Work Package 2 "Identification of relevant target substances in BREFs" of the HAZBREF project funded by Interreg Baltic Sea Region

Report

Approaches for a better use of available data to prevent or reduce releases of substances of concern from industrial installations

HAZBREF
Hazardous industrial chemicals in the IED BREFs

Interreg
Baltic Sea Region

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

HAZBREF in Brief

This report is a product of the HAZBREF project *"Hazardous industrial chemicals in the IED BREFs"*. HAZBREF is funded by the EU Interreg Baltic Sea Region Programme and the implementation period is three years from October 2017 until September 2020.

The overall aim of HAZBREF is to increase the knowledge base of the industrial sources and the reduction measures of substances of concern. HAZBREF will identify relevant chemicals used in industrial sectors, their use patterns, environmental characteristics and measures to prevent and reduce releases to environment.

On the EU level the main instrument to control industrial releases is the Industrial Emissions Directive (IED), particularly through the publication of BAT Reference documents (BREFs) and their key chapter: the BAT conclusions. This approach has achieved significant environmental gains in the EU, widely recognized by stakeholders. This project intends to further analyse whether BAT conclusions address hazardous substances in a systematic and comprehensive way. HAZBREF aims to develop a systematic approach that will help to exchange and utilize the existing information about substances of concern between different regulatory frameworks (IED, REACH, Water Framework Directive, Marine Strategy Framework Directive, EU provisions on Circular Economy, Stockholm POP Convention & HELCOM) in the preparation of BREFs.

This report looks at ways to address more comprehensively the use and risks of chemicals in BAT Reference documents, with a view to enhancing the capacity to manage industrial chemicals among both authorities and operators. The information gathered in BREFs is also useful for the Baltic Marine Environment Protection Commission HELCOM in the development of actions to reduce the inputs of hazardous substances to the Baltic Sea. HAZBREF also promotes the circular economy by proposing ways to better include circular economy aspects in BREFs.

HAZBREF outputs target both the policy and the enforcement level. On policy level the outputs will strengthen the links between different regulatory frameworks and their key players. On enforcement level at industrial installations the project will identify and test model solutions for chemicals management in industry.

The activities were carried out in four Work Packages:

- WP1 – Project management and administration (Lead Partner SYKE) including communication and dissemination of results;
- WP2 – Identification of target substances (Lead by UBA) that include:
  - 2.1 Identification and selection of target substances
  - 2.2 Fate of substances during emission treatment
- WP3 – Policy improvement (Lead by UBA) that include:
  - 3.1 Strengthening links between regulatory frameworks on different levels
  - 3.2 Developing method to include substance information into BREFs, improve communication and data flow
- WP4 – Best practices in chemicals management in industry (lead by IETU) that include:
  - 4.1 Sectoral guidance for three IED sectors (chemicals, textile, surface treatment of metals and plastics)
  - 4.2 Case studies in selected installations
  - 4.3 BAT descriptions and model permits
  - 4.4 Circular economy aspects.

The HAZBREF partnership includes 5 organisations from the Baltic Sea region: Finnish Environment Institute (SYKE) (Lead partner), German Environment Agency (UBA), Swedish Environmental Protection Agency (SWEPA), Institute for Ecology of Industrial Areas (IETU) and Estonian Environmental Research Centre (KLAB).

In addition, 27 associated organisations and a wide range of other stakeholders were involved in HAZBREF, such as ministries and governmental environmental and chemical agencies from several EU countries, permitting and supervision authorities as well as industries and environmental NGOs.

More information about HAZBREF can be found on our project website (www.syke.fi/projects/hazbref).

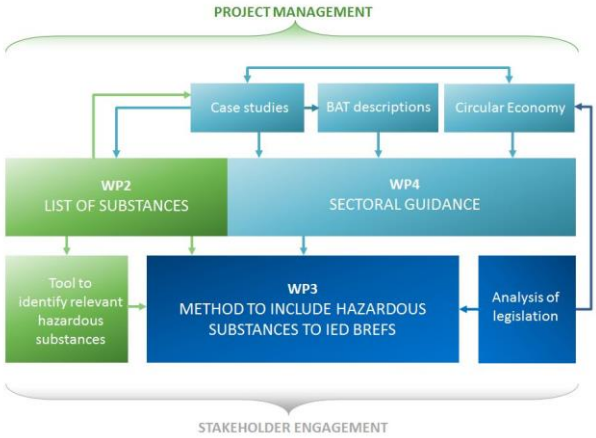

Figure 1: Overview of the design of the HAZBREF-project with its four work packages

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Abbreviations

AC	Article category (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Chapter R.12)
BAT	Best Available Techniques
BATC	BAT Conclusion
BCF / BMF	Bioconcentration factor / biomagnification factor
BEP	Best Environmental Practice
BOD / COD	Biological oxygen demand / chemical oxygen demand for degradation of substance mixtures in sewage treatment
BREF	Best Available Techniques Reference Document
BSAP	Baltic Sea Action Plan
CAS No.	A unique numerical identifier assigned by the Chemical Abstracts Service (CAS) to every chemical substance
CBI	Confidential Business Information
CLP Regulation	Classification, Labelling and Packaging Regulation (EC) No. 1272/2008; feeds into the Global Harmonised System (GHS) for Hazard Classification
CMR Substances	Carcinogenic, Mutagenic and Reprotoxic substances
CoRAP	Community Rolling Action Plan for substance evaluation (ECHA)
CSR	Chemical Safety Report
DE WGK	Deutschland Wassergefährdungsklassen
DG ENV	Directorate-General for Environment
EC	European Commission
ECHA	European Chemicals Agency
ED	Endocrine disruption
EEA	European Environment Agency
EIPPCB	European Integrated Pollution Prevention and Control Bureau
EQS	Environmental Quality Standards
ERC	Environmental Release Category
ES	Exposure Scenario
EU	European Union
HAZBREF	EU Interreg project “Hazardous industrial chemicals in the IED BREFs”

