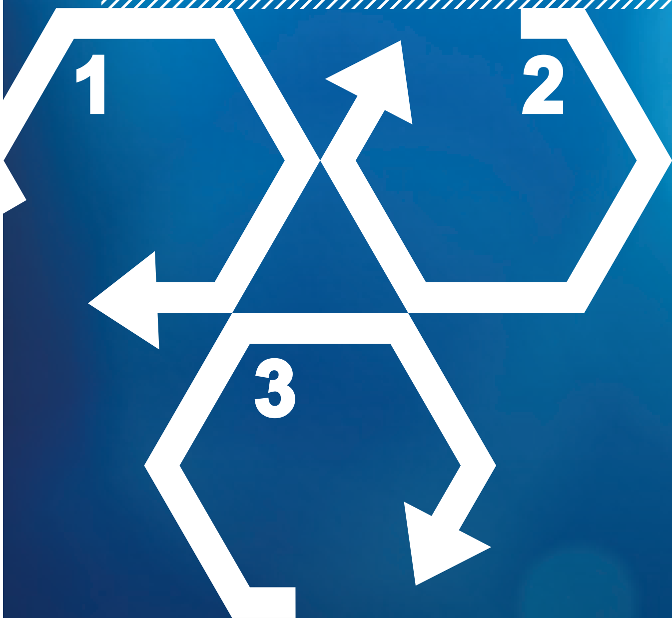
Guide on Sustainable Chemicals

A decision tool for substance manufacturers, formulators and end users of chemicals



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Preface

Sustainable chemicals – yes, but how? This guide helps you to select chemicals which are more sustainable.

The selection of sustainable chemicals has beneficial effects for occupational safety, consumer and environmental protection. In the medium run, sustainability leads to more innovative uses of chemicals, and is therefore also economically attractive. More sustainable products mean: fewer pollutants, greater acceptance, less adverse impacts on the environment and to society, with simultaneous success in the market.

The "Guide on Sustainable Chemicals" of the Federal Environmental Agency helps you as a manufacturer, formulators or end users of substances to put a greater emphasis on sustainability aspects: in the selection of substances and use of chemicals in the company. The guide furthermore assists companies in the implementation of the REACH task on the safe use of substances. If, during the process of substance selection, additional attention is reserved to sustainable chemicals, this will help ensure that the raw materials needed by the enterprises will be at their disposal over the medium and long term as well, and will not be restricted or prohibited as a result of administrative interference.

The guide comprises specific criteria for eight important test points on the sustainability of a substance:

- Mentioning in lists of "problematic substances" and physico-chemical properties
- Hazardous properties for human health and for the environment
- Mobility, greenhouse gas emissions and resource consumption
- Responsibility in the supply chains

Red, yellow or green? By means of these colors, the guide shows the results of an inspection: high need for action, indications of need for action or no evidence that the users of the guide should undertake any initiative. If data gaps appear, the color white is chosen.

Probably, the elimination of problematic substances will not be possible in all cases. Setting out use-specific criteria, the guide provides clues as to how the use of problematic substances can be made more sustainable.

This involves:

- The emission potential of use and related user groups
- The use amounts of the substance and the waste stage
- The substance's substitutability
- The substance's potential benefits and its innovation potential
- The guide in paper form focuses on the evaluation of substances, providing some clues on how companies may proceed in the evaluation of mixtures.

The guide in paper form focuses on the evaluation of substances, providing some clues on how companies may proceed in the evaluation of mixtures.

With the Access-based file **SubSelect**, an electronic version of the guide is now available in addition to the guide. SubSelect assists enterprises in evaluating the sustainability of substances and mixtures by using the same substance-related criteria as those described in the guide.

Index

Page 4 – 11

1.0

Introduction

Sustainable chemicals – yes, but how?

1.0 Introduction: Sustainable chemicals – yes, but how?

Sustainable chemistry comprises of many aspects. They range from the selection of inherently safe chemicals via the assessment of environmental impacts of product lines by lifecycle analysis to the implementation of ambitious social standards in the supply chain.

The background document of the environment agency on sustainable chemistry gives a good overview about the different aspects of this topic (Umweltbundesamt 2008).[1]

Neither today nor in the future, may sustainable chemicals have unacceptable (eco-) toxic impacts on humans and the environment. They may not or only insignificantly contribute to the depletion of natural resources. Furthermore, they may not cause or enhance socially precarious situations or unhealthy workplaces, however they are beneficial to the entire economy and to enterprises.

The sustainable use of (sustainable) chemicals aims at providing socially necessary products while minimizing resource consumption, reducing substance losses and controlling exposures by corporate, design oriented, organizational and technical means and at the same time enhancing healthy workplaces and fair social conditions.

1.1 Why sustainable chemicals?

The selection of sustainable chemicals can have advantages for the protection of workers, consumers and the environment. In the long run, sustainability leads to more innovative uses of chemicals and is therefore also economically attractive. Hence, a sustainable product is a product that is successful on the market, for which less dangerous substances are used and which have less adverse impacts on the environment and to the society than a comparable product.

[1] http://www.umweltbundesamt.de/uba-info-medien/mysql_medien.php?anfrage=Kennummer&Suchwort=3734

This guide also helps you to implement the REACH task of safe use. If you count on sustainable chemicals in your substance selection, these raw materials will be available for you in the medium- or long-term (and will not be restricted or prohibited through regulative steps).

1.2 Why this guide?

Numerous practical examples have been published on the implementation of single aspects of sustainability in enterprises[2]. However, up to now guidance supporting enterprises in a systematic manner to practically implement sustainable chemistry in their daily practice is missing.

This guide assists the selection of sustainable chemicals by providing criteria to distinguish between sustainable and non-sustainable substances. It can also support a more sustainable use of chemicals, by highlighting single aspects of the evaluation. The guide is not specific to certain industry sectors, but the criteria can be used across all fields of economy[3].

[2] For example the implementation of environmental or quality management systems, the manufacture of substances using catalysts (energy and resource savings), design for the environment integrating recyclability of products (reduction of material losses), the self-commitment to "codes of conduct" which exclude dangerous substances from products and reclaim compliance with workplace standards along the supply chain, and chemical leasing. For an overview we recommend the publication of Lißner and Lohse (2006) as well as Umweltbundesamt 2008.

[3] Here we want to mention an additional approach: the HACCP-concept ("Hazard Analysis and Critical Control Point"). It is implemented for managing risks along supply chains, mainly in the food industry, but can also be used to prioritize risk management in other sectors.

Note: There already are various different approaches to sustainability. A good overview has been published in the background document on sustainable chemistry of the Umweltbundesamt, which sets the focus on conceptual approaches.

1.3 For whom?

This guide is addressed to manufacturers, formulators and end users of substances and mixtures. It supports the integration sustainable aspects in their selection and the way chemicals are used.

End users of chemicals frequently demand specific technical standards of the products they use (substances and mixtures), like the uniformity of coloration achieved by a specific dye or a particular degree of light resistance of lacquers. In addition, requirements of workers' protection, consumer protection and environmental protection must be fulfilled. The consideration of sustainability aspects may trigger further demands, e. g. on conformity of actors in the supply chain with social standards.

Some enterprises have already implemented a sophisticated quality or environmental management system and are eager to substitute dangerous chemicals. However, small and medium sized enterprises (SMEs) normally have only little or no experience in the selection of sustainable chemicals. The guide aims particularly to support these companies.

1.4 Integration of "new" issues

For some aspects (e. g. avoiding chemicals with a high human toxicity) well defined decision criteria can be provided in this guide (e. g. classification as carcinogenic or mutagenic of categories 1, 2 and 3).

For other aspects these criteria don't exist yet, for example on resource consumption, reduction of greenhouse gas emissions and taking social responsibility. In many industry sectors "best available techniques" have been compiled in so called BREF documents which will lead to resource savings and emission reduction if implemented[4].

The evaluation of sustainability of chemicals is more than the traditional identification of dangerous substance properties, assessing exposures and characterizing risks. Therefore, this guide also provides support for the "new" issues – even though no fully developed and quantified criteria are available.

Demands for sustainable chemicals can be better accommodated (maybe even only then!), when they are integrated not only into a company's policy and goals but also in its quality or environmental management system (including standards for success monitoring). The implementation is normally a step-by-step process.

1.5 Contents and structure of the guide

This guidance sets the focus on potential impacts of substances on man and the environment and on social responsibilities in supply chains. Economic aspects are addressed to a minor extend only. Such aspects are treated in detail within the socio-economic analysis developed under REACH. It is introduced in chapter 2.2.6.

In this guide, the term "chemicals" means both substances and mixtures. The evaluation of sustainability, in particular regarding the substance-specific criteria is recommended to be performed primarily for substances as such. However, along their life-cycle they are in most cases included into mixtures (formulation) and either consumed or further processed into articles. This is reflected in the second set of criteria addressing the uses.

Formulators and end users of chemicals (= substances and mixtures) normally handle mixtures rather than substances. In this case we recommend to start the assessment of the mixture with substances of the mixture classified as dangerous. These substances are important for occupational health and environmental protection in companies. They are documented in section 3 of the safety data sheet of the mixture (in most cases, for substances which are not classified as dangerous the downstream user has no information

[4] *http://eippcb.jrc.ec.europa.eu/reference/*

on their properties (without a specific communication with his supplier[5]).

This guide consists of six chapters. The criteria for sustainable chemicals are introduced in Chapter 2, following this introduction. Substance-specific criteria, which only depend on the substance properties, are differentiated from use-specific criteria, which depend on the type of its application and use. The criteria in this guide are selected according to two guiding questions:

[5] *In case of mixtures consisting of many substances in a first step it should be clarified, which substances as lead substances are triggering the risk management measures for the mixture. Guidance for the identification of lead substances is given in Part III of the REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains. You can get the document from us. Write a short email to d.bunke@oeko.de.*

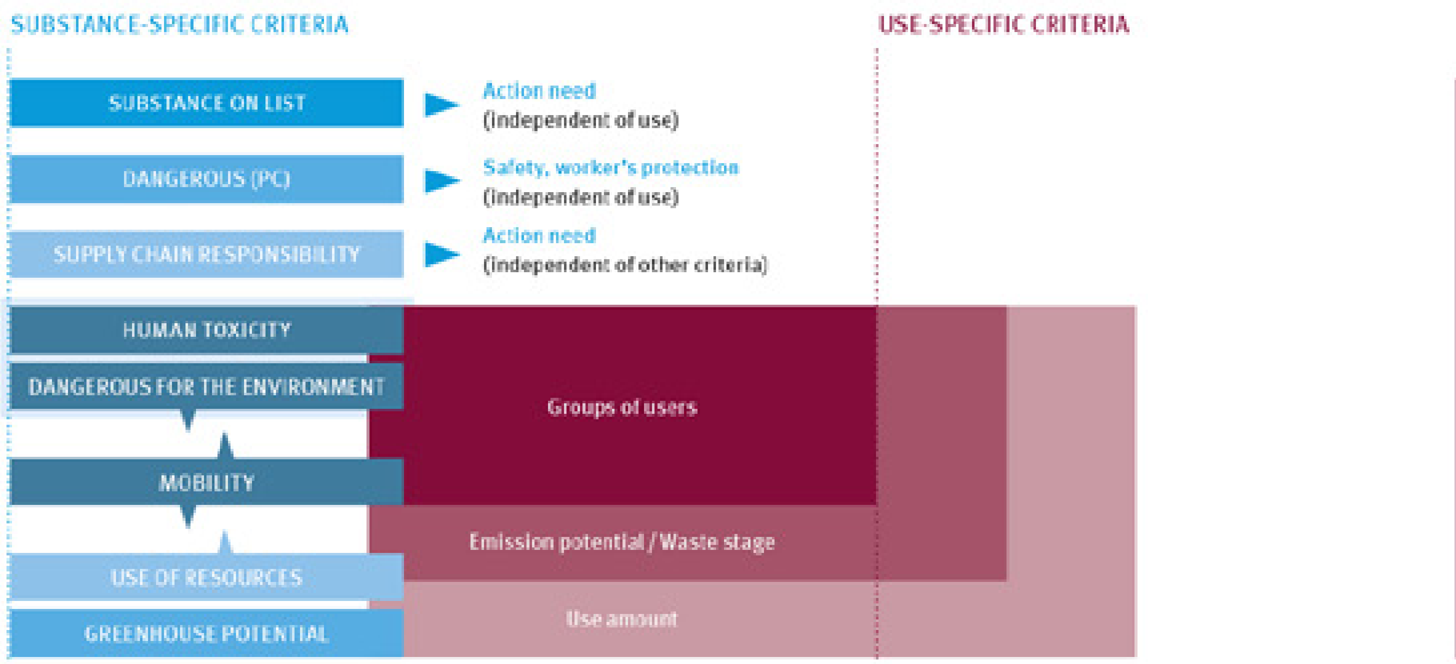
- Which criteria can be applied by enterprises in practice for the selection of substances and mixtures?
- What types of demands can enterprises pose their suppliers that exceed those of product labels such as the Blue Angel?

In Chapter 2.1.9, using some examples, you can see the outcome of the analysis and how you can compare substances.

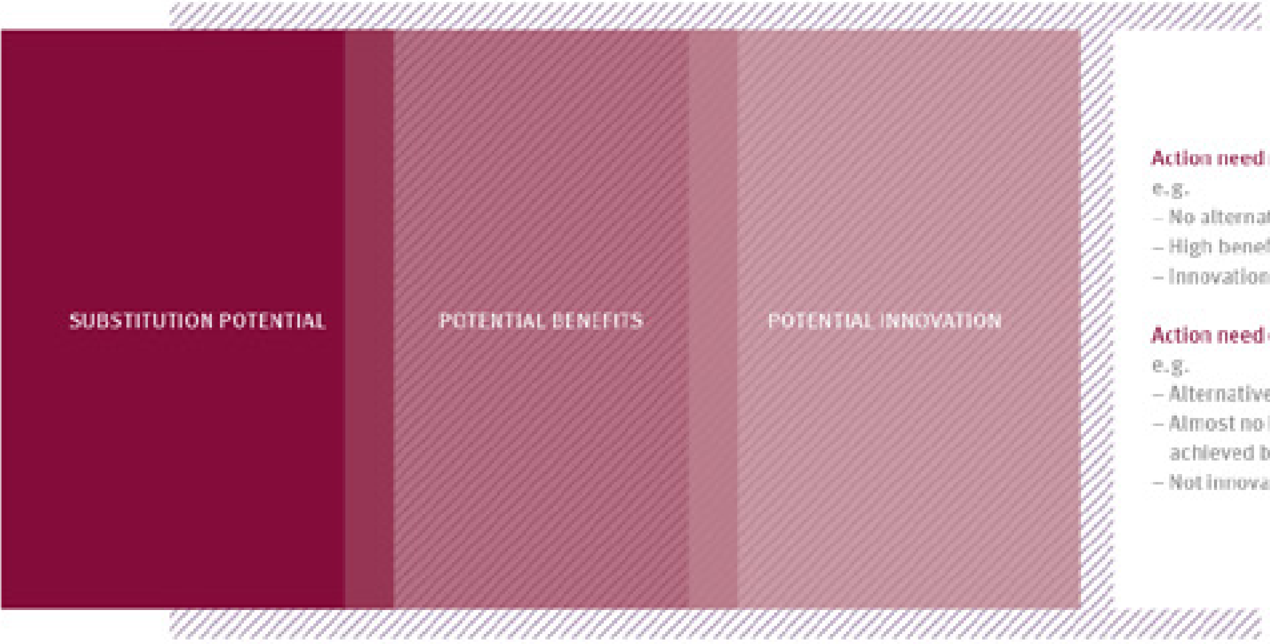
Following the description of the sustainability criteria, in Chapter 3 "golden rules" for the selection and use of sustainable chemicals are introduced, which can be understood as simplified and aggregated sustainability criteria. The "golden rules" relate to the selection of sustainable chemicals connected with some important rules regarding their safe application.

Figure 1

LINKAGE BETWEEN THE SUBSTANCE-SPECIFIC CRITERIA AND THE USE-SPECIFIC CRITERIA



In Chapter 4, we give an outlook with notes on SubSelect, the electronic supplement to this guide. Chapter 5 provides references used in this guide and abbreviations are explained in Chapter 6. The annexes contain links and further information sources on substance lists, specific criteria, data bases and assessment systems.



1.6 What does the result look like?

This guide provides criteria which can be used for a first assessment of the sustainability of substances and mixtures in your enterprise.

When analyzing the sustainability of chemicals using the following, substance-specific criteria will result in one of the following statements:

- No action is needed, because available information indicates that the chemical is not “problematic” (green)
- No action is needed, because the available information indicates problematic substance properties (yellow)
- There is a high priority to act, because the available information indicates very problematic substance properties (red)
- There is a need to gather further information, because no or little data is available (white).

The results of the substance based criteria can be compiled to a sustainability profile – in chapter 2.1.9 you can see an example. The application of the use-specific criteria can modify the evaluation of a substances sustainability judged only by the substance-specific criteria, because properties assessed as problematic may, due to the type of application, not cause any harm. Other aspects, such as very high benefits of the use of a substance, may justify the continuation of its use, although it was originally evaluated as non-sustainable.

Chapter 2.2 describes consequences of the application of the substance-specific criteria for the next step of the assessment, the application of the use-specific criteria.

Chemicals without problematic properties, which can be regarded as inherently safe will not be available in all cases. Nevertheless, there may be ways to optimize the use of problematic substances, for example by implementing risk management measures. The guiding questions are:

- How can the emission potential of a specific use be minimized?
- Which user groups will be exposed to the chemical?
- How can exposures be reduced?

You can find related support in Chapter 2.2 (use-specific criteria).

