials per subject of protection, exposure route and lifecycle step, i.e. the first assessment step. The ranking is performed in the same way as for substances.

2.6 Climate damage and ozone depletion

Table 24: Indicators on the intrinsic global warming potential

RED	YELLOW	GREEN
Listed in Kyoto-Protocol and GWP > 500 or		Solids at 20°C
GWP > 500	GWP 100 - 500	GWP < 100

Table 25: Indicators on CO_2-Emissions during production

RED	YELLOW	GREEN
> 10 kg CO_2 equiv./kg substance	1 - 10 kg CO_2 equiv./kg substance	< 1 kg CO_2 equiv./kg substance

Table 26: Indicators on ozone depletion

RED	YELLOW	GREEN
H420 or		No H 420 or
Listed in Montreal-Protocol		Not listed in Montreal Protocol
ODP > 0,02	ODP 0,0001 – 0,02	ODP = 0 or not halogenated or solid at 20°C

2.7 Resource consumption

Table 27: Indicators on energy consumption

RED	YELLOW	GREEN
> 100 MJ /kg substance	10 – 100 MJ/kg substance	< 10 MJ / kg substance

Table 28: Indicators on water consumption

RED	YELLOW	GREEN
> 100 Liter /kg substance	5 – 100 Liter /kg substance	< 5 Liter / kg substance

Raw materials use

Table 29: Indicators for renewable raw materials

RED	YELLOW	GREEN
Raw material cultivated in ecologically valuable areas or International standards of cultivation not followed or Cultivation in competition with food production.	Raw material cultivated sometimes/ in some ecologically valuable areas or International standards of cultivation are partly not followed or Cultivation is in competition with food production in some regions.	Raw material not cultivated in ecologically valuable areas and International standards of cultivation are followed and Cultivation not in competition with food production.

Table 30: Indicators for non-renewable raw materials

RED	YELLOW	GREEN
Raw material extraction has very negative social and ecological consequences or Raw materials is critical or Listed in EU CRM 2022 or ÖkoRess2	Raw material extraction has negative social and ecological consequences or Raw materials could become critical in the next years or Listed in ÖkoRess2	Raw material extraction has hardly any negative social and ecological consequences and Raw materials is not critical and Listed as not critical in ÖkoRess2

Examples of substances are given to support the answer:

- GREEN: Iron, mineral raw materials: gypsum, lime and sand.
- YELLOW: Natural gas and crude oil, aluminium and copper (critical environmental impacts possible during extraction; mentioned in ÖkoRess as raw materials with medium aggregated environmental impact potential)
- RED: Beryllium, gallium and niobium (listed as CRM EU 2020 and high aggregated environmental impact potential according to the ÖkoRess study (UBA ÖkoRess 2020).

Resources:

- List of critical raw materials in the EU by the EU Commission https://ec.europa.eu/docsroom/documents/42849
- Results of ÖkoRess II Project[9] https://www.umweltbundesamt.de/publikationen/oekoress-ii).

2.8 Circularity

The assessment does not consider the local waste infrastructure, nor any local legislation. Therefore, and because the final product and related waste treatment may not be known to the users of ChemSelect, the assessment is generic,

Substances and mixtures which are not incorporated into articles are generally considered well recoverable. The recovery potential of substances (as such or in mixtures) when included into articles depends on their function and the materials the article consists of.

ChemSelect considers state of the art in recovery and recycling and the indicators are largely based on expert judgement. They should be revised as waste treatment technologies develop.

2.8.1.1 Sub-criterion: Potential for recovery

Considers:

a. the ability to extract and recover a substance or mixture from the waste stream, and

b. the quality of the reused chemical or material, particularly with regard to maintaining the functionality of the chemicals.

For substances/mixtures that are used as such and do not become part of a material/product at the end of their life cycle, it is generally assumed that recovery and recycling are possible and that they can be used again with the same functionality. A measure of how well this recovery is possible is the share of recovered materials used in the production as input material.

[9] Umweltbundesamt, Texte 79/2020, https://www.umweltbundesamt.de/themen/kritische-rohstoffe-aus-umweltsicht-ermittelt

If substances or mixtures themselves become the material ("main building block"), are integrated into a material (additives) or are applied to a material/product (coatings, adhesives, etc.), the recyclability of the material becomes the basis for evaluation in ChemSelect.

For mixtures, the sub-criterion is evaluated for the mixture as a whole.

2.8.1.2 Assessment of substances/mixtures that are not integrated into a material or product

Table 31: Indicators for the recovery potential of chemicals which are not bound in/on/as matrix

Criterion	Green	Yellow	Red
Are recovered substances / mixtures used as input materials in the company conducting the assessment (own input)?	Yes	Partly	Bi

2.8.1.3 Assessment of chemicals that are included into/onto materials in products

Substances and mixtures used in materials or products require material and product-related assessment.