HELCOM	Baltic Marine Environment Protection Commission – Helsinki Commission
HPVC	High production volume chemicals (> 1000 tons/year)
IED	Industrial Emissions Directive 2010/75/EU
IMPEL	European Union Network for the Implementation and Enforcement of Environmental Law
Interreg	European Regional Development Fund for the Baltic Sea Region
IPPC	Integrated Pollution Prevention and Control Directive 96/61/EC
JRC	Joint Research Centre of the European Commission
KEI	Key Environmental Issue
MRSL	Manufacturing Restricted Substances List of the ZDHC Programme
NACE code	Nomenclature statistique des activités économiques dans la Communauté Européenne = sector of use category
NGO	Non-Governmental Organisation
NORMAN list	List of emerging substances from the Network of reference laboratories, research centres and related organisations for monitoring of emerging environmental substances
NPhEtox	Nonylphenolethoxylates
OECD	Organisation for Economic Co-operation and Development
PACT	Public activities coordination tool
PAHs	Polyaromatic hydrocarbons
PBT	Persistent, bioaccumulative and toxic
PC	Chemical product category (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Chapter R.12)
PCBs	Non-dioxin-like polychlorinated biphenyls
PCDD/F	Polychlorinated dibenzo-para-dioxins/furans
PE / PP	Polyethylene / polypropylene
PEC/PNEC ratio	Quotient of the predicted environmental concentration to the predicted no-effect concentration for a species (risk quotient)
PFAS	Perfluoroalkylated substances
PFBS	Perfluorobutane sulfonic acid
PFNA / PFOA	Perluorononanoic acid / Perfluorooctanoic acid
PFOS	Perfluorooctance sulphonate
PMT	Persistent, mobile and toxic substances of concern

POL sector	
POP Regulation	Persistent Organic Pollutants Regulation
PROC	Process category of use descriptors (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Chapter R.12)
QSAR	Quantitative structure-activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals, Regulation (EC) No. 1907/2006
RoI	Registry of Intentions
SDS	Safety Data Sheet
SIN list	SIN (Substitute It Now!) List developed by the International Chemical Secretariat (ChemSec)
SMILES code	Simplified Molecular Input Line Entry Specification code
SPERCs	Special Environment Release Categories
SPIN database	Database on the use of Substances in Products in the Nordic Countries
STM sector	Industrial sector of surface treatment of metals
SU	Sector of use category (ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Chapter R.12)
SVHCs	Substances of Very High Concern (under REACH)
SWEPA	Swedish Environmental Protection Agency
SYKE	Finnish Environment Institute
TWG	Technical Working Group (for the drawing up or reviewing of a BREF)
TXT BREF	Best Available Techniques (BAT) Reference Document (BREF) for the textiles industry
UBA	Umweltbundesamt, German Federal Environment Agency, Dessau-Roßlau
UNECE	United Nations Economic Commission for Europe
vPvB	Very persistent and very bioaccumulative
WFD	Water Framework Directive
WG CHEM	Working Group Chemicals
WP #	Work Package No. of HAZBREF
WWTP / STP	Waste-water treatment plant / sewage treatment plant
ZDHC	Zero Discharge of Hazardous Chemicals Programme (Industry Foundation)

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Preface

This report opens up the knowledge base on registered chemicals in the EU (the "ECHA data-base") with the intention to feed this information into the preparation of BREFs by the EIPPCB and to facilitate the implementation of BATs by installation operators.

The following persons have participated in WP 2 of the HAZBREF project and in the preparation of this report (Activity 2.1):

- from the Section IV 2.3 of the Umweltbundesamt in Dessau (Germany): Nannett Aust, Jürgen Fischer, Johann F. Moltmann (retired), Stefan Kacan, and other colleagues, as well as Consultants working for UBA – Barbara Werschkun (Strategy B) and Frank Riedel (IT solution for interactive scheme);
- from SYKE (Finland): Kaj Forsius, Emmi Vähä, Timo Jouttijärvi, Jukka Mehtonen, Pia Högmander (in particular for Chapter 3 on SVHC and other priority chemicals, as well as by commenting the report);
- from the Swedish EPA: Annika Månsson, Henrik Appelgren, Sven Bomark, Claes Debourg (in particular for the simulations of the behaviour of chemicals in wastewater treatment plants using SimpleTreat 4.0, i.e. Activity 2.2);
- from the Section III 2.1 of UBA participating in WP 3: Michael Suhr, Sandra Leuthold, Brigitte Zietlow;
- from the other HAZBREF project partners: Janusz Krupanek (IETU) and Karl Kupits (EKUK)
- the stakeholders of the HAZBREF project, in particular ECHA and TEGEWA, with suggestions and comments

We would like to express our special thanks to all involved parties for their continuous and beneficial co-operation and support, as well as their active participation in the conferences and webinars.