This guide does not provide a valuation method which ultimately maps the “sustainability” of a substance in figures. It is possible (but only with individual weighting). However, the “one-point”-rating can cause inadequate provision for the complexity of this topic. The guide with individual results for eight fields for the substance selection gives you clear references where to make a more in-depth assessment or where there is information demand- which is better than one figure which aggregates the individual findings.

We recommend a stepwise approach:

- For the first assessment data should be used which are readily available in the company. The resulting sustainability profile (see chapter 2.1.9) indicates areas which require further action.
- In the next step, further information is included. It might become necessary to use additional data sources. Some of them are described in Annex.

SubSelect – A tool for the evaluation and comparison of substances and mixtures

https://www.umweltbundesamt.de/dokument/subselect-instrument-zur-auswahl-nachhaltiger

SubSelect covers the assessment of chemicals on the basis of eight substance-specific criteria. Reference is made to the use-specific criteria of the guide as a means of assessing chemicals further.

If you have any questions regarding our instruments and about the sustainability of chemicals feel free to contact us:

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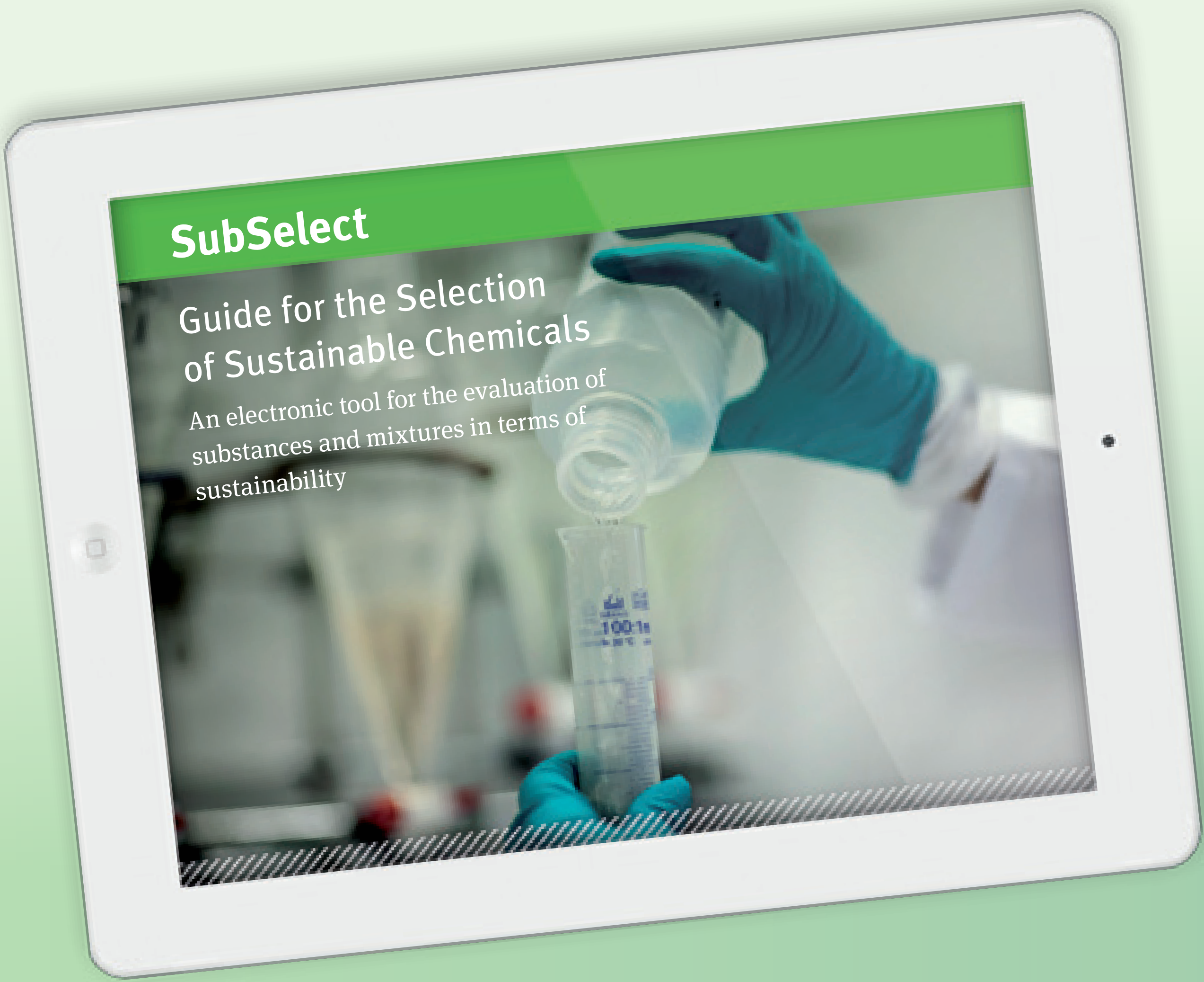
GET STARTED NOW!
It is worth attaching importance to sustainable chemicals. For you, your customers, your employees and the environment.

Further information on page 55 (see chapter "Outlook").



Page 12 – 45

2.0

Criteria for selecting sustainable chemicals

2.0 Criteria for selecting sustainable chemicals

The criteria for the selection of sustainable chemicals should enable companies to systematically implement sustainable chemistry in their daily practice.

Generally, substance-specific criteria which only depend on the properties of a substance (for instance its classification regarding hazardous properties) and use-specific criteria which mainly depend on the type of its use, like the substance amount at use, are distinguished. The substance-specific criteria are introduced in Chapter 2.1 and the use-specific criteria in Chapter 2.2.

The evaluation of sustainability is based on the following eight substance-specific criteria (step 1).

The application of the use-specific criteria to chemicals evaluated as "red" and "yellow" may be helpful in the prioritizing of action needs. For chemicals which have been evaluated as "white", more information should be obtained as a priority action to enable the assessment of the substances-specific criteria.

Figure 2 gives an overview of the possible options to act on, depending on the result of the evaluation.

Figure 2

CRITERIA, EVALUATION AND OPTIONS TO ACT

Criteria	RED	YELLOW	GREEN	WHITE
Substance on list	Substitution		No action need	Gather Information
Dangerous PC properties	Substitution Riskmanagement			
Human toxicity Dangerous for the environment (Mobility)	**Use-specific criteria** Priority **RED:** Substitution Priority **YELLOW:** Substitution or risk management			
Greenhouse potential	Substitution, Design increasing energy efficiency			
Resource use	Substitution, Design increasing material efficiency			
Supply chain responsibility	Request standards from supplier or change sourcing			

2.1 Substance-specific criteria for the evaluation of sustainability

For the evaluation of sustainability of chemicals, the following eight substance-specific criteria should be used as a first step. They refer to the substance itself-regardless of the situation of use

1. Mentioning in lists of "problematic substances"
2. Dangerous physicochemical properties
3. Human toxicity
4. Problematic properties related to the environment
5. Mobility
6. Emission of greenhouse gases
7. Resource consumption
8. Responsibility in the supply chain

In the following sections these eight criteria are described. We also discuss where you can find the information you need for the application of these criteria.

Some products require properties which automatically result in an assessment as being "less sustainable" (red sphere). E. g. can preservatives are used to prevent microbial degradation of lacquers. This requires a biocidal activity of ingredients which are therefore hazardous to the environment. In such cases a problematic property has to be accepted to achieve the required function of the product.

If criteria refer to properties which are essential for the function of the product, it might be that these criteria become less important for the overall assessment of the product.

If the function of a product requires problematic properties, it should be carefully checked whether it is possible to achieve the same function by a different product design. This includes alternative solutions without chemicals, e. g. constructive solutions for flame protection. In any case – including alternative solutions without chemicals – the assessment of the alternative solutions has to cover the different potential impacts on man and the environment (e. g. energy consumption in case of vegetation control using heat). Details on the assessment of substitutes are given in chapter 2.2.5 of this guidance.

The sustainability of chemicals based on their intrinsic properties is evaluated using tables with specific indicators, which are included at the end of each section. To improve understanding, the colors "green", "yellow", "red" and "white" are used to indicate the evaluation result. The following explains what each color means:

- **Green:** There are no indications of critical properties, no action needed.
- **Yellow:** There are indications of problematic properties; further analysis with use-specific criteria is necessary.
- **Red:** The substance is obviously problematic. Substitution possibilities should be assessed with high priority.
- **White:** Information is not sufficient for an evaluation. Further information should be gathered.

Some criteria consist of several sub-criteria. Here, the overall evaluation results from the integration of all sub-criteria into one. The sub-criterion with the worst evaluation determines the overall result (results are not averaged!). The sequence of "severity" is:

Red > **White** > **Yellow** > **Green**

The action requirement is highest for red and lowest for green. In case of "White" a high need for further action is required to get sufficient information for the assessment.

Note: The assignment of colors and indicators to the criteria is a proposal of the editors, which is based on the expertise of the persons involved.

Excursus:
In the past, much substance-related empirical data has been generated for assessing risks and classifying and labelling substances. This data, which was and is required among others in legislation on supply chain communication, is an important information basis for the evaluation of a substance's sustainability. In general they are communicated with the safety data sheets. Therefore, some of this data is explained in annex 5.

2.1.1 Mentioning on lists of problematic substances

Substances with particularly dangerous properties for man and the environment may already be regulated in different contexts (e. g. legislation or conventions, such as the Helsinki or Stockholm Convention). Corporate instruments may exist for managing these substances as well, such as the "Global Automotive Declarable Substance List" (www.gadsl.org) of the automotive industry. Legislation, conventions and private instruments may contain lists of substances to which they refer. If a substance is included in any of these lists, it is a strong indication that the substance is not sustainable.

Unfortunately, there is not "the one and only" list, but several exist. For the evaluation of sustainability of substances we recommend to use the following lists. They have origin from European or international regulations and conventions. They have been thoroughly discussed by experts and politically agreed.

- The candidate list for authorization under REACH,
- The list of priority and priority hazardous substances of the Water Framework Directive
- Persistent organic compounds regulated under the POPs-Convention
- Substances on the priority lists of OSPAR[6] and HELCOM[7]
- Substances affecting the climate according to the Montreal- and Kyoto-Protocol
- Ozone depleting substances according to the Montreal protocol
- The SIN ("Substitute it now")-list[8].

Not all of the substances on the SIN-list have been lawfully restricted. However they hold problematic qualities, so you should avoid or exchange these substances, as far as possible. Furthermore, it is possible that these substances will be lawfully restricted or prohibited in the future.

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[6] OSPAR: Convention on the protection of the marine environment of the North-East Atlantic.

[7] HELCOM: Commission on the protection of the marine environment of the Baltic Sea.

[8] http://chemsec.org/business-tool/sin-list/

You should check for all substances you use in your enterprise, if they are mentioned in one of these lists. Therefore, you only need the CAS-numbers of the substances. The testing on listing will then be easy and quickly possible.

In some (rare) entries of the problematic substances lists, there are no CAS-numbers. In this case a direct comparison of names is required. In the electronic instrument SubSelect (see Chapter 4) a analogy for these substances or element groups is supported. The lists are publicly accessible as some of them are regularly updated, we abstain from rendering these lists in the annex. Links to the web pages are compiled in Annex 1.

Substances are only included in lists of problematic substances, if they have been assessed by experts as of particular concern. It is to be noted that the lists are developed for a particular purpose (e.g. environmental protection) or from a particular perspective. Therefore, certain properties may dominate whether or not a substance is included. For a sustainability evaluation, in addition other criteria need to be tested. For this purpose, we have developed seven further substance related criteria, which will be explained in the following chapters of this guide.

For the criterion "mentioning on lists of problematic substance" there are only three possible results (see table 1): "Red" if the substance is listed on one of the lists, "green" if this is not the case and "white" if you haven't checked, yet. The listing of a substance as problematic substance is an important indication of critical (not sustainable) characteristics. For those substances, possibilities of replacement should be checked.

This is especially important for substances that are already on the REACH Candidate list due to their particularly alarming characteristics ("SVHC-substances", substances of very high concern). If your products contain any of these substances (in a concentration higher than 0,1 %), you have to inform your customers – and answer any of their questions concerning these substances (REACH Art. 33).

Table 1

USE AND EVALUATION OF THE CRITERION "MENTIONING ON SUBSTANCE LISTS"

Evaluation	RED	GREEN
Criterion: List of problematic substance	Substance is mentioned in one or more lists of problematic substances	Substance is not mentioned in any list of problematic substances.
Indicator	Problematic-substance lists (c.f. Annex 1)	

Note for evaluation, valid for this and all other tables:
"White" should be given if there is no further information for the evaluation criterion. It shows that there is a need for action to consult the information which is necessary for the evaluation.

2.1.2 Dangerous physicochemical properties

Substances with hazardous physicochemical properties are difficult to handle for workers. Alternatives with less dangerous physicochemical properties should be used or risk management measures implemented at workplaces, in order to prevent exposure and potential danger to workers. In addition, physicochemical properties could endanger installations (explosion, fire).

Some substances are used especially because of their (dangerous) physicochemical properties. For example, fireworks cannot be produced without the use of pyrophoric substances[9]. These substances will always be in the red sphere due to our criteria.

Physicochemical properties can be evaluated on the base of the classification of the substance. The necessary information should be available through the implementation of REACH, as a comprehensive data set is already required for substances manufactured or

[9] Note that the authors of this guidance consider this type of product as such as being not sustainable as a low societal benefit is contrasted with high risks to humans and the environment and high losses of materials and energy.

imported in amounts between 1 and 10 t/a[10]. Users of substances can find information in sections 2, 9 and 10 of the safety data sheets of the substances. If there are any doubts regarding the information, substance manufacturers should be consulted and the entries should be compared to information for evaluation from public databases, such as the "common substance data pool" (Gemeinsamer Stoffdatenpool von Bund und Ländern[11]) or the data base on classification and labelling.[12]

In table 2 the criteria for assessing the dangerous physicochemical properties of substances are shown. They refer to the indications of danger (H-phrases) of the substances. The assignment of the H-phrases to the colors has been derived from the "Easy-to-use workplace control scheme for hazardous substances" (Einfaches Maßnahmenkonzept Gefahrstoffe, EMKG) of the Federal Agency for Occupational Health and Safety. It supports enterprises' decisions on risk management measures to ensure safe use of substances and mixtures.

[10] This may take until 2018 for low volume substances which have been on the market before REACH entered into force.

[11] http://www.gsbl.de/index.html

[12] http://ecb.jrc.ec.europa.eu/classification-labelling/search-classlab/

Table 2

USE AND EVALUATION OF THE CRITERION „DANGEROUS PHYSICOCHEMICAL PROPERTIES

Evaluation	RED	YELLOW	GREEN
Criterion: Dangerous physical-chemical properties	Substance is explosive, oxidizing, very flammable or pyrophoric	Substance is flammable	Substance has no critical physical-chemical properties
Indicator: H-phrases according to CLP regulation*	H200, 201, 202, 203, 205, 220, 221, 222, 226, 228, 240, 241, 242, 250, 251, 260, 261, 270, 271	H 204, 221, 223, 224, 225, 252, 272, 280, 281, 290	No H-phrase indicating problematic physical-chemical properties

**C&L According to CLP-regulation: Classification and labelling of substances according to the European regulation on the classification, labelling and packaging of substances and mixtures.*
Some phrases can be assigned only in addition to other classifications according to the "old" classification and labelling rules (complementary labelling). The CLP regulation allows the independent assignment of these. if one or more of the H-phrases apply, a substance's dangerousness is increased in the evaluation about one level:

EUH001 – Explosive when dry
EUH006 – Explosive with or without contact with air
EUH014 – Reacts violently with water
EUH018 – In use, may form flammable/explosive vapor-air mixture
EUH019 – May form explosive peroxides

Remark for nanomaterials:

Particle size belongs to the physicochemical properties. Nano materials can be released from their matrices during use of the product and the waste phase. At present knowledge is limited about the fate and the hazardous properties of nanomaterials in waste treatment plants. As for all other chemicals the precautionary principle should also be applied to nanomaterials and expositions should be avoided, even if risks cannot be estimated exactly.

We suggest to first conduct an inspect, to find out where nanomaterials are used in your products. Therefore you need information about the particle size distribution of your materials. This information can be found in safety data sheet or in the technical bulletin. If this is not the case, you can inquire your supplier if there are any nanomaterials according to the EU definition in the material. For the evaluation of the particle size distribution the EU-commission's definition of 2011 is taken as a basis. According to this, "nanomaterial" is a natural, through processes incurring or manufactured material, containing particles in an unbound state, as aggregation or agglomerate, and at least 50 % of the particles in the particle size distribution have one or more sizes within the range of 1 nm to 100 nm (EU-Commission, 2011[13]). If you use nanomaterials, there is further need for action to exclude problematic properties or expositions (color yellow).

[13] *EU-Commission RECOMMENDATION OF THE COMMISSION of 18th October 2011 for the definition of nanomaterials, Pub.L.No. 2011/696/EU (2011). EU-Commission. Retrieved from http://eurlex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L2011:275:0038:0040:DE:PDF*

2.1.3 Human toxicity

Substances which are toxic to human health are to be avoided in general. They may cause harm to people during manufacturing as well as during the application of chemical products. The substance properties, which may cause irreversible and severe damage to human health, like cancer or which may damage the immune system, are evaluated as more problematic than those which cause reversible (curable) effects. Some properties are relevant not only for human health, but also for adverse impacts they may have on the environment (e. g. endocrine disruption).

The human toxicity of a substance refers to the substance as such. Firstly it is evaluated by itself, regardless of the use of the substance. However; the dangerousness to human health is determined by the type of use of the substance, its mobility and emission potential (c. f. Chapter 2.1.5. and Chapter 2.2.1). If a substance is manufactured and used only under strictly controlled conditions (e. g. biocides to avoid bacterial contamination of closed cooling circuits or lead sulfate in car batteries), toxic effects to humans cannot be excluded, but are, due to the estimated very low exposition, more unlikely than, for instance, in open applications like household cleaning agents.