When assessing the recovery potential, the basic rule is that all coatings, adhesives or other chemicals that are applied onto materials cannot be recovered (red rating), because the focus of recycling is on the recovery of the "main" materials. In some cases, the rating can still be given as yellow if the materials in downcycling still contain these substances and mixtures.

2.8.2 Sub-criterion: Potential to contaminate secondary materials

This criterion evaluates whether a substance (in a mixture) can be separated or destroyed during recycling, or whether it is "carried over" into the secondary material during the recycling process. The consideration of the risk of contaminating material flows is only limited to the second life cycle. The sub-criterion is linked to the recovery potential, because contamination of the secondary materials is only possible if there is recovery. The assessment does not consider if the contamination will actually cause damage to human health or the environment.

2.8.2.1 Assessment of chemicals that do not become part of a material/product

Two cases are distinguished:

1) Chemicals are not mixed with other chemicals during use → no contamination possible (= Green); no further assessment
2) Chemicals are mixed with others during use →
   a. Green: recovery of original chemical is possible after use
   b. Red: recovery of original substance is not possible due to mixing and lack of separability after the use.

2.8.2.2 Assessment of chemicals that do become part of a material/product

If the chemicals become the material → green. If they are additives or coatings etc. a separate assessment is needed.

2.8.3 Assessment of gases

The assessment is different for gases, and it is only checked if the release is intended. If this is the case the assessment is that the criterion is "not relevant" as recovery is not intended. Otherwise, it is checked if the released gas can be captured → green. If it is not possible to capture the gases, the recovery potential is red. In the last step, it is checked if cleaning of the captured gas is possible, the

assessment is red if the potential for contamination during this step is high and green, if it is very low etc.

2.8.4 Detailed assessment depending on the material

The following chapters list the assessment indicators by material type. These are not relevant for the evaluation of gases.

2.8.4.1 Ceramics and mineral construction materials

Table 32: Recovery potential in/on/as ceramics and mineral construction materials

Use	Green	Yellow	Red
Starting material of ceramics / construction material		Filling material	
Substance (in mixture) applied to ceramics/construction materials			No recovery

Table 33: Potential to contaminate secondary materials in/on ceramics and construction materials

Assessment	Case/substance/product
Red	SVHC not fixed part of ceramics / construction materials
Yellow	Substance (in mixture) applied to ceramics / construction materials but no SVHC (contained)
Green	Fixed part of ceramics / construction material (not water soluble/firmly bound)

2.8.4.2 Glass

Table 34: Recovery potential in/on/as glass

	Application	Green	Yellow	Red
Formulator	Starting material of glass	Container glass	Window glass, flat glass	Ceramic glass, Boro silicate glass, glass for tableware
	Substance (in mixture) applied to glass			Coatings not recycled
User	Starting material of glass	Container glass	Window glass, flat glass	Ceramic glass, Boro silicate glass, glass for tableware
	Mixture applied to glass			Coatings not recycled

Table 35: Potential to contaminate secondary materials in/on glass

Assessment	Case/substance/product
Red	Inorganic / heavy metals applied onto glass
Yellow	Pigments (→ downcycling) Glass from PV installations, leaded glass, glass from construction, ceramic glass Non-SVHC organic substances with decomposition temperatures > 1100 °C
Green	organic substances with decomposition temperatures < 1100 °C

2.8.4.3 Metals

Table 36: Recovery potential in/on/as metals and alloys

	Application	Green	Yellow	Red
Formulator	Substance (in mixture) that becomes alloy	All alloys		
	Substance (in mixture) that is applied to a metal article			Coatings are not recovered
User	Starting mixture for alloy	All alloys		
	Mixture that is applied to metal article			Coatings are not recovered

Table 37: Potential to contaminate secondary materials in/on metals and alloys

Assessment	Case/substance/product
Red	Metals not transferred to slags
Yellow	Inorganics; organics with decomposition temperatures > 1200 °C, metals that are transferred to slags
Green	Organic substances with decomposition temperature < 1200 °C

2.8.4.4 Paper

Table 38: Recovery potential in/on/as paper

	Application	Green	Yellow	Red
Formulator	Substance (in mixture) becomes paper	Paper fibres		Additives, coatings
	Substance (in mixture) applied onto paper			Coatings not recovered
User	Mixtures become part of paper during production			Additive mixtures
	Substance (in mixture) applied onto paper			Coatings not recovered

Table 39: Potential to contaminate secondary materials in/on paper

Assessment	Case/substance/product
Red	Mineral oils, bisphenols Substances with water solubility < 0,01 mg/l
Yellow	Pigments, other additives, glues, coatings Substances with water solubility of 0,01 mg/l – 1 mg/l
Green	Substances with water solubility > 1 mg/l, inorganic substances

2.8.4.5 Wood

No recovery is assumed (not relevant). Contamination of secondary materials is considered as yellow as sometimes wood is used to produce other materials and chemicals could be dragged over to secondary materials.