Disclaimer:

This report does not necessarily reflect the opinion of the sponsor, the European Regional Development Fund for the Baltic Sea Region Interreg, but that of the main contributors from UBA's Section IV 2.3 (Nannett Aust, Jürgen Fischer, Johann F. Moltmann), as well as other project partners with reference to the above-mentioned sub-chapters.

Executive Summary

The relation of the REACH Regulation and the Industrial Emission Directive (IED)

Chemicals used in the EU in industrial processes are registered, evaluated, authorised or restricted under the European Chemicals Regulation REACH (EC) No. 1907/2006 to ensure a high level of protection of human health and the environment. It is the task of manufacturers, importers or downstream users of chemicals to ensure that only those substances are manufactured, placed on the market or used, which do not adversely affect human health or the environment.

The industrial processes themselves, including the prevention and reduction of emissions and release of substances (of concern) into the environment, as well as the substitution of hazardous substances used at installation level, are subject to the Industrial Emission Directive 2010/75/EU.

This report analyses how these two key EU legal frameworks, REACH and IED, could benefit from each other, act complementary and best interact in a coherent manner to reduce emissions of substances of concern to the environment. For this the report focusses on how to select and utilise better available data.

The REACH instruments provide information for the safe use of a substance, e.g. on effects and exposure, obligations to substitute certain substances, or risk management measures. Making this information from the ECHA database of registered chemicals or Safety Data Sheets accessible in the BREF[1] elaboration process in a systematic and comprehensive manner, would strengthen implementation of measures via more complete BAT conclusions[1] with respect to the safe use of any substances of concern and the prevention and reduction of their emissions. While on the one hand, the information provided under REACH can be utilised in BREF reviews, on the other hand, REACH could also benefit from data gathered during BREF reviews and documented in BREFs or BAT conclusions, as far as the use and handling of hazardous substances is concerned.

Approaches for the identification of target substances relevant for BREF reviews in HAZBREF

This report describes approaches and tools to identify and assess substances of concern, presents substance data sources and provides guidance for substance evaluation, in order to characterise the relevance of substances for BREF reviews and BAT conclusions.

With the aim to minimise the release of chemicals of concern into the environment, it is in particular necessary to improve BATs for substances which pose concerns in ecotoxicological or human toxicological respect or with regard to their fate and behaviour in the environment.

In order to focus on the identification of (relevant) target substances in BREF reviews, it is firstly important that sectoral inventories of chemicals are drawn up. These chemicals inventories list and describe which chemicals are actually used in a given industrial sector and for which purposes and functionality. General data of retention potentials and aspects relevant for the assessment of the release potentials are of particular interest, too. The next step is to identify those substances that are already regulated by REACH and other EU Directives or

[1]) BAT: Best available techniques for the prevention and reduction of emissions of chemicals; BREF: BAT Reference Document containing BAT conclusions.

Regulations (e.g. SVHC or WFD priority substances), and to incorporate these legislative provisions into the BREF reviews as far as they are relevant for the determination of BAT. Finally, an examination of data from the ECHA database reveals those substances which, due to a high potential to be released and potential (eco)toxicological properties, are relevant target substances of concern for the preparation of BAT conclusions.

This report describes approaches and tools for assessment of substance properties of concern, presents substance data sources and provides guidance for substance evaluation, in order to characterise the relevance of target substances for BREF reviews and BAT conclusions.

Substances of concern and the interactive decision scheme as a tool for their identification

The HAZBREF project initially refers to hazardous substances as those which are "released from industries through discharges to waters, emissions to air and wastes (and which) have a harmful effect on the Baltic Sea environment". This interpretation covers harmful effects to the environment, as well as to humans via the environment.

Following the philosophy of the REACH Regulation, HAZBREF proposes to determine the "potential to be released" (through the WWTP), via the parameters adsorptivity / mobility and biodegradability / persistence. In addition, the intrinsic potential toxicity of the substance – which may qualify a substance as "relevant target substance" – is determined with the parameters for human toxicity (CMR and acute toxicity) and ecotoxicity (acute and chronic for different species). Both aspects have several degrees of importance, and the term hazardous should be reserved for high potential to be released and/or significant toxicity in this context. Thus, the definition of hazardous in this report is wider than based on CLP. The trigger values for decision-making regarding these parameters are those regularly used in chemicals safety assessment.

This report also provides means to systematically and efficiently gather and assess the crucial substance information from the ECHA database to be made available for the purpose of the BREFs, reviewing processes in order to facilitate the access and interpretation of substance information for operators of IED installations. This tool is designed as an interactive decision scheme based on the parameters of concern regarding fate, behaviour and effects. The scheme is presented in annex 6.

A promising approach was developed with the aim of establishing chemical groups via uses and chemical functions, e.g. provided by textile-processing sector itself. The analysis of these chemical groups then led to representative individual substances, for which a substance evaluation of the properties of concern could be carried out. Assuming that substances with similar functions and structural characteristics also show similar behaviour in the sewage treatment plant or have similar effects, recommendations can be given for the whole substance group in BREFs (i.e. BAT for elimination). As industrial installation operators are more likely to be informed about chemical functions and groups than about individual substances, this approach makes their work easier (see strategy B in annex 4).