For certain applications, substances are selected just because of their toxic properties, e. g. active substances in biocidal products and plant protection products, as well as pharmaceuticals. Here, the criterion will lead into the red sphere. Therefore, investigations should be made, if there are any less toxic alternatives or other ways of application that are more sustainable. Generally, the classification of a substance as harmful to human health is sufficient for the evaluation for most of the potential harmful effects on humans. Respective information can be found in the safety data sheet (c. f. Annex 5) in sections 2 and 11.

Substances that interfere with the endocrine system can cause severe damages to a human body. These substances are identified as "endocrine disruptive" and called "endocrine disrupting chemicals" (EDC): substances that disrupt the endocrine system. For the evaluation if your substance is an EDC, first, you have to check if there are any hints on endocrine effects in chapter 2 or 11 of the safety data sheet. Many as endocrine active identified substances are also listed on the SIN-list (see chapter 2.1.1). You can also look in dangerous substances databases for hints on endocrine activity, e. g. in GESTIS or in the database eChemPortal[14] (see Annex 3: Links on databases and evaluation instruments). An alert for endocrine activity is also given if there are structural similarities between your substance and substances that have already been identified as EDC.

In table 3 the criteria for assessing hazardous potential regarding humans are shown. As in the case of the assessment of physicochemical properties, they refer to the indications of danger (H-phrases) of the substances. The assignment of the H-phrases to the colors has been derived from the "Easy-to-use workplace control scheme for hazardous substances" (Einfaches Maßnahmenkonzept Gefahrstoffe, EMKG).

If workplace exposure estimations have to be made for the use of substances, appropriate estimation tools should be used, e. g. the EMKG tool (Easy-to-use workplace control scheme for hazardous substances" (Einfaches Maßnahmenkonzept Gefahrstoffe, EMKG) or the COSHH. In the EMKG tool of September 2009, the CLP regulation has been taken into account (BAUA 2009).

[14] The database eChemPortal has the following web-page: www.echemportal.org (last checked: 29th June 2016).

Table 3

USE AND EVALUATION OF THE CRITERION "HUMAN TOXICITY"*

Evaluation	RED	YELLOW	GREEN
Sub-criterion: Dangerous by Inhalation, ingestion and eye contact	Substance may cause severe health damage	Substance may damage health	Substance is not dangerous to human health
Indicator: Classification according to CLP-regulation	H300, 330, 340, 350, 350, 350i, 360, 360D, 360DF, 360F, 360FD, 361Fd, 362, 372, EUH032	H301, 302, 304, 314, 318, 319, 331, 332, 334, 341, 351, 361, 361d, 361f, 361fd, 37013, 371, 373, EUH029, EUH031	No classification other than "only" 335, 336
Sub-criterion: Dangerous upon skin contact	Substance may cause health damage if taken up via the skin	Substance damages skin	Substance has only light effects on skin
Indicator: Classification according to CLP-regulation	H310, 311, 314, Für hautresorptive Stoffe: 340, 341, 350, 351, 360, 360D, 360DF, 360F, 360FD, 361Fd 361, 361f, 361fd, 370, 372	H312, 315, 317 For skin-penetrating substance: 371,373	No classification other than "only" EUH066
Sub-criterion: Endocrine disruption	Proven endocrine disruptive substance (e. g. referred to problematic substances lists)	Indications for endocrine activity or structural similarity with endocrine disruptive substances	Not listed, no indications for endocrine disruption
Overall evaluation			

**The classification of the H-sentences within this evaluation is based on the "Einfache Maßnahmenkonzept Gefahrstoffe" of the German Federal Institute for Occupational Safety and Health (BAuA): http://www.baua.de/de/Publikationen/Fachbeitraege/Gd64.html*

Additional note:

Mineral fibers, dusts and substances that produce problematic combustion products can cause additional concerns for human.

Mineral fibers with a critical proportion of fiber length and diameter can cause chronic damages to human health. Such fibers should be replaced as far as possible. If you use mineral fiber in your enterprise, you should check if, due to the fiber characteristics, special health and safety measures are necessary. In the EMKG tool (see above) this topic is responded to. Dangerous fibers have to be classified appropriately. This classification has to be stated in the safety datasheet.

If you use mineral fibers you should check the information of the safety data sheets for the classification, e. g. through comparison with information in the dangerous substances database GESTIS[15].

Also **dusts** are particularly dangerous for humans, even if the substance is not classified as dangerous. Dusts can easily be released and inhaled. We respond to this quality in the criteria "mobility" (chapter 2.1.5). Notes to the exposure to dusts can be found in the EMKG tool mentioned above.

Mind that no **problematic combustion products** can emerge from the materials you use. That applies, for instance, to halogenated flame retardants. They should be replaced by halogen-free substances. This step also leads to the elimination of hazardous substances in the products. Currently a considerable amount of electronics is not professionally disposed but gets "disposed" outside of Europe under not monitored conditions. As a consequence, very adverse impacts on human health and the environment have been found. This is also related to the use of halogenated flame retardants. In the EMKG, the development of hazardous substances and their release of products is addressed.

2.1.4 Problematic properties related to the environment

Substances, which are persistent, bioaccumulative and toxic (PBTs) or very persistent and very bioaccumulative (vPvBs) are particularly problematic for the environment:

- They can concentrate in the environment (persistence and bioaccumulation) and in the long run may reach concentrations above which adverse effects are likely to occur,
- they cannot be recovered, once they have been released to the environment and
- they are transported via the atmosphere and biosphere and can be found far from their emission sources, even in pristine areas
- Furthermore, PBTs and vPvBs can accumulate in the food chain and damage human health.

Beside PBT and vPvB substances, further substances are problematic for the environment because they have the potential to harm the environment on a local scale – or in case of poorly degradable substances – on a larger scale. As criterion for these properties classification of substances as "harmful for the environment" is used.

[15] http://www.dguv.de/ifa/GESTIS/GESTIS-Stoffdatenbank/index.jsp

Attention: For some substances and mixtures persistency and high aquatic toxicity are required for the function of the product. Examples are biocidal products which are harmful for the environment. In these cases the criterion always indicates a low degree of sustainability.

The PBT/vPvB criterion is not applicable for elements because they cannot be degraded. Currently, there are no PBT-criteria for inorganic substances.

Where do you find the information you need for the evaluation? For substances for which PBT/vPvB properties have been found, this has to be noted in the safety data sheet (SDS). Information on persistence, degradation, bioaccumulation and aquatic toxicity are provided in sections 9 and 11 of the SDS. Data is available in the context of registrations under REACH[16].

In table 4 the use and the evaluation of the criterion "dangerous for the environment" is described. As before, three categories are defined (red, yellow, green). For the evaluation of PBTs/vPvBs, the criteria of REACH Annex XIII are provided (c. f. Annex 2). If all criteria are fulfilled, the substance is a PBT/vPvB.

Frequently, information on half-lives and on bioconcentration is not available. If there is a lack of data, estimations can be performed using indicative criteria on the degradability of a substance or its partitioning coefficient for octanol/water (LogKow): Substances which are inherently not degradable or are not easily

[16] *The registration of low volume substances (production or import volume between 1 and 10 ton per year) will be finalized by 2018. However, for these substances, the required data set to be generated will not allow a thorough PBT/vPvB assessment, as no BCF or half-life needs to be determined, but only the LogKow and easy degradability.*

Table 4

USE AND EVALUATION OF THE CRITERION "DANGEROUS FOR THE ENVIRONMENT

Evaluation	RED	YELLOW	GREEN
Sub-criterion: PBT/vPvB properties	The substance is a PBT/vPvB substance	Based on available information, it cannot be excluded that the substance is a PBT/vPvB substance*	No PBT/vPvB-substance
Indicator: Information from testing	Mention as PBT/vPvB-substance on a list/ in the SDB or implementation of the PBT/ vPvB-criteria**	H410 Aquatic toxicity: LC50 ‹ 0,1 mg/l	There are no indications that the substance is PBT or vPvB
Sub-criteria: Acute aquatic toxicity	The substance is highly dangerous to the aquatic environment	The substance is dangerous to the aquatic environment	The substance is not dangerous to the environment
Classification according to CLP-decree	H400	H410, 411, 412 and 413	Not H-phrase beginning with 4
Overall evaluation			

**It is possible that a substance is inherently not degradable and has a LogKow of more than 4. These are indications that the substance may be a PBT/vPvB. Further data is necessary for a comparison of the respective criteria (e. g. simulation test on degradability and/or study determining a BCF).*

***The criteria are given in the Annex.*

Table 5

USE AND EVALUATION OF THE CRITERION “MOBILITY”

Evaluation	RED	YELLOW	GREEN
1.Sub-criterion: Release potential in water	High solubility	Mittlere Wasserlöslichkeit	Niedrige Wasserlöslichkeit
Indicator: Solubility in water	› 10 mg/l	10 – 0,001 mg/l	‹ 1 µg/l
2.Sub-criterion: Release potential to air	High vapor pressure	Medium vapor pressure	Low vapor pressure
Indicator: Vapor pressure	› 100 pa (environment) › 25 pa (humans)	1–100 pa (environment) 0.5 – 25 pa (humans)	‹ 1 pa (environment) ‹ 0,5 pa (humans)
3.Sub-criterion: Long-range transport	Substance is transported over long distances	Indications or suspicion of long-range transport	No long-range transport
Indicator: Persistence, indications on long-range transport	Half-life in air › 2 days and vapor pressure › 1000 pa	Half-life in air between 1 and 2 days and vapor pressure ‹ 1000 pa	Half-life in air ‹ 1 day
4.Sub-criterion: Release potential at workplaces	Very dusty	Dusty	Not dusty
Indicator: Dosage form of manufacturer	Aerosols & gases, substance which form clouds of dusts, which remain in the air for a longer time	Substance which are pulverized but not too dusty, dust deposits quickly	Liquids, non-dusty solid sub-stances (pellets, waxes, granulates...)
The following sub-criteria are only relevant if the substance is used for the production of alloys and products			
5.Sub-criterion: General release potential of products and alloys	Use in mixtures, or intended release form articles	Is released unintentionally from articles	Stable embedding in matrix or containment inside articles
Indicator: Release (migration), integration in product matrices	Use in mixtures. substance is contained in articles, from which it is intended to be released	Substance is not used in mixtures and it is not known that it is released from the matrix during the lifecycle of the product	Embedding of substance in matrix or containment in inside product, no use in mixtures
Overall evaluation			

degradable (OECD screening test[17]) should be evaluated as persistent. Substances with a LogKow > 4 should be evaluated as bioaccumulative. It should be noted that these values are only indications of dangerousness and not sufficient for a classification as PBT or vPvB.

Substances classified as dangerous for the environment can have the resp. H classes: H400, H410, H411, H412 and H413.

2.1.5 Mobility

There are substances which can spread very far in air and water. Therefore, they can disperse in the working and natural environment and with low degradability can be transported over long stretch. A high mobility is particularly critical if substances also have a high human or environmental toxicity. Furthermore, high mobility may lead to high substance losses (this means a low resource efficiency).

[17] *http://www.oecd.org/chemicalsafety/risk-assessment/*

A substance's mobility is a property which can be assessed based on physicochemical properties. The mobility is also determined by its use (c. f. Chapter 2.2.1). In this chapter, only substance properties influencing partitioning and distribution in air and water, as well as the potential to penetrate the skin are discussed. The latter is relevant because if a substance cannot penetrate the skin, dermal exposure is less problematic.

Attention: There are substances used in applications requiring a high mobility. E. g. solvents in printing inks, which have to dry quickly to ensure smooth printing processes. Evaluating their mobility, they will always be in the red or yellow sphere. Therefore, the relevance of the criterion has to be assessed in relation to the use of a substance.

The information that is important for the evaluation of the mobility (e. g. vapor pressure) can be found in the safety data sheet in section 9 (partly also sections 2 and 11).

For the evaluation of mobility, five sub-criteria are used (see table 5). The last criterion is about the evaluation of the emission from products and alloys. This last criterion is not applicable to other products.

To evaluate the mobility, all sub criteria should be checked and then summarized in the overall evaluation. The sub-criterion with the most severe evaluation represents the overall evaluation.

A high mobility is especially relevant if the substance is dangerous for man or the environment or if it causes high losses of the substance. In this case it would lead to a loss of raw material and a decrease in resource efficiency.

Additional note on the mobility of persistent substances:

In the upper part of table 5, the water solubility is used to evaluate the possible release into water. For most substances, this is a good approach. Except for the substances that are not or hardly degradable. These-persistent-substances also carry the danger of pollute waters even if they are scarcely soluble. An evaluation of these substances with this table would lead to a wrong result ("green" due to alow water solubility). For the evaluation of the mobility of persistent substances another parameter is more appropriate: the partition coefficient Koc. It defines how a substance distributes in water and organic components ("organic carbon", "oc").

For persistent substances you can use the following classification to evaluate the mobility in water:

- Logarithm of the partition coefficient Koc (logKoc) > 4.5: green
  (the substance is adsorbed by the ground)
- LogKoc between 3 and 4.5: yellow
  (hints on critical mobility)
- Log Koc below 3: red
  (probably very critical mobility)

For some substances there is information available about the Koc in data bases, e. g. in the data base eChem http://ww.echemportal.org/echemportal/index?pageID=0&request_locale=en). For salts (ionizing substances) measured data is required.

2.1.6 Emission of greenhouse gases due to manufacture of raw materials or of the substance itself

Production of chemicals can cause emission of gases which contribute to global warming. Carbon dioxide (CO_2) is the best known greenhouse gas[18]. These emissions can occur in the upstream chain – for production of raw materials – and during the production of the substance itself. They are measured as CO_2-equivalents. Normally, the driving factors for these emissions are the energy consumption and transports for obtaining raw materials. Substances with a high greenhouse potential in their upstream chains, therefore, often have a high energy consumption value in their production (c.f. Chapter 2.1.8). In single cases also other parts of the life cycle can be connected to high greenhouse gas emissions. (pot whale)

The absolute values of CO_2-equivalents emitted along the lifecycle of a substance (e.g. "20 kg CO_2-equivalents / kg substance") normally have a low expressiveness. The evaluation is done in a comparative manner using different substances or products for comparison. The amounts of the substance needed in order to fulfil a certain function should be used as point of reference, rather than a total amount of a substance. The amount of CO_2-equivalents identified as being emitted for the production of 1 kg of a substances has to be multiplied with the amount needed to perform the function, in order to compare alternatives. This approach allows comparing alternative solutions which differ in the amount of substances they need.

Often very specific data is missing to estimate the greenhouse potential. Similar raw materials usually have the same values and the criterion leads to the same results for similar substances.

Information on the greenhouse gas of a substance can be found, for example in the data base Probas of the German Environment Agency (c.f. Annex 3). In the table in annex 9 you can see the greenhouse gas emissions for the production of 1 kg of frequently used substance. If a specific substance cannot be found in the table or the data base of Probas, for a first evaluation, data can be taken for substances that are produced in a similar way (similar resources, similar process of manufacture). The compilation of a greenhouse gas balance for a substance is highly acknowledgeable, but very time and resource consuming.

[18] In addition to CO_2 emissions, other greenhouse gases such as Methane or SF_6 are taken into account with different environmental impact than CO_2. To calculate the environmental impact, all emissions according to their respective effectiveness are calculated as CO_2 and the greenhouse potential is depicted as CO_2 equivalents.

Table 6

USE AND EVALUATION OF THE CRITERION "GREENHOUSE GAS EMISSIONS"

Evaluation	RED	YELLOW	GREEN
Criterion: Greenhouse gas emissions	High emissions of greenhouse gases	Medium emissions of green-house gases	Low emissions of greenhouse gases
Indicator: aggregated green-house gas emissions as CO_2-equivalents / kg substance	> 10 kg (see annex 9)	1 – 10 kg (see annex 9)	< 1 kg (see annex 9)
	In any case a comparative case-by-case assessment considering the functional unit is necessary.		

Excursus:
Meanwhile, producers of some products (e.g. construction materials) develop environmental product declarations (ePd). These consist of a product-specific greenhouse gas balance, among others. Such environmental product declarations would enable users of chemicals to reliably compare greenhouse gas emissions. In 2009, the international chemicals association (ICCA) published eco balances of selected chemicals (ICCA 2009)[19].

The indicator for the criterion greenhouse potential is the amount of CO_2-equivalents emitted for the production of a substance. As first step, it should be assessed what amount (in kilogram) of a substance is necessary for a respective use. Only then can a comparative assessment be performed.

For a first estimation, we have grouped the substances into three categories: Substances with high, middle and low greenhouse gas emissions. On average, 2 kg CO_2-equivalents are released if 1 kg of an inorganic or organic substance is produced. For a first estimation the following advice can be given: releases of greenhouse gases will be less relevant for a substance if they amount half to this value[20].

A value of below 1 kg CO_2-equivalents/kg substance is given in the following table as an indication for low relevance. However, if very high amounts of a substance are used, even low greenhouse gas emissions per kilogram may result in a high total amount. Here, possibilities should be checked to reduce emissions of greenhouse gases – including the assessment of the benefits of a use (c.f. Chapter 2.2.6).

[19] *ICCA International Council of Chemical Association 2009: Innovations for Greenhouse Gas Reductions. A life cycle quantification of carbon abatement solutions enabled by the chemical industry. July 2009 https://www.americanchemistry.com/Policy/Energy/Climate-Study/Innovations-for-Greenhouse-Gas-Reductions.pdf*

[20] *1 kilogram of CO_2 equivalents is of the order of magnitude the amount of CO_2 that is generated when using 1 kilowatt-hour of energy (the exact value is 650 grams/kWh). The average annual energy consumption of a family house in Germany corresponds to 1800 kWh.*

The values provided in table 6 are first indicators for the evaluation, referring to information from the life cycle assessment data base PROBAS (see annex 3.1). For more comprehensive statements, a comparative case-by-case assessment is necessary, which does not relate to a fixed amount of the substance (1 kg), but to the amount necessary to fulfil the desired function.