2.8.4.6 Leather

Table 40: Recovery potential in/on/as leather

	Application	Green	Yellow	Red
Formulator	Substance (in mixture) that is applied onto leather	Substance is retained with its function		
user	Substance (in mixture) that is applied onto leather		Substance retained, function unclear	

Table 41: Potential to contaminate secondary materials in/on leather

Assessment	Case/substance/product
Red	
Yellow	All substances and mixtures
Green	

2.8.5 Polymers / Plastics

Table 42: Recovery potential in/on/as plastics

	Application	Green	Yellow	Red
Formulator	Substance (in mixture) that becomes part of the plastics	Plastics is recovered (with additive) for similar use (e.g. PET bottles)	Plastics is recovered (with additive) but for less lower value use (e.g. park benches, construction elements for roads)	Plastics is incinerated (with additive), littered or landfilled (e.g. flame retarded parts of EEE)
	Substance (in mixture) that is applied onto plastics			No recovery
User	Polymer mixture becomes plastics	Plastics is recovered for similar use (e.g. PET bottles)	Plastics is recovered but for lower value use (e.g. park benches, construction elements for roads)	Plastics is incinerated, littered or landfilled (e.g. special plastics)
	Mixture is applied onto plastics			No recovery

Table 43: Potential to contaminate secondary materials in/on Plastik

Assessment	Case/substance/product
Red	Dissolved additives
Yellow	
Green	Additive covalently bound to the plastics

2.8.5.1 Polymer / synthetic fibres textiles

Table 44: Recovery potential in/on/as textiles (fibres)

	Application	Green	Yellow	Red
Formulator	Monomer, synthetic fibre, additive	Fibres		Additive, monomers
	Additive not integrated in textile		If no fibre mixture	No recovery
	Substance (in mixture) applied onto textile			No recovery
User	Mixture becomes textile		If no fibre mixture	
	Substance (in mixture) applied onto textile			No recovery

Table 45: Potential to contaminate secondary materials in/on textiles

Assessment	Case/substance/product
Red	Dissolved additives
Yellow	
Green	Additive covalently bound to the matrix

2.8.5.2 Polymer / rubber

Table 46: Recovery potential in/on/as rubber

	Application	Green	Yellow	Red
Formulator	Substance (in mixture) becomes rubber		Rubber for material re-use	Rubber is incinerated or landfilled
	Substance (in mixture) applied onto rubber			Coatings are recovered
User	Mixture becomes rubber		Rubber for material re-use	Rubber is incinerated or landfilled
	Mixture applied onto rubber			Coatings are recovered

Table 47: Potential to contaminate secondary materials in/on Gummi

Assessment	Case/substance/product
Green	
Yellow	All substances
Green	

2.8.5.3 Composite materials

Since composite materials are generally difficult to separate, applications in this type of material are generally rated red in terms of recovery potential. Since recovery is not assumed, contamination of secondary materials is not relevant (light blue).

2.9 Responsibility of the supplier

2.9.1 Responsibility of the supplier for workers in relation to the product

Table 48: Indicators for the responsibility of the supplier for workers

RED	YELLOW	GREEN
The safety data sheet contains no, implausible or incomprehensible information or the supplier does not answer inquiries about occupational safety regarding a product or It is known that the company has problems with occupational safety.	The safety data sheet mainly contains standard phrases; the supplier does not clearly answer inquiries about occupational safety regarding a product.	The safety data sheet contains comprehensive and understandable information on workers protection The supplier answers to inquiries about occupational health and safety well

2.9.2 Responsibility of the supplier for the environment

Table 49: Indicators for the responsibility of the supplier for environment

RED	YELLOW	GREEN
Problems in environmental protection are known or The supplier does not respond to inquiries about environmental protection	Supplier has a (non-certified) environmental management system or There are some indications that the supplier causes problems in environmental protection	Supplier has a -certified environmental management system or Supplier publishes environmental or sustainability reports

2.9.3 Responsibility of the supplier for workers social environment

Table 50: Indicators for the responsibility of the supplier for social environment

RED	YELLOW	GREEN
The supplier does not respond to inquiries about the company's social commitment. Cases of child labour at the supplier are documented.	The supplier confirms that it implements a social “Code of Conduct”. There is evidence of child labour at the supplier.	The supplier has a social code of conduct, the implementation of which is independently verified The supplier trains or The supplier participates in social projects outside the company

2.10 Substitution potential

The criterion is only relevant, if the results show that a substance should be substituted; i. e. in the summary of the sustainability profile: One of the three criteria “Special Concern”, “Risk indications” and “Life Cycle Effects” has the colour red.