In parallel, chemicals from different existing priority chemicals lists under different legislations (WFD substances and REACH SVHC) were linked with use information from the ECHA database and SPIN database. The purpose was to determine, whether it is possible to actually link the REACH use descriptors of priority chemicals to different IED industrial sectors. The high relevance of these hazardous substances is beyond question and their use is regulated to varying degrees in the respective regulations, alongside to the IED. However, it turned out, that linking the substances to different IED sectors could not be done in a straightforward way as

the use descriptions based on the data in ECHA and SPIN databases are not specific enough. Therefore, the results need further verification by sector experts (compare strategy A, C and D).

Conclusions and recommendations

The main outcome of this report is that it has been successfully demonstrated how to generically assess the environmental fate and toxicological relevance of chemicals based on the analysis of substance properties. The steps described for installation operators are also applicable for the BREF review.

It is helpful that right away or at least during the extended frontloading phase of the BREF revision, sectoral inventories of chemicals be drawn up or made available[2] by operators for their facilities. Also, industrial associations could establish chemical registers for their sectors. It is also important to derive generic schemes for technical functions and chemical functions for the substances used, so that it is finally known which chemicals or chemical groups are actually used for which purposes (and with which release potentials). The knowledge about individual substances actually used can be significantly expanded, if the composition of chemical products and mixtures (given by trade names) is disclosed, not only with regard to the anyway mandatory information on the content of SVHC.

However, it turned out, that linking substances to different IED sectors based on the data in ECHA and SPIN database could not be done in a straightforward way as the use descriptions are not accurate enough. Therefore, the results need further verification by sectors experts in order to incorporate the relevant BREF specific substances into the BREFs. The currently available use descriptor system under REACH should be revised to better fit use description in IED sector.

The next step is to identify those substances that are already regulated in other directives and regulations and to reflect relevant findings and recommendations for safe handling in the BREFs (e.g. SVHC or WFD priority substances).

Finally, different approaches are needed to identify the "substances of concern" which, due to a high "potential to be released" and potential (eco)toxicological properties, are relevant target substances for the preparation of BAT conclusions.

A streamlining of the regulatory frameworks is recommended, in particular with regard to the timeframes for substance evaluation under REACH or WFD and BREF revision. This might accelerate the introduction of recommendations for chemical management from other regulations into BREFs where relevant. Support for the early identification of emerging substances of concern is frequently provided by voluntary, standard-based sectoral programmes (e.g. ZDHC in the textile processing sector), which can often react more quickly than legislation. A link to list of substances of concern in other regulations and voluntary lists make more sense than rigid lists of substances in the BREFs themselves.

An improvement in co-operation between the actors involved is required: Exchange of data and information on chemicals (more transparency on substance properties, hazard potentials, uses, substance flows, elimination measures) along the value chain; improvement of information on

[2] It is to be noted that Art. 12 of IED requires that an application for a permit should include, inter alia, a description of […] the substances used by the installation (see par.1, point (b)). This type of information might be readily available (and sometimes organised in the form of preliminary inventories).

the use of substances in databases; establishment or enhancement of chemical product registers; harmonisation of the objectives and instruments of sustainable chemicals management among the actors and institutions involved; improved use of the own resources of the actors involved.

The valuable tool of Safety Data Sheets should be made more readily usable for downstream chemicals users - with improvements, updates and more realistic emission scenarios that reflects different usage conditions including worst case emissions.

1 Introduction

1.1 The relation between REACH and IED

Chemicals used in the EU in industrial processes are registered, evaluated, authorised or restricted under the European Chemicals Regulation REACH (EC) No 1907/2006 to ensure "safe-use" of these chemicals. The industrial processes themselves, including the reduction of emissions and substitution of uses of hazardous substances at installation level are subject to the Industrial Emission Directive (IED, Directive 2010/75/EU), which includes the determination and application of best available techniques (BAT) for use and discharge of chemicals at chemical installations. These two key EU legal frameworks address the issue of chemical pollution from different angles, which leads to the question how REACH and the IED could benefit from each other or how they could best interact in a coherent manner[3]. One main difference between the REACH Regulation and the IED is that REACH covers the risk management over the entire life cycle of a chemical, while the IED perspective is on the use and possible release of a substance in industrial installations (gate-to-gate approach). For further elaboration of the relations of REACH and IED, please refer to WP 3 (Suhr et al. 2020).

REACH aims at the safe use and handling of substances and mixtures on the European market. For all substances produced in or imported to the European Union in quantities of one ton or more per year, per company, information about uses and hazardous properties shall be provided in a registration dossier. It is the task of manufacturers, importers or downstream users to ensure that they manufacture, place on the market or use only those substances that do not adversely affect human health or the environment.

The REACH instruments provide information, e.g. on effects and exposure, obligations to substitute certain substances or risk management measures for the safe use of a substance. Use of this information in the BREF elaboration process would strengthen implementation of measures via more complete BAT conclusions with respect of the safe use of any substances of concern (including possibly their substitution) and the prevention and reduction of their emissions. By these means, the common objective of the IED and REACH – achieving a high level of protection of human health and of the environment – is easier to reach. Therefore, one option to improve the interaction between REACH and the IED is to assess, as a matter of routine, if substances of concern potentially used in industrial installations are emitted from the installation, and which measures are available to prevent and reduce their release.