First of all, you should estimate the substance-related greenhouse gas emissions of ten substances that have the highest consumption amounts in your enterprise. Compare the results with the other CO_2-emissions in your establishment – e.g. from the energy supply. Then, you can evaluate if it is profitable to engage in the assessment of the substance-related greenhouse gas emissions more deeply. One approach is that the substance related greenhouse gas emissions add up to more than 10 % of their total-CO_2-release.

If yes, it can be useful, to investigate selectively if there are any chemical substitutes which are known to release less greenhouse gases.

2.1.7 Resource consumption for the manufacture of raw materials and the substance

For the production of chemicals substances raw materials, water and energy are consumed[21]. They build the material base of our society and are called "resources"[22]. High resource consumption is not sustainable. Therefore substances should be specifically selected that have low resource consumption.

The evaluation of the resource consumption for the manufacture of a substance requires considering the upstream chains of a raw material or substance. This is in particular:

- Production of raw materials (e.g. extraction and transport of mineral oil, excavation and transport of minerals or metal ores, cultivation of renewable resources);
- Refining of raw materials (purification) as well as
- Chemical synthesis

The type of raw materials reflects another aspect of sustainability (fossil raw materials, renewable materials). Furthermore, the amount of waste produced per amount of manufactured substance (including waste from upstream chains) is an indicator of resource efficiency.

The identification of specific quantitative data on resource consumptions (including upstream chains) requires a comprehensive analysis of processing steps and uses of materials. This detailed analysis is normally too extensive to perform in addition to every day company work. Therefore, we present you a simplified approach in this guide. It allows you a first, qualitative evaluation providing a sufficient set of criteria and indicates where to intensify the sustainability evaluation.

The absolute values of the consumption of energy, raw materials and water are normally not very expressive. Only the comparison of two alternatives results in selective judgements regarding the resource efficiency of a substance.

The following Table 7 provides as a rough indication some benchmarks to distinguish "high", "medium" and "low" relevance of the criterion. The figures are based on information from the data base PROBAS. If a substance is used in high amounts, the criterion should be taken into account anyway.

As stated above, for of the criterion "resource consumption" further case-by-case evaluation is required.

Excursus:
Renewable resources can be non-sustainable if their cultivation is connected to high resource consumptions, e.g. in form of fertilizers and pesticides. Their cultivation could compete with other land uses, e.g. the production of food or require high water consumptions (e.g. cotton). Packaging made of corn starch is an example of a product that has been negatively assessed in lifecycle analyses (high energy and material consumption).

Chapter 4.1 of the background paper of the German environment agency on sustainable chemistry* describes more in detail sustainability aspects of renewable raw materials. In Germany two sustainability regulations exists referring to different kinds of bio fuels. They contain specific criteria for sustainability, e.g. protection of areas with high value for nature protection, protection of peat bog, sustainable agricultural use and greenhouse gas emission reduction potential (BGB 2009).

**http://www.umweltbundesamt.de/uba-info-medien/mysql_medien.php?anfrage=Kennummer&Suchwort=3734*

[21] The resource efficiency of the manufacture of a substance is to be correlated with the benefits of its use regarding the resource use along the supply chain, in order to obtain a full picture. However, this requires in-depth knowledge on the uses and application processes of a substance and is a very complex task, which cannot be elaborated in this guide.

[22] In a holistic perspective, additional production factors would be included, such as the use of machines and auxiliary materials or land consumption. In order to make the criterion manageable at company level, only the above mentioned factors are used.

Table 7

USE AND EVALUATION OF THE CRITERION "USE OF RESOURCES"

Evaluation	RED	YELLOW	GREEN
Sub-criterion 1: Availability of raw materials and manufacturing effects			
A) RENEWABLE RESOURCES	The raw material is renewable; however, its production and use have severe negative ecological and social impacts	Although the raw material is renewable, its use is partly ecologically and socially critical	The raw material is renewable and its production and use is related to only few negative ecological and social impacts.
Indicator: Sum of the points from the central questions	**1 point or less**	**2 or 3 points**	**4 points**
Central question	**1-minus-point per "yes"**		**1 point per "yes"**
Availability of raw materials and manufacturing effects	Is the raw material available only in low amounts? (e. g. Lithium) Is the production of the raw material resource intensive, e. g. due to mining or very complicated purification processes? (e. g. Beryllium) Does the production of raw materials cause negative social and/or ecological impacts in the countries of their origin? (e. g. gold, diamonds, shale glass)		Is the raw material available in sufficiently high amounts? (e. g. silicon, iron, mineral-oil) Is the production of the raw material resource not intensive? (e. g. iron, mineral-oil) Does the production of raw materials cause not many negative social and/or ecological impacts in the countries of their origin? (e. g. sodium chloride, clay, mineral-oil)
B) FOSSIL RAW MATERIALS, NON-RENEWABLE	The raw material is fossil and its production and use have severe negative ecological and social impacts	The raw material is fossil and the ecological and social impacts of its production and use are only partly critical	The raw material is fossil; however, it is available in sufficient amounts and its production and use is related to only few negative ecological and social impacts
Indicator: Sum of the points from the central question	**0 points or less**	**1 or 2 points**	**3 points**
Central questions	**1-minus-point per "yes"**		**1 point per "yes"**
Availability of raw materials and manufacturing effects	Is the raw material available only in low amounts? (e. g. Lithium) Is the production of the raw material resource intensive, e. g. due to mining or very complicated purification processes? (e. g. Beryllium) Does the production of raw materials cause negative social and/or ecological impacts in the countries of their origin? (e. g. gold, diamonds, shale glass)		Is the raw material available in sufficiently high amounts? (e. g. silicon, iron, mineral-oil) Is the production of the raw material resource not intensive? (e. g. iron, mineral-oil) Does the production of raw materials cause not many negative social and/or ecological impacts in the countries of their origin? (e. g. sodium chloride, clay, mineral-oil)
Sub-criterion: Energy consumption	High energy consumption	Medium energy consumption	Low energy consumption
Indicator: Data on energy consumption	More than 100 MJ/kg (see annex 10)	Between 10 and 100 MJ/kg (see annex 10)	Less than 10 MJ/kg (see annex 10)
	A case-by-case assessment is necessary. First reference point: the criterion is probably less meaningful if the energy consumption is below 10 MJ/kg and probably more meaningful if the value is above 100 MJ/kg		
Sub-criterion: Water consumption	High water consumption	Medium water consumption	Low water consumption
Indicator: Data on water consumption	More than 100 l/kg (see annex 11)	Between 5 und 100 l/kg (see annex 11)	Less than 5 l/kg (see annex 11)
	A case-by-case assessment, taking the functional unit into account, is necessary note: the criterion might be less relevant if water consumption is below 5 l/kg substance. it might be highly relevant if water consumption is above 100 l/kg substance.		
Total evaluation			

Substances for which low resource consumption has been identified can be used inefficiently and therefore also non-sustainably. According to the Rio-declaration[23], renewable resources should be consumed only to the extent they regenerate. A translation of this principle into company practice means to check if the global consumption of a specific raw material exceeds the regenerated amount. Indicators for excessive use can be declines of respective "populations" or stocks, increased prices due to scarcity or literature reviewing the use and cultivation of renewable resources. Provisions, rise in prices due to raw material scarcity, information on renewable resources in the references.

The use and evaluation of the criterion "Use of resources" is shown in table 7. For each of the three blocks there are a number of questions. The answers to these questions results in plus or minus points.

The waste phase and the possibility to recycle materials from waste streams are of high importance for the sustainability of a substance. See chapter 2.2.4 for details.

Evaluation – Indications for a more detailed assessment:

The above listed criteria can also be used to compare substances in detail, (type of raw material, consumption of energy and water, amount of waste). Respective data have been compiled in the context of lifecycle analyses (LCA) and other methods for the assessment of materials and processes. However, they are of course not available for all substances.

In Annex 3, data bases are listed which may be helpful for a detailed evaluation. If two substances are compared it is important that the same methods and data bases are used for both substances.

The differences within the above categories can be identified more clearly in a detailed evaluation. Since such evaluations can be very time consuming, they should only be started if it has been determined that the resource consumption is decisive for the evaluation of the sustainability of a substance.

We recommend, firstly, evaluating the sub-criteria "water consumption" and "energy consumption" of the ten substances that have the highest consumption amounts in your enterprise. Compare the results with the other water and energy consumptions in your establishment and the potential savings, here. This facilitates the estimation of substance related water and energy consumptions.

[23] The Rio Declaration has been stated during the conference of the United Nations for Environment and Development, taking place in Rio de Janeiro from June, 3.–14. 1992 (see http://www.quetzal-leipzig.de/printausgaben/ausgabe-02-umwelt-und-entwicklung-in-lateinamerika/erklarung-der-unced-19093.html).

Excursus:
As already mentioned in the previous chapter, for some products of different sectors, environmental product declarations (ePd) are available. The product related analysis includes an inventory of environmental indicators, among other the consumption of energy and the generation of wastes. Such environmental product declarations could enable users of substances and mixtures to make a comparative assessment based on sound data on resource consumption for the manufacture of substances.

2.1.8 Responsibility in the supply chain

This criterion can be used to assess whether the supplier of a substance takes the environmental and social responsibility that is needed. If the quality of raw materials is the same, normally the price is decisive for the choice of suppliers. If raw materials are selected according to their sustainability, the conditions of environmental protection and workplace health and safety are important for their manufacture and in the purchasing decision. The standards on environmental and workers protection (safety and health at the workplace, fair pay etc.) can be very different across the world. However, big differences may also exist between enterprises located in the same region.

Damage of the environment at the location of raw materials production equally needs consideration in this criterion as conditions at workplaces and social standards. The exchange about the addressed questions can help explain different prizes of the same substances. The conscious buying decision for raw materials that are more sustainable, supports establishments or regions that do justice to produce sustainable.

Taking responsibility for the environment and social conditions should be checked, first for suppliers from which high amounts of raw materials are obtained. Additionally and preferably, suppliers, for which little information is available, should also be approached.

Suppliers should feel responsible for environmental protection and agreeable social conditions not only within, but also in the nearer context of their companies. In order to check this, you need information on the suppliers themselves.

Information sources could be statements on corporate policies or sustainability and environmental reports in the context of certified management systems (workers protection: BA 18000; quality: ISO 9000; environment: ISO 14000 or EMAS). Furthermore, the willingness of the inquired suppliers to provide information, the overall service and the quality of chemicals supplied can be used as criteria. The existence of “Codes of Conduct”, requiring compliance with social standards and the engagement in social projects (social sponsoring, specific projects for the environment or on sustainability, research) may also be evaluated positively. Information reviewed by independent auditors should be weighted higher than that which is “purely voluntary”.

The use and evaluation of the criterion “Responsibility in the supply chain” is shown in table 8. The answers to the key questions result in plus or minus points which are summed up. The higher the commitment to comply with protection standards at workplaces and for the environment is, the higher is the overall score and the more responsible and hence sustainable is a supplier.

These criteria should help you to make a first assessment of your supplier. It will show you with whom the exchange about assumption of responsibility is most important.

Table 8

USE AND EVALUATION OF THE CRITERION "RESPONSIBILITY IN THE SUPPLY CHAIN"

Evaluation	RED	YELLOW	GREEN
Sub-criterion 1: Responsibility for workplaces at the supplier	The supplier doesn't care about workers protection.	Supplier complies with legal requirements on workers protection	Supplier values workers protection very high
Indicator: Sum of the points to the central questions	**Less than 0 points**	**0 points**	**1 point**
Central questions	**1 minus point per "yes"**	**0 points per "yes"**	**1 point per "yes"**
Management system, risk management at work	Problems are known in occupational health and safety (e. g. accidents, high rate of sick-leaves) The supplier does not respond to inquiries on occupational health and safety	The supplier confirms to run a systematic management system for health and safety at the workplace	The supplier runs a documented management system for health and safety at the workplace (with external auditing)
Sub-criterion 2: Responsibility for the environment	Supplier doesn't care about environmental protection	There are indications that environmental legislation is complied with.	Environmental protection is very important to the supplier
Indicator: Sum of the points to the central questions	**Less than 0 points**	**0 points**	**1 point or more**
Central questions	**1 minus point per "yes"**	**0 points per "yes"**	**1 point per "yes"**
Supplier's responsibility for environmental protection	Problems are known regarding environmental protection (e. g. accidents) The supplier does not respond to inquiries on environmental protection	The supplier confirms to run a non-certified environmental management system	The supplier has a certified environmental management system The supplier publishes environmental or sustainability reports
Sub-criterion 3: Social responsibility of the supplier	No involvement in social activities in and outside company	There are indications that social standards are important to the supplier.	Improvement of social conditions is important to the supplier
Sub-criterion: Water consumption	High water consumption	Medium water consumption	Low water consumption
Indicator: Sum of the points to the central questions	**Less than 0 points**	**1 points**	**2 points or more**
Central questions	**1 minus point per "yes"**	**1 point per "yes"**	
Indicator: Social activities and goals	The supplier does not respond to inquiries regarding social activities of the company	Supplier has "code of conduct", is social sponsor and provides training in the company. The supplier participates in social projects outside the company	
Total evaluation			

Note: *If information is missing to judge on this criterion, the color white should be assigned. This indicates that information should be gathered.*

Table 9

SUSTAINABILITY PROFILE OF A SUBSTANCE

Substance-specific criteria	RED	WHITE	YELLOW	GREEN
Mentioning on problematic substance lists				
Physicochemical properties				
Human toxicity				
Dangerousness for the environment				
Mobility				
Greenhouse potential				
Resource consumption				
Responsibility in the supply chain				

2.1.9 Summary of evaluation

The application of these eight criteria gives you a first analysis of the sustainability of a substance. We recommend placing the findings for the single criteria in a table, as shown below.

This sustainability profile shows you where there is need for information or action regarding the substance assessed. It can also indicate whether substitution of the substance by a less problematic should be taken into account.

An aggregated evaluation of a substance across all criteria with only one characteristic (e. g. a single number) is not the goal of this guide. However, a summary of the results after the application of the single criteria is possible. Admittedly, this approach endangers the single results of each criterion of not being valued or used sufficiently enough.

Therefore a final evaluation (e. g. “red”, “yellow”, “green”) of a substance is not aspired (see Chapter 1.6. “What does the result look like?”). Furthermore, the intention of this guide is to enable you to make selective improvements in different fields with the results of the evaluation.

The sustainability profile also facilitates the comparison between two or more substances. With the example of two dyes – phenolphthalein and thymolphthalein – table 10 shows how such a comparison could look like.

Table 10

COMPARISON OF SUSTAINABILITY PROFILES OF PHENOLPHTHALEIN AND THYMOLPHTHALEIN

Substance-specific criteria	Phenolphthalein	Thymolphthalein
Mentioning on substance lists	RED	GREEN
Physicochemical properties	GREEN	GREEN
Human toxicity	RED	GREEN
Dangerousness for the environment	GREEN	GREEN
Mobility	YELLOW	YELLOW
Greenhouse potential	YELLOW	YELLOW
Resource consumption	YELLOW	YELLOW
Responsibility in the supply chain	WHITE	WHITE

Phenophthalein is listed as a substance of very high concern on the candidate list. It has a high toxicity for humans. Evaluating the greenhouse potential and the mobility, there is no difference between the two substances. There is no information on the consumption of resources and the responsibility in the supply chain yet.

2.2 Use-specific criteria for the evaluation of sustainability

The use-specific criteria for the evaluation of the sustainability of a substance or mixture should be used to better value or weight the results of the evaluation of substance-specific criteria. The use-specific criteria are described in a more qualitative way, compared to the substance-specific criteria. Due to the high variety of uses of substances and mixtures, no structure can be defined that includes the majority of cases and no generally applicable and unambiguous indicators can be defined. This chapter therefore supports the reflection of the results of the first evaluation steps.

We recommend considering the results of the application of the substance-specific criteria in the following way:

- A need for action due to “substances on lists” (criterion 1)“ dangerous physicochemical properties” (criterion 2) and “responsibility in the supply chain” (criterion 8) is independent from the use-specific criteria.
- For substances with dangerous properties regarding man and the environment (criteria 3 and 4) the use-specific criteria should be checked in any case.
- For the substance-specific criteria “Greenhouse gases” and “resource consumption” (criteria 6 and 7) especially the use-specific criteria “Emission potential” and “Use amount” are important.
- The use-specific criteria 5 to 7 (“substitution potential”, “benefits potential” and “innovation potential”) can modify (enhance / decrease) the weight of the substance-specific criteria “Substance on list” (criterion 1) , “Dangerous physicochemical properties” (criterion 2), “Human Toxicity” (criterion 3), “Problematic properties regarding the environment” (criterion 4), “Mobility” (criterion 5), “resource consumption” (criterion 7) and “Greenhouse potential” (criterion 6).

For substance manufacturers, formulators and users of substances and mixtures, which have come to the conclusion to substitute a chemical because of its sustainability profile, this chapter can still be helpful in focusing the search for alternatives.

To evaluate the sustainability of chemicals, in this second step, seven criteria are proposed that relate to the use:

1. The emission potential
2. The user groups
3. The used amount
4. The waste stage
5. The substitution alternatives
6. The benefits of a chemical / its use
7. The innovation potential of a chemical / its use

In the following chapters these seven criteria are described. Main points are the meaning of the criteria, the applicability, the information basis, the relevance related to the substance-specific criteria and the evaluation.