Table 51: Indicators on the substitution potential

Colour Sub-criteria	RED	YELLOW	GREEN
Availability of alternatives	No references to alternatives (in databases etc.)	Occasional mention of alternatives in databases/literature	Information about directly applicable alternatives
Characteristics of the use	• Substance used in mixtures with >10 ingredients and/or • Final use in article or very specific processing aids and/or • Very high performance requirements (e.g. temperature, friction) and or • Substance is essential and/or • Long-lasting external assessment and certification processes for process or product and/or • Very specific or very rare function	• Substance used in mixtures with 5-10 ingredients and/or • Final use in article or processing aids but generally replaceable and/or • High performance requirements (e.g. temperature, friction) and or • Substance could be avoided in general • Short external assessment and certification processes for process or product and/or • Function needed in different uses	• Substance used as such in < 5 ingredients and/or • Use as substance or mixture without integration in article and/or • No specific performance requirements (e.g. room temperature, no friction) and/or • Any substance could be used • No external assessment and certification processes for process or product and/or • Frequent function
Regulatory pressure	The substance is not on the candidate list or comparable regulatory lists and is not discussed as a problem substance.	/ The substance group has not yet been discussed as problematic.	The substance or substance group has been discussed as problematic for 1 – 2 years. The substance or group of substances has been discussed and/or as a problem substance for more than 2 years The substance or substance group is on the candidate list, in REACH Annex XIV, XVII or comparable lists

A Annex

A.1 Formulas to calculate the exposure potentials

Table 52: Calculation of the exposure potential

Protection goal, lifecycle step	Equation	Comment
Worker formulation, dermal	$EP_{T,S} = R_{T,S} * F_T * F_M$	
Worker formulation, inhalative	$EP_{T,S} = R_{T,S} * F_{mob} * F_T * F_M$	If NOT agas or liquid → F_{mob} = dustiness, otherwise Vp
Worker use mixture, dermal	$EP_{T,S} = R_{T,S} * F_{conc} * F_M * F_T$	
Worker use mixture, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_{mob} * F_M * F_T$	F_{mob} → if solid: dustiness, otherwise Vp
Worker processing article, dermal	$EP_{T,S} = R_{T,S} * F_{conc} * F_T$	
Worker processing article, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_T$	F_{mob} from Vp
Worker service life, dermal	$EP_{T,S} = R_{T,S} * F_{conc} * F_T$	
Worker service life, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_{mob} * F_T$	F_{mob} from Vp
Worker waste, dermal	$EP_{T,S} = R_{T,S} * F_{conc}$	
Worker waste, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_{mob}$	F_{mob} from Vp
Consumer, use mixture, dermal	$EP_{T,S} = R_{T,S} * F_{conc} * F_M * F_T$	
Consumer, use mixture, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_{mob} * F_M * F_T$	F_{mob} from dustiness (if solid) or vapour pressure
Consumer, use mixture, oral	$EP_{T,S} = R_{T,S} * F_{conc} * F_M * F_T$	
Consumer, service life, dermal	$EP_{T,S} = R_{T,S} * F_{conc} * F_T$	
Consumer, service life, inhalative	$EP_{T,S} = R_{T,S} * F_{conc} * F_{mob} * F_T$	F_{mob} from Vp
Consumer, service life, oral	$EP_{T,S} = R_{T,S} * F_{conc} * F_T$	
Environment, formulation, water	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = water solubility F_M from formulation F_T from biodegradability
Environment, formulation, air	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from formulation F_T half-life air
Environment, formulation, soil	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_{mob} = water solubility
Environment, use mixture, water	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	

Protection goal, lifecycle step	Equation	Comment
		F_M from formulation/use F_T from biodegradability
Environment, use mixture, air	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from formulation/use F_T half-life air
Environment, use mixture, soil	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from formulation / use F_T from biodegradability
Environment, processing article, water	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = water solubility F_M from use F_T from biodegradability
Environment, processing article, air	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T half-life air
Environment, processing article, soil	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T from biodegradability
Environment, Service Life, water	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = water solubility F_M from use F_T from biodegradability
Environment, Service Life, air	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T half-life air
Environment, Service Life, soil	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T from biodegradability
Environment, waste, water	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = water solubility F_M from use F_T from biodegradability
Environment, waste, air	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T half-life air
Environment, waste, soil	$EP_{T,S} = R_{T,S} * F_{mob} * F_M * F_T$	F_{mob} = from Vp F_M from use F_T from biodegradability