Criteria for determining best available techniques (BAT) are, for example, the reduction of emission or the use of less hazardous substances (Annex III, 3. IED). Under the IED-regime, BREFs and their corresponding BAT conclusions already address to a certain extent the use and potential release of chemicals which are used in particular industrial activities. The perception of the IED stakeholders, in general, is that IED addresses the most relevant pollutants. However, this project intends to further analyse whether the magnitude of potentially hazardous substances is addressed in a systematic and comprehensive manner. In order to minimise the release of substances of concern into the environment, it is in particular necessary to improve the currently "best available techniques" (BAT) for the removal of substances which show a hazard potential either in (eco-)toxicological respect or with regard to their fate and behaviour in the environment (e.g. persistence, mobility or high bioaccumulation). By the application of

[3]) This chapter contains some unmarked passages which were also used in the report of HAZBREF Activity 3.1 (Analysis of the interfaces, links or gaps between the different pieces of EU legislation and marine convention, Suhr et al., January 2020) and *vice versa*, due to the contribution of WP 2 to chapter 3. of the Activity 3.1 report (REACH and the IED).

BAT conclusions authorities and operators should have the guarantee that releases of potentially hazardous chemicals are reduced at least to a level where hazards or concerns resulting from such chemicals are acceptable. This is usually below and not identical with a risk quotient below 1 according to REACH, and at the best at zero emission.

Information about restricted substances and substances of very high concern (SVHC) according to REACH are available in Annexes XVII and XIV of REACH and on the Candidate List. The inclusion of a substance in the Candidate List (currently 211 substances[4]) results in immediate obligations for suppliers of the substance and for articles and mixtures containing the substance above a concentration of 0.1% (w/w). REACH covers harmful effects to the environment, as well as to humans via the environment. The BAT-based approach of the IED obviously addresses substances classified as acute toxic and CMR, or substances classified as hazardous, but according to the REACH SVHC definition, the release of substances with environmental concern, e.g. PBT- and vPvB-substances, from installations should be avoided too.

A "Strategy to review the chemical BREFs" (EC, JRC, EIPPCB, 2007) gives some insight, how substances of importance for BREFs related to the chemical industry have been identified at that time. On the one hand, a list of 40 substances was developed based on conspicuous substances already identified by experts or listed in Annex I of the old IPPC Directive (96/61/EC) – this could be called 'listing by acclamation'. On the other hand, substances posing a “key environmental issue” were identified by expert judgement taking into account information on production volume, number of producers and installations in Europe, environmental impacts, and unit processes and operations not covered by existing BREFs. Assessment trigger values for these fate information criteria are not provided, unlike as for many hazard criteria.

The IED (from 2010) does not directly refer to the REACH Regulation (earlier from 2006) and the information on hazardous substances REACH provides. In contrast, Guidance Documents following REACH explicitly address 'the prevention and control of emissions to the environment from industrial sites following the principles laid down in the IED and the BREFs' (cf. Guidance on Information Requirements and Chemical Safety Assessment, Part D: Framework for exposure assessment, Version 2.0, August 2016, page 11 ff.):

'The particular role of REACH in the interaction with the other pieces of legislation is the generation and communication of substance specific information with regard to the hazards intrinsic to the substance, the properties determining the behaviour of the substance and the required conditions to ensure safe use all along the supply chain (including waste treatment). Downstream users will know best how their installation or product is designed in order to comply with the different legislations they are subject to. However, the REACH information brings a substance-focussed dimension to safe use of chemicals that complements the site-specific approach (taken under IED or the Chemical Agents Directive (CAD) and the Carcinogen and Mutagens Directive, CMD)' (ibid. page 12)[5].

The challenge is to combine both approaches in an intelligent and less burdensome manner.

'The integrated approach is one of the main pillars of the IED. This means that the permits must take into account the whole environmental performance of the plant, covering

[4]) https://echa.europa.eu/candidate-list-table (accessed 09.02.2021).

[5]) Statement quoted from page 12 of the above-mentioned REACH-Guidance that can be obtained via the ECHA website at: https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment .

e.g. emissions to air, water and soil, generation of waste, use of raw materials, energy efficiency, noise, prevention of accidents, and restoration of the site upon closure.

When applying for the permit the operator has to provide information on (not an exhaustive list):

- the substances used in or generated by the installation;
- the sources, nature and quantities of emissions from the installation into each medium and their effect on the environment;
- the technology and other techniques for prevention or, if not possible, reducing emissions from the installation.

Substance specific information provided in exposure scenarios will support operators in identifying the most relevant substances (in terms of hazard), their environmental fate and measures to prevent or reduce emissions' (ibid. page 13).

While on the one hand, the information provided under REACH can be utilised in BREF reviews, on the other hand, REACH could also benefit from data gathered during BREF reviews and documented in BREFs (in particular the chapters "techniques to consider in the determination of BAT" or BREF annexes dedicated to the use of chemical substances in a sector) or BAT conclusions as far as the safe use and handling of hazardous substances is concerned (see Figure 2).