2.2.1 Emission potential of the use of a substance or mixture[24]

In this guide, the "emission potential of a use" is understood as an estimation of the amounts of a substance (as such or contained in mixtures or articles) which are released along its lifecycle. The releases could occur from industrial installations to the environment, to the workplaces or from products into the living environment. These releases normally result in a contact with man or the environment (exposure) and potentially may cause damage.

Substances are not sustainable if they exhibit problematic substance properties and if they are released during their use, which may finally cause adverse effects in man and the environment. If substances are of very high concern, low releases can already be critical.

Furthermore, a high emission potential is equal to high losses of the substance indicating an inefficient use of resources. Therefore this criterion is relevant in relation to the resource consumption as well.

The criterion "emission potential of use" is related to the criteria "user groups" (Chapter 2.2.2) and "mobility" (Chapter 2.1.5) because the emission potential depends among others on how mobile a substance is and whether or not it is used in a correct manner.

The explanation and support of a comprehensive assessment of emissions along the lifecycle of a substance is not possible in this guide. Publications on this topic can be found on the web in much detail, for example:

- The VCI REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains introduces to the topics exposure assessment and communication in the supply chain with several recommendations on the implementation in practice[25].

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[24] *Further explanation to this criterion is provided in Annex 6.*

[25] *The "REACH guidance on exposure assessment and communication in the supply chain" including examples can be received from Dirk Bunke. Just write a short request to d.bunke@oeko.de.*

- The guidance document of the European Chemicals Agency (ECHA) on information requirements and chemical safety assessment describes a method for assessing exposures and characterizing risks from the use of chemicals[26].

Substance manufacturers, which have to assess the safety of a substance in a REACH registration, should use that information in the evaluation of sustainability. Important information for the evaluation of sustainability is e. g. if a high degree of risk management is necessary to ensure safe handling and use of a chemical or if certain uses are not safe.

Emissions at the **workplace**[27] could result from evaporation, dusting or skin contact of the chemical and the worker. The degree of release depends on the type of processing and the conditions of use. Emissions into the living environment of consumers may result from the use of chemical mixtures (e. g. air fresheners, paints) through the formation of aerosols, evaporation or dusting or e. g. through the use in water (dish washing agent). Furthermore, articles may release substances (e. g. plasticizers in PVC-flooring).

The **environmental** emission potential equals to the sum of all emissions of the substance from mixtures and articles, which are released to the environment via the air, water or soil.

Relevance related to the substance-specific criteria: A high emission equals a high loss of substance. This is an ineffective use of resources. Therefore the criterion “Emission potential” is relevant for the criterion “Resource consumption” (chapter 2.1.7). The criterion “Emission potential” has to be seen together with the criterion “User groups” (chapter 2.2.2) and the criterion “Mobility” (chapter 2.1.5), because the emission of a substance depends on its mobility and the way of handling the substance.

Applicability of the criterion: The criterion can be applied to any type of substance (as such or as component of a mixture or article). The criterion is not very expressive for substances which are only used as intermediates, as their lifecycle is very short and normally strictly controlled. The lifecycle of substances used as processing aids normally ends with their actual use inside a mixture (they are not included in any articles), but includes the waste phase of product residues.

Information basis: Information on the use of a substance as such or in mixtures and articles are either available (purpose of product) or have to be requested from the users (communication with customers).

Evaluation: In table 11, 12 and 13, examples of uses with very high and very low emission potentials are given. In the first table this is related to the substance-specific criteria “dangerous for the environment” and “resource consumption”. In the second table it is related to the “dangerousness for the worker” and in the third table to the “dangerousness for the consumer”, the latter two being a more differentiated view on the “human toxicity”.

The high emission potentials can enhance the importance of the evaluation of the substance-specific criteria (dangerous for man and the environment, resource consumption, i. e. yellow ⇢ red) and low emission potentials can attenuate them (red ⇢ yellow)

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[26] *The guidance is available at the European Chemicals Agency: http://guidance.echa.europa.eu/guidance_en.htm*

[27] *Guidance for a detailed assessment of emissions and exposures of dangerous substances at workplaces can be found in the “Easy-to-use workplace control scheme for hazardous substances” (Einfaches Maßnahmenkonzept) of the Federal Agency on Occupational Health and Safety, including help for practical risk management measures.*

Table 11

INDICATORS FOR THE EVALUATION OF THE EMISSION POTENTIAL OF USES RELATED TO THE ENVIRONMENT*

Influencing factors	Critical uses, high emission potential	Less critical uses, low emission potential
Use of the substance as such or in mixtures	Open use in the environment, in private households in crafts, use in small industry	Chemical synthesis Use in large installations, automated processes
Relevance of use regarding water emissions	Use in aqueous systems or in direct contact with environmental media	Substance or mixture does not come into contact with water
"Containment" of installation	Open or semi-open installation, wastewater and exhaust gas are generated	Substance or mixture is used in closed systems or installations**
Other conditions of use of substance or mixture	Processing at high temperatures and high pressures, mechanical stress (abrasion, formation of dusts)	Processing at room temperature or less, no extreme conditions
Disposal of production wastes or wastes from consumer mixtures	No specific disposal, consumers products disposed with wastewater or household waste	Disposal by destruction or systematic collection and recovery/recycling
State-of-the-art of end-of-pipe technologies	Capture of emissions according to state-of-the-art not ensured All chemicals for consumers	Exhaust gas and wastewater are cleaned and disposed of according to legal requirements
Substance as part of articles	Flat products, coatings, outdoor use, abrasion	Compacted products, indoor use, no abrasion
Disposal of articles containing the substance	Wide dispersive use, no special collection or disposal system, normally part of household waste	Small group of users, specific waste regimes exist (e. g. electric devices, cars etc.)
Influence of mobility (water and air to be viewed upon separately)	Mobile substances or substances which don't react with article matrices	Substances with low mobility, substances which are firmly embedded in article matrices

**Source: Federal Environment Agency: Guidance for the use of environmentally sound substances – part 2, Berlin 2003; http://www.umweltbundesamt.de/wasser-e/themen/stoffhaushalt/umweltvertraegliche-stoffe/inventare.htm. The table has been slightly modified.*

***As preliminary guiding value an annual loss of materials of less than 0.001 to 1 % compared to the input amount to the system can be used. The target values have to be defined specifically for sectors, substances and processes.*

Table 12

INDICATORS FOR THE EVALUATION OF THE EMISSION POTENTIAL OF USES RELATED TO THE WORKPLACE

Influencing factors	**Critical uses, high emission potential**	**Less critical uses, low emission potential**
Use of the substance as such or in mixtures	Use in installations with low technical standards, professional use in crafts	Installations for chemical synthesis, installations with high technical standards (automated processes)
Type of use – dosage of substances and mixtures	Manual dosage of powders and liquids, direct feeding of dusty or volatile chemicals	Simple dosage (closed pipes, ready-to-use packaging), immobilization, e. g. by compounding
Type of use – processing	High energy or fast processes, low degree of automation. Open, manual use (e. g. spraying, cutting, immersion)	Automated processes, low energy or slow processing. organizational or technical separation of worker and chemical
Disposal and cleaning	No separation of wastes Disposal is not regulated, cleaning and maintenance is conducted untrained personnel	Separate disposal through specified waste management company, cleaning and maintenance by expert companies (incl. abatement equipment)
State-of-the-art of workers protection	No management system for workers health, few emission reduction measures Use by professional users, use at "mobile" work-places	Existing management system for workers health, regular risk assessment at workplaces and emission reduction measures implemented.
Influence of mobility (volatility more important than solubility, LogKow for dermal contact)	Mobile substances	Low mobility of substances

Table 13

INDICATORS FOR THE EVALUATION OF THE EMISSION POTENTIAL OF USES RELATED TO CONSUMERS

Influencing factors	Critical uses, high emission potential	Less critical uses, low emission potential
Type of use of substance or mixture	Manual dosage of powders and liquids	Ready-to-use packaging, tabs, high viscous mixtures
Type of use application	Spray applications "open uses", e. g. wiping, direct contact with skin and lungs	Use inside machines (e. g. washing), use in specific equipment (e. g. silicone cartridge guns), direct contact is low
Waste disposal	Complicated disposal (e. g. paints), cleaning of equipment necessary	Disposal without refilling or cleaning No waste is generated
Substance as part of articles	Substance is not firmly embedded in article matrix, ca e. g. leach or evaporate during use	Substance is integrated in article matrix or inside closed sub-parts
Influence of mobility (water and air to be viewed upon separately)	Mobile substances or substances which are not firmly embedded in an article matrix	Substances with low mobility or which are firmly integrated in article matrices

Recommendation: Enterprises should create an overview which processes are characterized by specifically high substances' releases. For these processes emission reduction potentials at workplaces or to the environment as well as improvements of product qualities (healthier products for consumers) and cost savings are very likely to be high. Hints on how to compile such an overview can be found in the REACH Practical Guide on Exposure Assessment and Communication in the Supply Chains[28].

2.2.2 User groups of a substance

Substances are used as such, in mixtures and as part of articles by different groups of persons and in different environments. For the evaluation it is important whether particularly vulnerable user groups handle the substance, such as children or handicapped people. In principle these groups, which require a higher degree of protection, should not be exposed to chemicals, which may cause harm to human health. In this case, not only the use of the substance in whatever form is relevant, but also if it is released[29] (c. f. Chapter 2.1.5 "mobility" and Chapter 2.2.1 "emission potential").

Relevance related to substance-specific criteria: In relation to the user groups, only the criterion "human toxicity" is considered, although other criteria could also be relevant. If vulnerable user groups are identified, the evaluation results of the criterion human toxicity should be modified (yellow à red and even higher urgency for white).

Information basis: The uses of a substance need to be known as well as the user groups (consumers, vulnerable groups, workers) of the end product.

[28] The REACH-guide can be received from Dirk Bunke. Just write a short request to d.bunke@oeko.de.

[29] Here, the criteria "mobility" and "emission potential" are not considered. However, it is recommended to view the use amount in conjunction with these criteria, because for example even sensitive or vulnerable groups users may not be at risk, if the substance has a low mobility and is used in closed systems.

Table 14

USE AND EVALUATION OF THE CRITERION "USER GROUPS"

Substance-specific criteria	Enforcement	Attenuation
Substance is on lists of problematic substances	**Use should be avoided for any user group**	
Substance is dangerous to human health	Substance is used in products for children or for vulnerable groups. Substance is used indoors.	Substance as such and in mixtures is only foreseen for use by professional users. Substance is used only in consumer articles, which don't give rise to releases to indoor environments.
Substance is volatile and dissolves well in water	Substance is only used in products for professional users.	Substance is used in consumer products and for indoor use. Substance is used in articles from which they are intentionally released (e. g. pens, fragrance candles).

Evaluation: Vulnerable groups, such as children and pregnant women, should not come into contact with chemicals which are toxic to human health at all. Workers are often exposed to high amounts of substances and at higher frequencies. Consumers could be exposed to emissions of substances form products inside their homes.

In table 14, for each criterion it is assumed that a "yellow" evaluation has been concluded for the mobility of the substance in the first steps. Using the examples, it can be derived if the substance-specific characteristics are enforced or attenuated by the types of user groups.

2.2.3 The use amount

There are no harmonized definitions of which amounts are a "high" or "low" amount. Under REACH, registration requirements distinguish between amounts of 1 to 10, 10 to 100, 100 to 1000 and above 1000 t/a. The amounts should be considered in relation to the dangerous properties: for a substance of very high concern (SVHC) an amount of 1 t/a may already be very high.

For articles containing SVHC the concentration limit of 0.1% (weight/weight) set in REACH Art. 7.2 is a reasonable order of magnitude. In Europe, a concentration above this limit triggers the legal requirement to make a notification to ECHA as described in REACH Art. 7.2.

In order to avoid non-sustainable impacts on man and the environment, in case of complex articles this concentration limit should refer to the homogeneous materials within the article. Especially the substance-specific criteria "Human toxicity" (chapter 2.1.3),

Table 15

USE AND EVALUATION OF THE CRITERION "USE AMOUNTS"

Substance-specific criterion	Significance of amount as indicator
Substance is mentioned on lists of problematic substances	Independent of other criteria. The use should be phased out or at least use amounts should be minimized.
Dangerous pc-properties	Dangerous pc properties are mostly independent of used amounts.
Substance is dangerous to human health	Workers › kg/day = high; mg/day = low. For cmr substances the exposure levels can be critical depending on the type of use even if only a few grams per are day applied. Substances in consumer products should be contained in concentrations below the classification limits (low amount). If substances are incorporated in articles critical amounts are difficult to evaluate and the criteria "emission potential" and "mobility" should be applied instead.
Substance is dangerous to the environment	Critical amounts depend on the degradability of the substance. For non or only slowly degradable substances, low volumes can already be critical. For easily degradable substances, this criterion should not be applied.
Pbt/vpvb-substances	Any type of use should be avoided independent of the amount.
Mobility	Any type of use should be avoided independent of the amount. The linking of use mobility and use amounts is not meaningful.
Resource consumption	The higher the production or use amounts, the higher the resource Consumption. Indication for "high" = more than 1,000 t/a
Global warming potential	The higher the production or use amounts, the higher the emission of greenhouse gases. Indication for "high" = more than 1,000 t/a
Origin of raw materials	The higher the use amount and the more expensive the substance, the higher the financial support for questionable production methods or social conditions. Indication for high: more than 1 ton per year.

"Problematic properties related to the environment" (chapter 2.1.4), "Mobility" (chapter 2.1.5), "Emission of greenhouse gases" (chapter 2.1.6and 2.1.7) and "Resource consumption" have to be seen in connection with the amount used.

Relevance related to substance-specific criteria: High use amounts can enhance the importance of some substance-specific criteria. The higher the resource consumption or the emission of greenhouse gases for the production of a substance, the higher the weight of these criteria in the overall evaluation is. In particular if large amounts of the substance are produced or used. Vice versa, if a substance is used in small amounts, the importance of the criteria "resource consumption" and "greenhouse gas emissions" should be decreased.

Applicability of the criterion: The criterion can be applied to any substance or mixture. Manufacturers should relate to the substance amount they produce. Formulators could either assess amounts of a substance used in a mixture or the amount of the mixture as such. Users of mixtures can identify the use amount of a component by multiplying the concentration in the mixture with the total amount of the mixture used[30].

Information basis: The own manufactured or used amount (company information) or market volumes of the substance in the EU can be used.

Evaluation: The use amount as isolated indicator is fairly meaningless. Therefore, in table 15 the substance-specific criteria are used as basis for the assessment of use amounts. The high amounts enhance a negative evaluation of the substance-specific criteria and low amounts attenuate them.

Recommendation: Enterprises should in a first assessment use their substance inventory in order to get an overview of which of the critical substances are used in particularly high amounts.

2.2.4 Waste stage

Some substances may cause risks for man or the environment when they become waste. Generally, the recovery of substances from wastes should be aspired to save resources and energy. However, recycling could be problematic if substances contaminate a material stream and reach new products.

Sustainable substances should either fully degrade or mineralize during disposal (no waste in the long run) or be designed in a way that they can be fully recycled without loss in quality[31]. Although some indicators of potential problems during the waste phase exist, it should be assessed case-by-case whether or not they are relevant and if they change the overall evaluation a substance's sustainability.

The final product, in which the substance is used, is of high significance in this assessment, as it normally determines the disposal pathways.

Relevance related to substance-specific criteria: If a substance or a product containing a substance becomes waste (because the substance is not completely degradable or is not recycled), the substance-specific criteria get more importance.

The evaluation of the waste phase can enhance the results of the criteria "Human toxicity" (chapter 2.1.3) and "Problematic properties related to the environment" (chapter 2.1.4), "mobility" (chapter 2.1.5) and "Resource consumption" (chapter 2.1.7), if indications of problems during the waste phase exist.

Applicability of the criterion: For substances which don't occur in wastes, e. g. because they are almost fully emitted during their lifecycle (e. g. solvents) or because they react with other substances (intermediates, reactive additives) the criterion is not applicable.

Information basis: In order to assess the waste phase, the substance manufacturer or user has to identify the likely disposal pathways of the products (mixtures or articles in industrial, professional and consumer uses) the substance is used in and assess potential problems in relation to the substance properties.

Evaluation: The following list presents combinations of waste technologies and substance properties, which may cause risks to man and the environment. In the evaluation of sustainability related to the waste stage of a substance they have to be seen as less sustainable[32]:

- Metal containing compounds can be destroyed in waste incineration installations and distributed widely in the environment (if no abatement techniques are applied).
- PBTs/vPvBs can be released to the environment in different disposal processes, e. g. evaporation or leaching in landfills.

[30] The concentration in a mixture is only specified in the safety data sheet if the substance is classified as dangerous. It may be useful to contact the supplier for more information.

[31] Due to this, substances have to be stable and easily separable.

[32] The ECHA guidance document on information requirements and chemical safety assessment (IR/CSA – R18) contains a part on assessing risks of substances in their waste stage, including guidance on quantitative assessments. This part of the guidance is currently under revision.

- Through thermal and biological processes in landfills, dangerous degradation products could be formed and reach the environment.
- Problematic substances could contaminate material streams in recycling processes and be contained in products manufactured from recovered materials.
- If substances are not recovered as such or as part of materials (e. g. plastics, metals), they are "lost" (inefficient use of resources).
- Halogenated compounds can lead to the formation of dioxins and furans in thermal processes. These reactions can be enhanced by some metals, e. g. copper, which function as catalysts.
- Substances with high water solubilities could reach surface waters in different processes of waste collection, separation and treatment.
  - Workers in waste treatment installations can be exposed to dangerous substances in products and chemical wastes (without knowing thereof), if articles are dismantled (opening of closed containers, e. g. batteries, dangerous operating fluids in cars) or shredded (dust formation). These situations don't normally occur during the use of a substance as such and in products.
  - Nanoscale substances can disaggregate/deagglomerate and be separated from the product. The behavior and dangerous properties of nanomaterials in waste treatment installations, including physicochemical risks are largely unknown. In particular for nanomaterials the precautionary principle should be applied: risks, which cannot be assessed, should be prevented in the first case.
  - It can be assumed that wastes from industrial installations are properly disposed of. This is not the case for wastes from professional users or consumers. For example, electric and electronic equipment is still disposed of as household waste instead of being separately collected and treated. Therefore a lower content of hazardous substances is more important for products for professional and private uses.