This very clearly sets the frame for identifying target substances in this report.

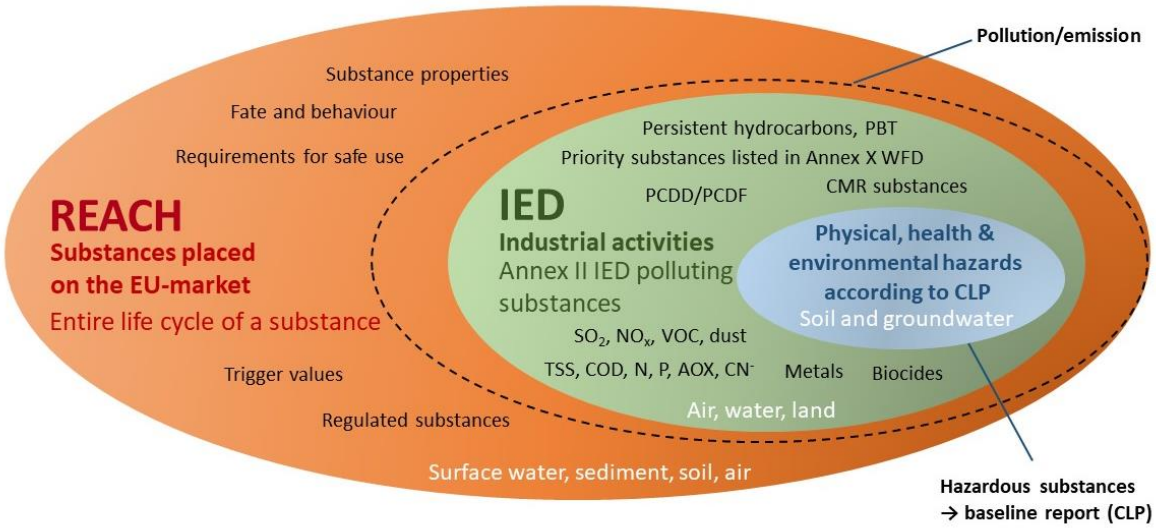

Figure 2: Scope of REACH and IED in comparison regarding substances, activities and compartments considered (Suhr and Aust, 2020).

This figure shows the overlap between REACH and IED. REACH comprises around 26.000 substances while the IED addresses nearly 40 substances. There are differences between the compartments addressed. REACH addresses the risk caused by a substance to surface water,

sediment, soil and air, while the IED addresses air, water and land, respectively soil and groundwater. REACH takes the full life cycle of a substance into account while the IED concentrates on industrial activities.

1.2 Wastewater treatment as central means for elimination of substances of concern

The process to produce articles and mixtures is in general complex and often various chemicals are used. The industrial use of chemicals implies an environmental release of chemicals from different sources in the production process (see Figure 3).

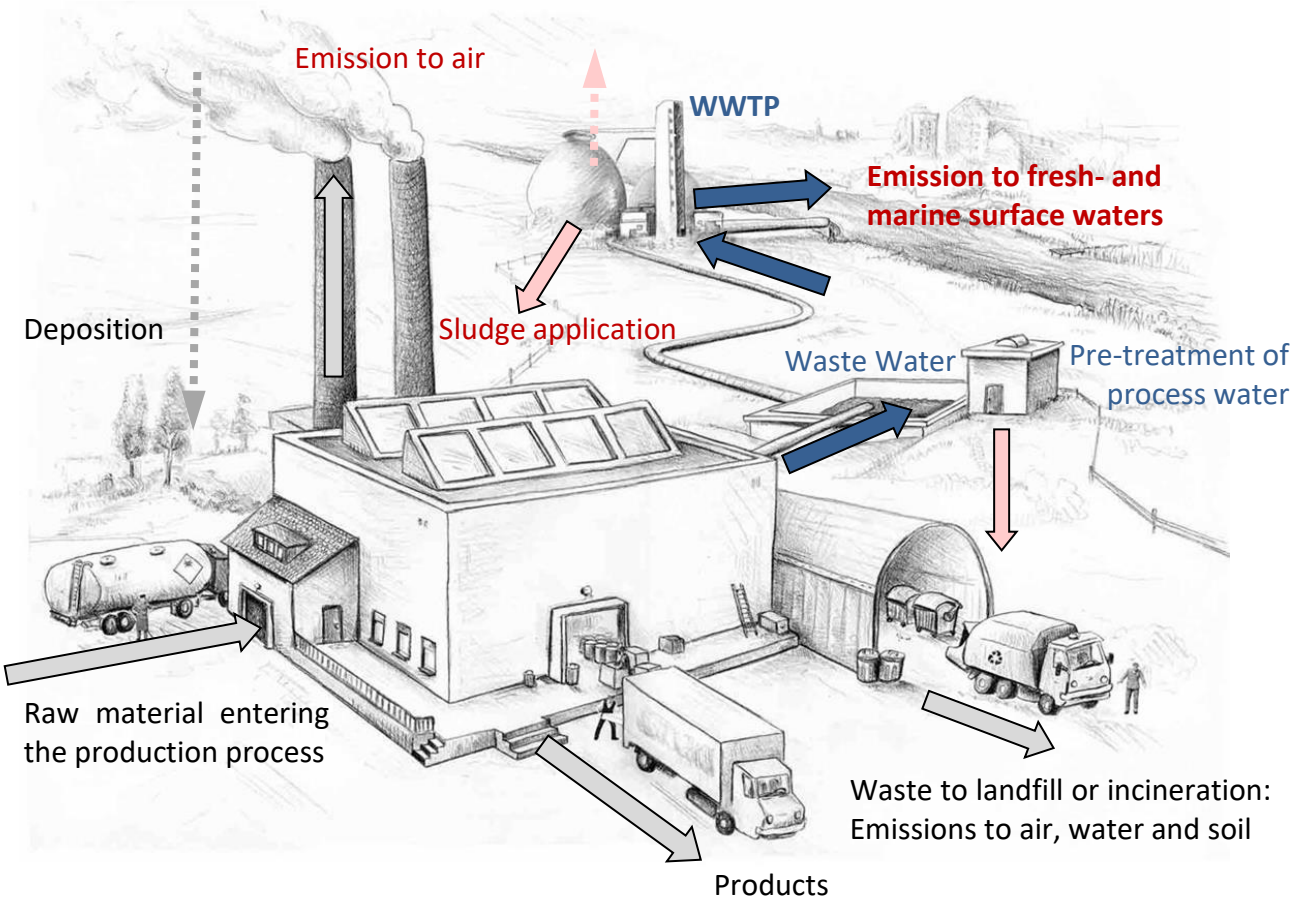

Figure 3: Possible releases from a production process

The red and blue arrows show the release paths considered in HAZBREF; blue arrows: substances entering the waste water; red arrows: possible emissions from the wastewater treatment process → subject for BAT (light red arrows: emission pathways not in the main focus in HAZBREF); grey arrows: possible emissions from different other sources in the production process

The amount of chemicals in use, the multiple ways how these substances are released into the environment and their fate and behaviour in the WWTP as well as in the environment have to be considered in environmental protection. This is in line with the spirit of the Industrial Emission Directive (2010/75/EU) to protect the environment as a whole.

In order to prevent environmental releases of industrial used chemicals, a detailed analysis of specific production processes and the fate of a substance through these processes has to be

performed. The outcome of this survey delivers information on possible environmental release paths and the quantity of substances released by a specific path. In the HAZBREF context the analysis is limited to those chemicals, which end up in wastewater. Beyond the direct discharge of substances with process waters into an industrial WWTP, it also has to be considered that substances may enter wastewater indirectly. For example, if substances are emitted to air in and then these exhaust gases are cleaned with liquid scrubbers. The polluted scrubber liquids also may be released into wastewater.

Every WWTP is designed for a certain cleaning capacity. This capacity is calculated on the expected load and quality of pollutants in the sewage and on the flow rate the WWTP is working. The effluent water has to fulfil certain release criteria. The intrinsic substance properties, as well as the equipment of the WWTP determine the potential of a considered substance to be released into the environment (Riffat, 2012; Bauhaus Universität Weimar, 2013). The better the equipment is matched to the substances entering the wastewater system, the better is the elimination rate from waste water. Due to its intrinsic properties, a substance can be distributed between the compartments air, effluent water, suspended matter and sludge. Therefore, depending on the composition of sewage as a sum of various substances with its unique properties, different measures of sewage treatment are required. Substances can be eliminated from the wastewater system e.g. by mechanical separation, by adsorption to particles, by biological degradation or by chemical treatment. The biological degradation in water as well as in sludge occurs aerobically (oxygen is needed) or anaerobically (under oxygen deprivation). Conventional wastewater treatment is very effective for removing solids from water. Therefore, suspended solids are often well manageable.

Because the specific substance properties affect the fate and behaviour in a WWTP and in the receiving environment, it is important to characterise the physical-chemical properties of the substance to be used. This information is needed to decide how the sewage containing the regarded substance has to be treated. The findings have to be matched with the features that are currently available in the WWTP. Further action is needed when using the chemical and/or in operating this WWTP to prevent environmental releases of the substances.

Besides the intrinsic substance properties, the amount of the substance entering the WWTP is crucial, too. Micro-organisms use substances as source for energy and as resource for life building blocks. However, at a certain concentration even readily biodegradable substances may act as a toxicant. At this point the biological elimination rate declines rapidly and substances could not be retained by the WWTP anymore and are released into the environment. If general treatment criteria in effluent water, like biological or chemical oxygen demand (BOD, COD), do not comply with the respective limit values, this could be an indicator for this situation.

Additionally, the possibility of a secondary release should be checked, too. For example, if a persistent substance or a persistent transformation product adsorbs to sludge, pay attention that the contaminated sludge is disposed appropriately or incinerated. Contaminated sludge has not to be applied e.g. to agricultural soils. Hence, in cases where the main fraction of relevant chemicals/substances are ending up in the sludge, it is important to address the handling of the sludge according to procedures outlined at e.g., regional-, national- and/or EU level, or elsewhere. In addition, if substances to a large extent end up in sludge, they should be taken into account already in the front loading process of relevant BREFs.