The above examples show that additional adverse impacts may occur during the waste stage. Therefore, the waste stage is of high relevance in the assessment of sustainability. If one or more of the above listed items applies to the substance, this is to be evaluated as not sustainable.

2.2.5 Substitution potential

The substitution potential of a substance is a criterion applying rather to the alternatives of a use of a substance, than the substance itself. The substitution potential affects all of the substance-specific criteria.

The substitution potential describes the degree of availability of alternatives to the use of a problematic substance or mixture. If the use could be replaced by other substances / mixtures or by other measures, e. g. improved product design or change of processing techniques, and if this is economically and technically feasible, the substitution potential enforces all negative evaluations of sustainability criteria, because of the potential to avoid the use of the substance or mixture.

If no alternatives are available, the further use of the substance or mixture (and if possible, the implementation of measures to reduce the non-sustainable aspects of the use of the substance) is inevitable and a negative evaluation of sustainability may be acceptable. However, the availability of alternatives should be checked regularly to take into account the technical progress and new information and substitution experience.

Because substitution is a complex process, no details can be provided in the frame of this guide and no concrete substitution scenarios presented. Practical support can be obtained from corresponding publications, for example the "technical rules for dangerous substances 600" (TRGS 600) 43[33] by the Federal

[33] *www.baua.bund.de/nn_78960/de/Themen-von-A-Z/Gefahrstoffe/TRGS/pdf/TRGS-600.pdf*

Agency on Occupational Health and Safety. A good overview is given in the publication of Lißner and Lohse 2006. In Annex 7, some basic considerations on substitution are discussed which can be used for a first assessment.

You can find good examples for substitution and a lot of useful help regarding this topic on the webpage of the project "Subsport". "Subsport" is the short term for substitution portal[34]. The case examples are particularly demonstrative.

In this chapter we introduce only the guiding principles for consideration in substitution decisions:

- Substitution should maintain or even improve the quality of a product.
- Substitution should not lead to an increase or shift of risks for man and the environment. Overall the risks should be reduced (for all subjects of protection).
- Substitution can only be successful, if the technical precondition exists not only in the own company, but also at the customers'. This requires for example considering if technical processes are fine-tuned to a specific substance or mixture, which would require a change of the technological process if the substance or mixture were replaced.
- Substitution is only a sustainable solution, if society and corporate costs for the use of alternatives remain under the costs of potential damage.

In substitution-tasks problematic substances are often exchanged with structural very similar substances. This so-called "1:1"-substitution is easy because in most cases, no changes need to be, made in the process (except the substitution of the substance). It often leads to the problem that after a while another substitute needs to be found: Often, the used similar substance carries the same problematic characteristics as the substance initially used. Medium or long term, substitution solutions using structurally different substances ("power system change") or totally different solutions are more secure. This can be, for instance, changes in the product design which make the use of flame retardants unnecessary.

Relevance related to substance-specific criteria: The substitution potential has relevance to all substance-specific criteria. As said above, if a substance cannot be substituted, the substance-specific criteria become less important. However in case of a substance which has to be considered as less sustainable according to these criteria, it has to be checked.

Applicability of the criterion: In principle it can be assessed for any substance or mixture whether its use can be avoided or not. From this perspective, the criterion can be applied to any substance or mixture and any of their uses. The possibilities to substitute decrease and are more complex, the more specific the functionality of a substance or mixture, or the more essential it is for the product or process it is used in.

Information basis: Different types of information are necessary to assess alternatives (substitution). These are among others:

- Company internal sources for the assessment of financial feasibility of substitution
- Demands and statements of customers regarding the quality of products and processes
- Public data bases on alternatives
- Information on substance properties, uses and potential exposures and risks
- Technical experience on substitution

Evaluation: Each enterprise has to decide for each case, whether or not the sustainability evaluation requires (or justifies) a substitution. The "simpler" and "cheaper" a substitution, the higher the substitution potential is and the more negative evaluations of sustainability are to be weighed. The evaluation cannot be standardized and no indicators can be given.

[34] *http://www.subsport.eu/?lang=de*

2.2.6 Benefit potential

The benefit potential of a substance or mixture influences, like the substitution potential, the evaluation of all substance-specific criteria. The benefit potential consists of the quality of the (end) products, the societal and environmental benefits from its use and the corporate benefits.

Substances can have very different functions in mixtures and in articles into which they are included. In order to determine the benefit potential, the relevance of the substance for the quality or functionality of the end product is to be identified. The functions of substances in end products can be allocated to different categories. One possible differentiation is introduced in the following and further explained in Annex 8.

Benefit potentials of substances are in most cases realized only in the end product they are used in. The benefits can be distinguished into:

- Quality of (end) products. The substance contributes significantly to the product quality (e. g. long life spans, safety, weight), e. g. surface coatings for protection against damage
- Function of (end) products. The end product has got a high societal benefit which is realized to a high extent through the use of the substance. E. g. fire extinguisher foams
- Environmental benefits of products comprise of e. g. the improvement of product quality or the use of the product to improve the environmental quality (environmental technologies, e. g. photovoltaic).
- Benefits for the company. High profit can be made with the product which uses the substance.

Relevance related to substance-specific criteria: The evaluation of the benefit potential through a specific functionality of a substance, mixture or end product can influence the overall result of the evaluation of all substance-specific criteria. If benefits are very high, negative sustainability profiles may be acceptable or relativized.

The approach of balancing costs and benefits is pursued among other in socio-economic analyses (SEA)[35]. A complete SEA is very complex and cumbersome but leads to valuable information to evaluate the sustainability of a substance. By using "common sense", societal costs and benefits can be identified at a much rougher level, which although being much less differentiated and not "proven" frequently results in the same conclusions as a detailed SEA.

Applicability of the criterion: The criterion is applicable to all substances.

Information basis: The functionalities of substances are based on their properties and are normally known and intended by substance manufacturers and users.

The functionalities of mixtures are achieved by combining single substance and their properties are normally well known as well. However, sometimes the interaction of substances is important in mixtures, which may hinder the clear identification of contributions of the substance which is evaluated.

If substances are used in articles, only very superfluous functions as well as those which have a very high benefit can be unambiguously attributed to single substances. In most cases this is not possible, in particular for bulk chemicals with different uses. Here, the article as such should be submitted to a benefit assessment and issues of product design become more important.

Evaluation: The evaluation of the benefits of the use of chemicals can, depending on the type of actor, be viewed upon differently. This is particularly true for products which are very profitable for companies but are critical with regard to their impacts on the

[35] The socio-economic analysis aims at a structured compilation of societal benefits and costs of a certain issue. In the past, such analyses have among others been performed in the frame of the "existing substances program" of the EU in order to identify those measures, which lead to the highest risk reduction in the use of a substance and which are connected with the lowest costs and highest societal benefits. In a SEA, different parameters are quantified and described as costs and savings. Under REACH, the socio-economic analysis will be applied by industry in the context of applying for an authorization of a use of a substance. A separate guidance document is intended to be developed.

environment or society. The criterion should be used to analyze benefits of a product, but doesn't suffice to support an in-depth discussion of different stakeholders on the benefits of a substance.

There can be cases in which you use problematic substances for a certain purpose – e. g. flame protection with halogenic flame retardants. Examine in these cases, if there are any substitutes that give you the same result but avoid the problematic qualities of the "standard solution". You can find details on this matter in chapter 2.2.5.

2.2.7 Innovation potential

In all economic areas, the sustainability of products should be aimed at. The criteria for sustainable chemicals can influence the direction of innovation in a positive way, if already applied in the early stages of product development. Herewith, the market position of the innovating company may also be improved.

The chances generated through the use of sustainable substances (avoiding problems of no sustainable products, improving overall product qualities etc.) related to product and process innovations and the penetration of innovative products on the markets used should be considered as a "plus" in the evaluation of sustainability of products. The possibility to transparently document and communicate aspects of sustainability is very important in this context.

Sustainable substances not having any problematic characteristics for humans and the environment won't be restricted. That means for you and your production processes: These substances will be available for you in the medium and in the long term (if they don't decrease due to other reasons). This secures your direction in product and process related decisions.

The sustainability of substances and products plays a role especially in ecologically-sensitive markets (ecologically produced products, like organic foods, clothing or furniture). In the future, demands for such products will be even higher for substances, which are contained in consumer products with high relevance for human health (e. g. clothing, cosmetics, products for infants, construction products for indoor use). The manufacture and use of sustainable substances is also important in filling respective company policies with life.

Relevance related to substance-specific criteria: The innovation potential has relevance to all substance specific criteria. It enhances the importance of positive results of the application of these criteria.

Applicability of the criterion: The connection between the uses of sustainable substance with innovation activities is rather a question of the design of the innovation processes and its timing, than a question of the evaluation of sustainability of substances. The criterion can be applied to any substance or mixture.

Information basis: The criterion can be applied using internal knowledge of markets, products and production processes.

Evaluation: Different actors in society can achieve very different results in assessing the innovation potential of the use of a specific substance. This is the case especially for products which might offer a high economic potential, however they have to be considered as problematic regarding their impacts on man and the environment.

In this situation the criterion proposed at least supports a transparent analysis of the innovation potential of a substance or a mixture.

Page 46 – 51

3.0

Golden rules

3.0 Golden rules

The following "nine golden rules" summarize the most important principles of sustainable chemicals. Of course, this is only possible by making some rather rough simplifications. Therefore, the following rules do not replace the detailed explanation of the previous chapters, but highlight the core issues for you to consider and facilitate orientating chemicals management towards sustainability.

RULE 1

If possible, only use substances (as such, in mixtures or in articles) which are not mentioned on lists of problematic substances! This way you avoid losing raw materials because of legitimate restrictions.

RULE 2

Using problematic substances assess the different uses and potential users of the substance as such. If the substance cannot be exchanged you have to take responsibility for the consequences of its use. Never only evaluate the substance in isolation but think through the entire lifecycle!

RULE 3

As much as possible use substances which are not dangerous to human health (in particular none, which are classified as carcinogenic, mutagenic or reprotoxic), which are easily degraded, don't bioaccumulate and don't widely disperse in the environment! With these substances you have to put less effort in risk management measures.

RULE 4

Don't use substances, which require a high degree of risk management according to the easy-to-use workplace control scheme for hazardous substances or the COSHH approach!

RULE 5

Prefer substances which are available in excess or made from renewable resources to substances which are scarce and produced from fossil raw materials! On the one hand, you will pay less for them. On the other, they will probably still be available for you in 20 years.

RULE 6

Avoid long-distance transports at any stage of the supply chain, in particular for substances which you use in high amounts! Transport always correlates with higher environmental stress.

RULE 7

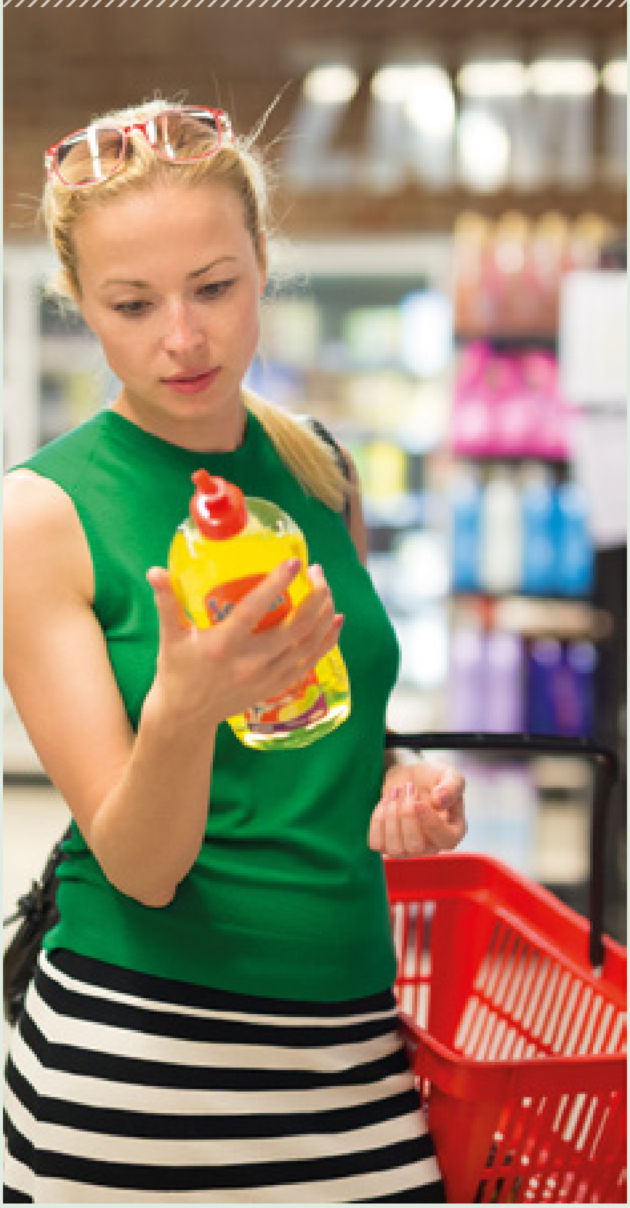
Pay attention to a low energy and water consumption of substances you use in large amounts as well as to a low generation of wastes in manufacturing and use! That way you conserve limited resources.

RULE 8

Assess whether your suppliers conform to high environmental and social standards. Select substances considering the transparency of the supply chain and the commitment of its actors to sustainability! That is how you support enterprises that do their responsibility in the supply chain justice.

RULE 9

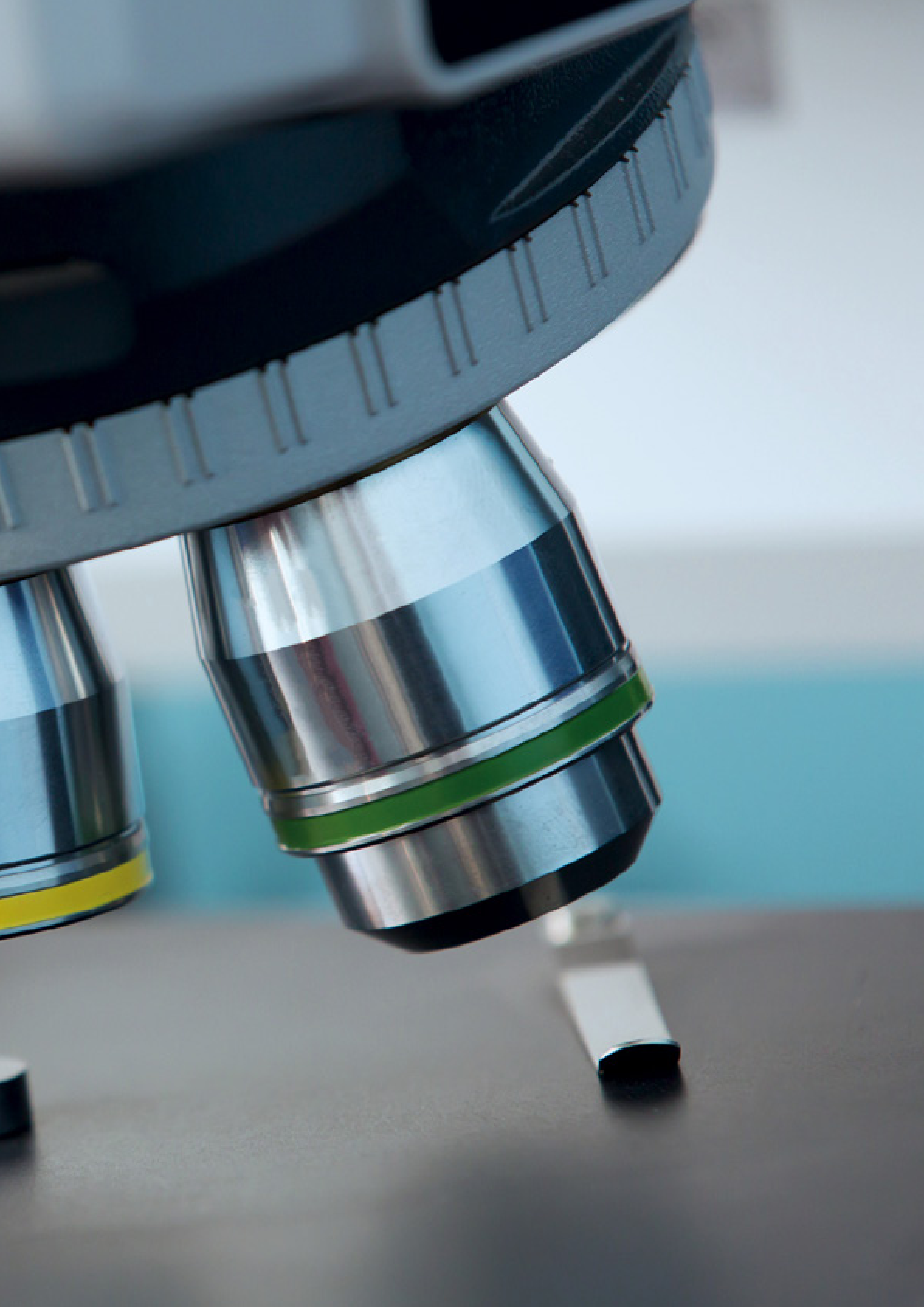
Furthermore products should not be put on the market for which a societal benefit and a benefit for consumers can not be identified.



Page 52 – 55

4.0

Outlook



4.0 Outlook

This guide should help you to consider aspects of sustainability in selecting their chemicals.

This guide should help you to consider aspects of sustainability in selecting their chemicals.

The criteria introduced in Chapter 2 enable analyzing which aspects of a substance require action or further information gathering or if an exchange of problematic substances by less problematic substances might be wise. If a problematic substance cannot be replaced, the substance-related criteria help you to create the use of this substance more sustainable.

With the Access-based file SubSelect, an electronic version of the guide is now available in addition to the guide. SubSelect assists enterprises in evaluating the sustainability of substances and mixtures by using the same substance-related criteria as those described in the guide. It facilitates the evaluation at many points, since the procurement data is deposited in the access-file, for instance the current version of the problematic substances lists. The following picture shows you the start page of SubSelect.

An essential aspect of attractiveness thanks to SubSelect is the opportunity to assess mixtures and not just individual substances, using the criteria you learned about in this guide. SubSelect saves substance data that has been entered once.

You can get SubSelect and this guide here in German and English:
https://www.umweltbundesamt.de

Your work with the guide for more sustainability can also be used for your public relations. It can also be used for internal trainings or for the exchange with your suppliers or customers.

If you have any questions regarding our instruments, about the sustainability of chemicals or about the ways of support in evaluation feel free to contact us:

- Christopher Blum, Umweltbundesamt
  christopher.blum@uba.de

- Antonia Reihlen (SubSelect), Ökopol
  reihlen@oekopol.de

- Dirk Bunke (Leitfaden), Öko-Institut
  d.bunke@oeko.de

Get started now! It is worth attaching importance to sustainable chemicals. For you, your customers, your employees and the environment.

SubSelect – A tool for the evaluation and comparison of substances and mixtures

https://www.umweltbundesamt.de/dokument/subselect-instrument-zur-auswahl-nachhaltiger

With the Access-based file SubSelect, an electronic version of the guide is now available in addition to the guide.
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GET STARTED NOW!
It is worth attaching importance to sustainable chemicals. For you, your customers, your employees and the environment.

Page 56 – 57

LI

Literature

Literature

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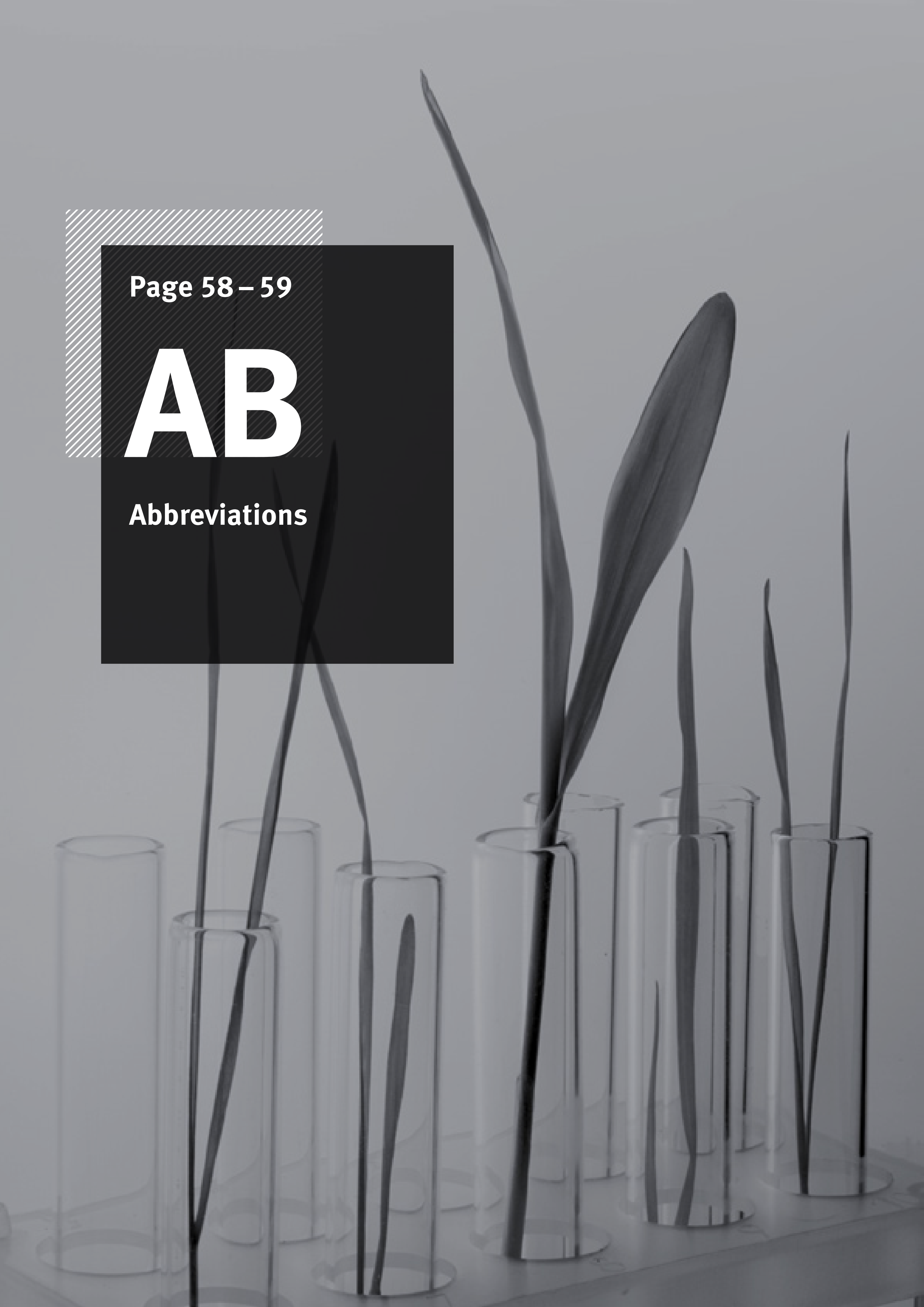

Page 58 – 59

AB

Abbreviations

Abbreviations

ARTICLE	An object with a special shape, surface or design which determines its function to a greater degree than does its chemical composition
BAT	Best available techniques
BCF	Bioconcentration factor
BREF	Best available techniques reference document
CAS	Chemical abstract service
C&L	Classification and labelling
COSHH	Control of substances hazardous to health. Approach from great britain for the derivation of risk management measures for work place
CLP	Classification, labelling and packaging
CMR	Carcinogenic, mutagenic or reprotoxic substance
DNEL	Derived no effect level
DPD+	Method to identify lead substances in mixtures based on the dangerous preparation directive
ECHA	European chemicals agency
EDC	Endocrine disrupting chemical
EMKG	Einfaches maßnahmenkonzept gefahrstoffe (simple concept of measures for dangerous substances) = easy-to-use workplace control scheme for hazardous substances Epd: environmental product declaration
EXPOSURE	Exponere (lat): to be set out; contact between a chemical substance or a physical or biological agent on the one hand and an organism or an environmental compartment on the other.
HACCP	Hazard analysis and critical control point
LCA	Lifecycle analysis
LC50	Lethal concentration; concentration causing 50 % of test organisms to die
LOGKOW	Logarithm of the partitioning coefficient between water and octanol
MIXTURE	A mixture or solution composed of two or more substances (clp regulation). This term replaces the term “preparation”.
PBT	Persistent, bioccumulative and toxic substance
PC	Physicochemical
PEC	Predicted environmental concentration
PNEC	Predicted no effect concentration
REACH	Registration, evaluation and authorization of chemicals (new European chemicals regulation)
SME	Small and medium sized enterprises
SVHC	Substance of very high concern
VPVB	Very persistent and very bioaccumulative substance

Page 60 – 72

AN

Annex

Annex

Annex 1: Links to substance lists

REACH Candidate list of substances of very high concern and background information about the list:	http://echa.europa.eu/chem_data/candidate_list_table_en.asp https://echa.europa.eu/support/authorisation/substances-of-very-high-concern-identification
Water Framework Directive – priority and priority hazardous substances of the:	http://ec.europa.eu/environment/water/water-framework/priority_substances.htm
Helcom list of substances of possible concern and background information:	http://www.helcom.fi/about-us/convention/annexes/annex-i/ http://www.helcom.fi/
Ospar list of substances of possible concern and list of substances for priority action:	http://www.ospar.org/work-areas/hasec/chemicals/possible-concern http://www.ospar.org/work-areas/hasec/chemicals/priority-action
Ospar list of substances for priority action:	http://www.ospar.org/work-areas/hasec/chemicals/priority-action
Stockholm Konvention POPs:	http://chm.pops.int/TheConvention/ThePOPs/ListingofPOPs/tabid/2509/Default.aspx http://chm.pops.int/ https://www.umweltbundesamt.de/themen/chemikalien/chemikalien-management/stockholm-konvention
Montreal protocol:	http://ozone.unep.org/
Substitute-it-now (SIN) list:	http://chemsec.org/business-tool/sin-list/

Annex 2: PBT/vPvB – Criteria of REACH Annex XIII

Criterion	PBT	vPvB
Persistence		
Half-life in marine water or	› 40 days	› 60 days
Half-life in freshwater or estuaries or	› 40 days	› 60 days
Half-life in marine sediments or	› 180 days	› 180 days
Half-life in freshwater sediments or estuarine sediments or	› 120 days	› 180 days
Half-life in soil	› 120 days	› 180 days
Bioaccumulation potential		
Bioconcentration factor	› 2 000	› 5 000
Toxicity		
Concentration, below which no effects are observed in marine or freshwaterorganisms (no-observed effect concentration – noec)	‹ 0,01 mg/l	Not applicable
Substance is or	Carcinogen (cat 1A or 1B), mutagen (cat 1A or 1B) or reprotoxicant (cat 1A, 1Bor 2)	
Classification according to CLP Regulation	Specific target organ toxity-repeated exposure (STOT RE Category 1 or 2)	

Annex 3: Links to databases and evaluation instruments

3.1 PROBAS Database of the Federal Environmental Agency

In the Probas database, information on different materials and processes are compiled. For a defined reference amount of a product (e. g. 1 kg of copper), the required inputs are provided (energy, materials, water). The energy consumption is expressed as aggregated values (KEA/KEV), which describe the cumulated energy consumption along the supply chain (table "resources"). The water consumption can be extracted from the table "inputs". In the table "wastes" the amounts of waste produced along the supply chain are listed. http://www.probas.umwelt-bundesamt.de/php/index.php

3.2 MIPS-concept of the Wuppertal institute for climate, environment and energy GmbH and further LCA tools

MIPS stands for "material input per service unit". According to this concept, the environmental impacts of a substance, material, product or service are calculated using the material consumptions necessary for their manufacturing or supply. On the MIPS web pages an excel file is provided for structuring respective data collection. Furthermore, lists with material intensities of different raw materials and chemicals are given. Related to the current guide, the values for material and water consumption can be used. Energy consumptions and the renewability of raw materials are not considered by MIPS. However, self-standing evaluations can be done. http://www.wupperinst.org/de/projekte/themen_online/mips/index.html

The Directorate Research of the European Commission provides tools and data bases for lifecycle analyses on their website free of charge. http://lca.jrc.ec.europa.eu/lcainfohub/directory.vm

Annex 4: Further public available sources of information

This annex describes some sources for additional information. It is not complete, however if offers valuable help to work with the sustainability criteria. In many cases sector-specific information is available. For this the respective associations should be contacted.

Review on sustainable chemistry:
The background document of the environment agency on sustainable chemistry gives a good overview about the different aspects of this topic. It can be downloaded from: http://www.umwelt-bundesamt.de/uba-info-medien/mysql_medien.php?anfrage=Kennummer&Suchwort=3734

Approaches to set sector-specific priorities in risk management:
The HACCP concept ("Hazard Analysis and Critical Control Point" has been developed especially for the food industry. However its principles can be applied in other sectors of industry, also. More details can be found at: http://www.bfr.bund.de/cm/234/fragen_und_antworten_zum_hazard_analysis_and_critical_control_point_haccp_konzept.pdf

Sector-specific documentation of best available techniques:
Saving of resources and costs can be achieved by implementation of best available techniques. They are documented for many sectors in the so-called BREF documents, see: http://eippcb.jrc.ec.europa.eu/reference/

Sector-specific lists of problematic substances:
The “Global Automotive Declarable Substance List” of the automotive industry is a corporate instrument for the management of problematic substances. It is publicly available (www.gadsl.org). Lists of problematic substances which can be relevant for all branches are documented in Annex I of this guidance.

Data bases on hazardous substances:
Examples for public available data bases on hazardous substances are “Der gemeinsame Stoffdatenpool von Bund und Ländern” (http://www.gsbl.de/index.html) and the European data base on classification and labelling, Joint Research Center, Ispra, Italy (http://ecb.jrc.ec.europa.eu/classification-labelling/search-classlab/). Data on more than 5000 dangerous substances are available in GESTIS, the hazardous substances information system of the German statutory accident insurance (http://www.dguv.de/ifa/GESTIS/GESTIS-Stoffdatenbank/index.jsp, last checked on the 29th of June 2016). Here, you can find, for instance, the H-phrases of a substance and information on its water solubility, its vapor pressure and other physicochemical characteristics.

The international portal eChem contains very extensive data on physicochemical characteristics as well as data on hazardous qualities for humans and the environment (http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en, last checked on the 29th of June 2016).

Identification of risk management measures for work places:
The “Easy-to-use workplace control scheme for hazardous substances” (Einfaches Maßnahmenkonzept Gefahrstoffe, EMKG) of the Federal Agency for Occupational Health and Safety supports enterprises’ decisions on risk management measures to ensure safe use of substances and mixtures. It is based on a limited amount 44 Leitfaden nachhaltige Chemikalien of information which are available in companies (e. g. in safety data sheets http://www.baua.de/de/Themen-von-A-Z/Gefahrstoffe/EMKG/EMKG__content.html).

Guidance on chemical safety assessment, exposure assessment and risk characterization:
The explanation and support of a comprehensive assessment of emissions along the lifecycle of a substance is not possible in this guide. However, publications on this topic can be found on the web in much detail.

The European Chemicals Agency publishes an comprehensive Guidance on Information Requirements and the Chemical Safety Assessment. It describes – besides others – the methods for assessing exposures and characterizing risks from the use of chemicals46. ECHA publishes further guidance on all topics related to REACH (see http://guidance.echa.europa.eu/guidance_en.htm).

For the structured communication on uses the so called “Use Descriptor System” has been developed in the framework of REACH. It is described in Part R12 of the ECHA Guidance on information requirements mentioned above.

The VCI REACH guidance for practitioners introduces to the topics exposure assessment and communication in the supply chain with several recommendations on the implementation in practice. The guidance and the case studies can be received from Dirk Bunke. Just write a short request to d.bunke@oeko.de

Exposure estimation tools:
Several instruments have been developed to support the tasks of exposure estimation and risk characterization. An overview is given in Part IV of the above mentioned REACH Practical Guide. Last year the second version of the exposure estimation tool ECETOC TRA (“Targeted Risk Assessment”) has been published. It is available for free (http://www.ecetoc.org/tra).

Guidance for Substitution:
Guidance for substitution is given in a publication of the Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAUA) (Technische Regel Gefahrstoffe (TRGS) 600, www.baua.bund.de/nn_78960/de/Themen-von-A-Z/Gefahrstoffe/TRGS/pdf/TRGS-600.pdf).

A good overview on the topic is given in the publication of Lißner and Lohse (Lißner, L.; Lohse, J. (2006); Braucht Substitution mehr Staat oder mehr Markt? In: UWSF – Z Umweltchem Ökotox 18 (3) 193 – 200).

Annex 5: Classification of substances and safety information in the supply chain

Three of the eight substance-specific criteria described in chapter 2 of this guidance are based on the existing classification of a substance (physicochemical properties, human toxicity and ecotoxicity (c. f. chapters 2.1.2, 2.1.3 and 2.1.4). This information is to be generated by manufacturers and importers and is normally available at the end users of chemicals in form of safety data sheets, REACH information or product labels. Information on the dangerousness for the environment (c. f. Chapter 2.1.4) and on the mobility (c. f. Chapter 2.1.5) is normally contained in the safety data sheet as well. Therefore, some basic information and legal background is given on this information source.

By the end of 2010, substances may be either classified or labelled according to the EU Dangerous Substances Directive (67/548/EEC or the German TRGS 200 respectively) or according to the European Classification and Labelling Regulation (CLP-regulation, EC/1272/2008).

The placer on the market may choose which of the systems he applies or even if he uses both simultaneously. By 2015, all substances are to be classified and labelled only according to the CLP-regulation.

Under REACH, manufacturers of substances are required to compile and / or generate information in the scope of its registration. The extent of information depends on the registered annual volume. Parts of this information are to be forwarded to the downstream users of substances and mixtures via the safety data sheet. The information is to be provided in accordance with REACH article 32 and the results of tests and studies are to be provided directly, if possible. Information which is not (yet) available or not legally required for the registered tonnage as specified in the Annexes VI – XI of REACH should be indicated in the safety data sheet (remark “not tested” or “information not available”).

Downstream users of substances and mixtures receive respective safety information from their suppliers. In the transition period of REACH, they should pay particular attention to new information on a substance as such or contained in mixtures, especially after its registration.

The lack of information about the properties of substances and mixtures in the safety data sheet and / or those marked with “not applicable” are not transparent, as it is not clear if tests have been performed to show that a dangerous property is not present or if no tests sufficient for a classification have been performed. If information is ambiguous, the supplier of substances or mixtures should be consulted to clarify the information basis[36]. This is particularly relevant when alternatives are compared in the context of assessing substitution possibilities.

If a substance or mixture is not classified as dangerous[37], in principle no safety data sheet must be provided[38]. However, other properties of a substance or mixture (e. g. dustiness) may require the communication of risk management measures to ensure safe handling. According to REACH article 32, suppliers/manufacturers have to communicate such information. The format for forwarding this information is not legally defined.

[36] If a substance is not classified because no data are available, at a later stage it can turn out to be of higher concern than the substance to be substituted. It would neither be sustainable nor economically reasonable to take a decision based on an incomplete data basis. In this case it is to be decided if new data are awaited or if a substitute is excluded due to lack of data, if own data are generated or substitution is implemented despite the lack of information.

[37] According to REACH, a safety data sheet has to be provided also for PBTs/vPvBs and substances on the candidate list for authorization, even if they are not classified.

[38] Unless the substance is of very high concern and listed on the candidate list for authorization.

Annex 6: Further information on the emission potential

Relevance of the emission potential:
The emission potential expresses, what amount of a substance is lost or released during its lifecycle and what exposures and pressures for man and the environment may result. Emissions are normally assessed for single substances, rather than for several substances at the same time. If mixtures are assessed, the emission potentials are to be evaluated separately for its components, reasonably for those with the highest mobility and / or the most severe dangerous properties for humans or the environment.

Emissions from products and processes can be reduced by implementing risk management measures, which should be considered in the assessment of the emission potential, if the respective information is available in the company[39].

Lifecycle of a substance:
In order to review the emission potential of a substance (as such or as a component of a mixture or article), all of its uses need to be considered. Normally, each use is a sequence or combination of the following lifecycle stages:

- Manufacture (or import)
- Formulation / mixing of mixtures (frequently several mixing steps in one or several companies)
- Use of a mixture in processes (as processing air or for the manufacture of articles, in which the substance is integrated into)
- Use of the article (service life)
- Disposal of the articles and production wastes, which are produced along the lifecycle.

Depending on the type of substance and its uses, each of the lifecycle steps may occur once, more than once or not at all. Some substances are used in different applications and hence, several lifecycles should be assessed. According to the European chemicals regulation REACH, for all substances registered in amounts exceeding 10 t/a and which are classified as dangerous, an emission estimation and exposure assessment is to be performed. The instruments supporting this assessment are for example a system to describe uses in a standardized way (use descriptors[40]) and simple models[41] for estimating emitted amounts of a substance from processes and products.

The aim of the so called chemical safety assessment under REACH is the identification of risk management measures, which are necessary to ensure safe handling and use of a substance along its entire lifecycle, including the use in articles and the waste disposal stage.

[39] In order to remain manageable, this guide is limited to a first and rough estimation. Furthermore, emissions with view to sustainability, even if they do not lead to exposures because of appropriate risk management measures, should be prevented, in order not to lose substances (resource consumption).

[40] C. f. the guidance document by the European Chemicals Agency on information requirements and the chemical safety assessment, part D. This guidance is available on the website of the European Chemicals Agency (http://guidance.echa.europa.eu/guidance_en.htm.).

[41] E. g. ECETOC TRA Version 2. An easy to understand description of instruments on exposure assessment can be found in the in-depth chapter on exposure assessment of the REACH guide for practitioners (The REACH-guide can be received from Dirk Bunke. Just write a short request to d.bunke@oeko.de)

Annex 7: Substitution

When deciding on substitution, the replacement of critical substances with less critical alternatives, as well as other measures such as a different product designs or organizational and technical measures in the production process are relevant. In any case, various factors influence which option is most efficient or feasible in a specific context. In the following, some of these factors are briefly introduced. For detailed information, specific literature on substitution should be consulted.

Maintaining or improving product quality:
The use of alternatives should improve the quality of a product towards more sustainability; in no case should it worsen the product quality. The qualities to maintain or improve are e. g. the lifespan of the product, safety functions during use, the practicality of a product or a product's weight (material input).

If the product design is changed and thereby the use of a critical substance is phased out (e. g. constructive flame retardation instead of the use of chemical flame retardants) sustainability can be realized through the adoption of that change in other products. This could happen either as a "technological spill over", where a systematic change is used across different technologies or simply through the integration of the changed product into complex articles as a component.

The quality of products is sometimes defined by the customers, who may demand certain characteristics or qualities. In these cases, the question of the availability of alternatives is limited by these demands – sometimes with very low tolerances. On the other hand, if customers define their quality criteria with respect to the content or the absence of certain substances, the search for alternatives is obviously welcome and not limited by any conditions.

No shift of risk, no increase of total risk:
If non-sustainable substances are replaced by other substances, any risks for human health or the environment should be carefully observed that they are not increased. This can be ensured if the substitute has less dangerous properties for human health and the environment (c. f. Chapter 2.1.3 and 2.1.4), if it less mobile (c. f. Chapter 2.1.5) and / or is used in significantly lower amounts (c. f. Chapter 2.2.3).

For non-chemical alternatives, but also if alternatives are used, further risks have to be considered:

- If a substance is replaced by technical measures, risks for workers may shift from chemical stress to physical or other stress[42]

- Substitution may result in the loss of safety of the product, which could be an indication for a worse quality (e. g. higher flammability due to the abandonment of flame retardants).
- A changed (substance) design could deteriorate the manageability of products.

Technical preconditions in the own company and at the customers':
The alternatives for non-sustainable substances have to be applicable in existing technology, not only inside own production processes, but also at the customers'. In particular in sectors where complex and very fast production processes occur (e. g. newspaper printing) or very complex articles are manufactured (e. g. electronic devices), production processes and machines are fine-tuned to the use of particular chemicals. In substitution processes, the entire supply chain and all related conditions and technical requirements are to be assessed.

Economic issues:
The substitution of substances is connected to different types of economic risks: the technical feasibility, the frequently missing information on the dangerous properties of substitutes (and resulting difficulties in comparing alternatives), the financing of research activities, the practical and technical implementation of substitution, as well as the risk of lower acceptance of new products on the market. Substitution may at the same time offer many opportunities to increase product quality, enforce approaches for sustainable innovation and thereby improve the market position or enter new markets.

Each enterprise has to assess substitution issues for itself, balance risks and opportunities connected with a substitution and make a respective decision.

[42] For example can solvent-based paints be replaced if a drying installation is used. The dryer my expose workers to higher temperatures and potentially higher levels of noise by the exhaust gas system of the drying installation.

Annex 8: Benefit potentials

The benefit potentials can be allocated to different areas, which are briefly described in the following.

Quality of (end) products:
The functionalities of substances[43], which improve product qualities in the sense of sustainability, are for example functionalities that:

- Prolong the lifespan (e. g. reduced deterioration due to weathering by the use of UV-stabilizers or corrosion inhibitors);
- Reduce the material consumption for the manufacturing of a product (e. g. lower material density through the use of nanomaterials);
- Enhance safety or enlarge the benefits of other products (e. g. lubricants increase safety and reduce abrasion of machinery).

Societal benefits:
To evaluate the societal benefits of a substance, the function of the end product is to be assessed as well as the potentially caused impacts on human health. For example, the societal benefit of fragrances in erasers, CDs or similar articles can be questioned. However, a significant benefit can be seen in the use of silver in textiles which makes clothes better tolerable for persons with neurodermatitis. The use of biocides in metal working fluids improves workers' health by preventing or at least significantly reducing the growth of pathogenic bacteria.

For the reflection of societal benefits, the following questions should be answered:

- What qualities does a substance add or contribute to an end product?
- What benefit does society have from the existence of that property? Are there indications that the function is wanted or objected to?
- Does the property enhance the health conditions of consumers and workers?

Environmental benefits:
Environmental benefits are realized by improving product quality (prolonged lifespan, resource savings) and frequently overlap with the previously mentioned items. Further environmental benefits of substances can be seen in that they (contribute to) improve the quality of the environment. Some examples are environmental remediation technologies: chemical wastewater cleaning, use of chemicals for the remediation of environmental damage. Further benefits regarding sustainability are always connected to a chemical, when it is important for the function of a product that replaces technologies carrying heavy environmental burdens (e. g. silica in solar cells instead of energy production based on fossil fuels like coal).

Economic benefits:
A sustainable decision on the manufacture and use of chemicals must also consider the economic consequences for enterprises. Normally, it is not possible to immediately phase out the production or use of a chemical, which has been evaluated as not sustainable. The economic survival of companies is to be ensured and may relativize the non-sustainability of chemical. However, sustainability of products should gain a higher importance in the long-term goals of companies.

[43] If the sustainability of materials or end products is evaluated, further and other criteria are relevant as compared to assessing chemicals only, e. g. the possibility to repair or dismantle products for recycling. The following explanation is limited to functionalities of sustainability, which can be evaluated and influenced by manufacturers and users of chemicals.

Annex 9: Greenhousegas emissions of substances

The following table contains information about the amount of greenhouse gas emissions of often used substances. This amount is specified as kg-CO_2-equivalent. It shows how much CO_2 is emitted by producing 1 kg of a substance. The data origins from the life cycle assessment data base Probas of the Umweltbundesamt (see annex 3.1). The following evaluation is applied:

- Values below 1 kg CO_2-eq/kg substance: green
- Values between 1 and 10 kg CO_2-eq/kg substance: yellow
- Values above 10 kg CO_2-eq/kg substance: red

Name	kg CO_2-eq/kg substance	Color
Inorganic substance*	2	Yellow
Organic substance*	1.9	Yellow
Asphalt	0.2	Green
Bauxite	0.2	Green
Biocide	25	Red
Calcium chloride $CaCl_2$ (high purity)	0.5	Green
Calcium hydroxide $Ca(OH)_2$	0.8	Green
Carbon black	0.4	Green
Carbon monoxide, CO	4.1	Yellow
Carbon tetrachloride	1.5	Yellow
Chlorine	1	Green
Chlorine (Mix)	0.5	Green
Clay	1.2	Yellow
Distilled water	0.5	Green
Fluoric acid (high purity)	0	Green
Formaldehyde	0.5	Green
Hydrogen	1.7	Yellow
Hydrogen	8.7	Yellow
Hydrogen peroxide	5.5	Yellow

*without further specification

Name	kg CO_2-eq/kg substance	Color
Industrial diamonds	7,000,000	Red
Melamine	1	Yellow
Metallizing past	0.03	Green
Methanol	0.5	Green
NaOH mix	0.4	Green
NF_3 (high purity)	21	Red
Nitric acid	1.6	Yellow
Nitrogen (liquid)	0.4	Green
Oxygen (liquid)	0.4	Green
P_4 (Phosphorus)	8.7	Yellow
PEG+DPM (high purity)	2.2	Yellow
Phenol	2	Yellow
Phosphoric acid	3	Yellow
Phosphoric paste	0.05	Green
Phosphorus trichloride	3	Yellow
Plant protection product	5.4	Yellow
$POCl_3$ (high purity)	4.8	Yellow
Polypropylene granulate	2	Yellow
Propylene glycol	2	Yellow
SF_6 (high purity)	10	Yellow
SiC	1.3	Yellow
SiC (high purity)	6	Yellow
$SiCl_4$	4.6	Yellow
Silane (high purity)	53	Red
Silicon (technical)	9.5	Yellow
Silicon-EG	61	Red
Soda	1	Yellow
Sodium silicate	1.9	Yellow
Solvent (high purity)	2.6	Yellow
Sulfuric acid	0	Green
Thermal oil	7	Yellow
Toluene	1.7	Yellow
Urea	0.7	Green
Xylene	1.7	Yellow

Annex 10: Energy consumption of substances

The following table contains information about the amount of energy consumption related to the substance production of often used substances. This amount is specified by the unit Mega Joule / kilogram substance. The data origins from the life cycle assessment data base Probas of the Umweltbundesamt (see annex 3.1). The following evaluation is applied:

- Energy consumption below 10 MJ/kg substance: green
- Energy consumption between 10 and 100 MJ/kg substance: yellow
- Energy consumption above 50 MJ/kg substance: red

Name	MJ/kg	Color
Inorganic substance*	27	Yellow
Organic substance*	65	Yellow
2-Propanol (high purity)	10	Yellow
Acetic acid	14	Yellow
Aluminum fluoride	0.6	Green
Ammonia	0.07	Green
Ammonium nitrate	0.2	Green
Bauxite	0.65	Green
Benzene	10	Yellow
Biocide	281	Red
Bitumen	6.3	Green
C_2F_6 (high purity)	152	Red
Calcium chloride $CaCl_2$ (high purity)	0.01	Green
Calcium hydroxide $Ca(OH)_2$	0.17	Green
Carbon black	4.9	Green
Carbon Monoxide	68	Yellow
Carbon tetrachloride	27	Yellow
CF_4 (high purity)	153	Red
Chlorine (any process)	17	Yellow
Chloroform	26	Yellow
Clay	18	Yellow
Clay	0.9	Green
Cumene / Cumol	9.8	Green
Distilled water	0.13	Green
Ethanol (high purity)	3.6	Green
Ethylene	7.1	Green
Ethylene oxide	5.7	Green
EVA	40	Yellow

* without further specification

Name	MJ/kg	Color
Fertilizer (P, N, K)	0.11	Green
Fertilizer-K	19	Yellow
Fluorine	149	Red
Formaldehyde	0	Green
Glycerin	119	Red
Hydrofluoric acid	0	Green
Hydrogen	64	Yellow
Hydrogen peroxide	41	Yellow
Industrial diamonds	106,000	Red
Melamine	28	Yellow
Metalizing paste	213	Red
Methanol-Substance	9.8	Green
NaOH (all but membrane)	11	Yellow
NaOH (only membrane process)	8.8	Green
NaOH 50 %	4	Green
NF_3 (high purity)	351	Red
Nitric acid	0.07	Green
Nitrogen (liquid)	7.5	Green
Oxygen (liquid)	7.0	Green
P_4 (phosphorous)	196	Red
PEG+DPM (high purity)	6.1	Green
Phenol	9.1	Green
Phosphoric acid	0.78	Green
Phosphoric paste	0.8	Green
Phosphorus trichloride	64	Yellow
Plant protection product	198	Red
$POCl_3$ (Phosphorous trichloride)	92	Yellow
Polypropylene; granulate	29	Yellow
Propylene glycol	16	Yellow
SF_6 (high purity)	167	Red
SiC	13	Yellow
SiC (high purity)	154	Red
$SiCl_4$	98	Yellow
Silane (high purity)	1072	Red
Silicom	47	Yellow
Silicom (technical grade)	149	Red
Soda	14	Yellow
Sodium silicate	20	Yellow
Solvents (high purity)	40	Yellow
Sulfuric acid	0.4	Green
Thermal oil	109	Red
Toluene	0.7	Green
Urea	12	Yellow
Xylene	0.7	Green

Annex 11: Water consumption of substances

The following table contains information about the amount of water consumption related to the substance production of often used substances. This amount is specified by the unit Liter/kg substance. The data origins from the life cycle assessment data base Probas of the Umweltbundesamt (see annex 3.1). The following evaluation is applied:

- Water consumption below 5 l/kg substance: green
- Water consumption between 5 and 100 l/kg substance: yellow
- Water consumption above 100 l/kg substance: red

Name	Liter/kg substance	Color
Inorganic substance*	46	Yellow
Organic substance*	8	Yellow
Acetic acid	3.7	Green
Aluminum fluoride	6.4	Yellow
Ammonium nitrate	99	Yellow
Asphalt	1.4	Green
Bauxite – import mix	0.2	Green
Benzene	5.6	Yellow
Biocide	14	Yellow
C_2F_6 (high purity)	272	Red
Calcium chloride $CaCl_2$ (high purity)	1.3	Green
Calcium hydroxide $Ca(OH)_2$	2.0	Green
Carbon black	2.2	Green
Carbon tetrachloride	114	Red
Carbonmonoxide, CO	2.1	Green
CF_4 (high purity)	282	Red
Chlorine (all but diaphragm)	95	Yellow
Chlorine (Diaphragm)	153	Red
Chloroform	102	Red
Clay	1	Green
Clay, mix	8.6	Yellow
Cumene/Cumol	5.7	Yellow
Distilled water	1.03	Green
Ethanol (high purity)	3.4	Green
Ethylene	5.6	Yellow
Ethylene oxide	4.5	Green
EVA	6.1	Yellow
Fertilizer-N	1.9	Green
Fertilizer-P	234	Red
Fertilizer-K	61	Yellow

* without further specification

Name	Liter/kg substance	Color
Fluoric acid (high purity)	101	Red
Fluoric acid (high purity)	101	Red
Fluorine	155	Red
Formaldehyde	43	Yellow
Glycerin	257	Red
Hydrogen	1.8	Green
Hydrogen	6.7	Yellow
Hydrogen peroxide	13	Yellow
Industrial diamonds	109,700,000	Red
Melamine	230	Red
Metalizing paste	1.6	Green
Methanol	2.5	Green
NaOH (Diaphragm)	138	Red
NaOH mix	42	Yellow
NF_3 (high purity)	270	Red
Nitric acid	126	Red
Nitrogen (liquid)	0.00003	Green
Oxygen (liquid)	0.00003	Green
P_4 (Phosphorus)	61	Yellow
PEG+DPM (high purity)	4.8	Green
Phenol	5.2	Yellow
Phosphoric acid	172	Red
Phosphoric paste	2,8	Green
Phosphorus trichloride	95	Yellow
Plant protecion product	32	Yellow
$POCl_3$ (high purity)	103	Red
Polypropylene-Granulate	43	Yellow
Propylene glycol	6.7	Yellow
SF_6 (high purity)	174	Red
SiC	65	Yellow
SiC (high purity)	34	Yellow
$SiCl_4$	171	Red
Silan (high purity)	1819	Red
Silicom (all but EG)	47	Yellow
Silizom-EG	207	Red
Soda	66	Yellow
Sodium silicate	57	Yellow
Solvent (high purity)	2.5	Green
Sulfuric acid	40	Yellow
Thermal oil	35	Yellow
Toluene	5.3	Yellow
Urea	80	Yellow
Xylene	5.3	Yellow

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