1.3 The context of WP 2 in the HAZBREF Project and target groups of the report

The previous Chapter 1.1 clearly described the basic challenge of HAZBREF and the work assignment for REACH stakeholders. Chapter 1.2 points to appropriate means for elimination of substances of concern via wastewater treatment. Chapter 1.4 briefly addresses the objectives of this report. Solution approaches in chronological order are described in annex 1. *Chapter 1.5 gives an overview on the final approach to identify relevant target substances for BREF review.*

This Chapter 1.3 shows how the work on the basic issues of HAZBREF is divided between the different WPs and how our findings are incorporated into the modification of the frontloading process which is essential for the report of HAZBREF Activity 3.2 (Suhr et al. draft). This forms the context for WP 2.

During the initial phase of the work underlying this report, it became obvious that the identification of target substances for BREF review has to start with a selection of registered substances in Europe[6] by focussing on their use in specific industrial sectors (i.e. textile finishing industry, surface treatment in the IED context, polymers and fertiliser additives – as representative sectors within HAZBREF), while also considering their intrinsic properties. Such hazard and environmental fate information is available in the ECHA database and requires sophisticated search strategies. The problem with this approach is, that searching in ECHA database usually results in a large number of substances[7], which for practical reasons has to be narrowed down with respect to their possible relevance for BREFs. This may be carried out by applying criteria related to industrial use of hazardous substances and their partition to the compartments air, water, products or waste (cf. HAZBREF Activity 2.2, Appelgren et al. 2019).

The purpose of work by Appelgren et al. (2019) was to obtain generic knowledge about the fate of a subset of industrial chemicals in typical wastewater treatment and feed information into the creation of a decision scheme for the identification of substances of concern for BAT candidates. Based on the results and conclusions for the presented methodology (SimpleTreat 4.0), substances, that are likely to be released to wastewater treatment effluents, may be identified in advance and thus trigger specific actions in industrial wastewater treatment plants or before that in modifying industrial processes.

The relationship of this report and the HAZBREF Activity 3.2 final draft report "Method to include information on hazardous and other substances of concern more systematically into BREFs" (Suhr et al. 2021 draft) is that this report identifies and quantifies the substance properties of concern, opens substance data sources and provides guidance for substance evaluation. The report demonstrates how these findings can be incorporated into a modified frontloading phase of the BREF revision. The aim is to promote the systematic use of the

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[6]) ECHA has created a mapping tool of all registered substances called the chemical universe in which each substance is assigned to a pool indicative of the regulatory actions already initiated or under consideration for that substance (News 4.12.2019: https://echa.europa.eu/fi/-/mapping-the-chemical-universe-list-of-substances-by-regulatory-action-published). It also identifies those substances for which the need for suitable regulatory actions still needs to be determined. https://echa.europa.eu/fi/universe-of-registered-substances .

[7]) Note that the prioritisation of substances is context dependent. The SVHC identification under REACH, the selection of priority hazardous substances under the WFD, SIN lists etc. justify a ban, phase-out or substitution (ultimately also a minimisation in the environment) with the intrinsic hazard potential of the substances, while the relevance for installation operators primarily results from the elimination of the substances, which, however, increases if the (eco-)toxicological potential increases.

existing substance data (mainly in the ECHA database) for a targeted development of BAT conclusions.

It is important to differentiate between the stakeholder groups: This report addresses both experts of the Sevilla process and operators of installations while the interactive scheme was developed mainly for the installation operators. HAZBREF WP 3 is addressed to the EIPPC-Bureau and the experts from the Technical Working Groups, while WP 4 addresses chemicals management at facility level. In principle, it would be desirable to identify target substances for BREFs and BAT conclusions based on real production processes in industrial installations, from which relevant chemicals are identified ("reality check"). However, reality checks conducted as case studies will hardly cover all processes and substances used in a respective branch and the results will only represent a part of the branch.

1.4 Objectives of Work Package 2 of HAZBREF

The overall aim of the HAZBREF Project is to improve the knowledge base of industrial emissions of chemicals of concern to be considered in BREF revision. This improvement is achieved by providing supporting information on substance properties, which will enable installation managers to characterise the substances used in the respective installation with regard to various concerns (cf. Chapter **Error! Reference source not found.**) and to choose appropriate risk reduction measures and abatement techniques.

It is the intention of this report to characterise substances with regard to the properties which determine their fate in wastewater treatment, i.e. adsorptivity / mobility, degradability, water solubility and volatility (cf. Chapter 2.3.1). In addition, substances with an ecotoxicological or human toxicological concern (cf. Chapter 2.3.2) should be flagged for additional risk reduction measures. This characterises the relevance of substances for BAT conclusions.

In addition, information on the substances for which regulations of different legal contexts (e.g. REACH and WFD) are already in place is provided in Chapter 3.3. These regulated substances and the (non-regulated) substances of concern (SoCs; Chapter 2) from the chemical universe complement each other and they should be considered duringthe BREF processes.

However, the attempt to *a priori* create sector-specific substance lists with the help of use descriptors from registration data from the ECHA database or hazardous substances lists showed to be difficult in the project (as an example the textile processing sector was analysed) as will be shown in Chapter 4.1. The use descriptor SU textile under REACH includes besides textiles in the narrow sense also leather and fur industry. Chemicals use in these three branches differ very much and the variety of processes in the textile, leather and fur industry is very large. Thus, combining these industries under one use descriptor certainly does not make sense and should be changed for the future. However, analysing ECHA database might be a useful starting point for other sectors. This could make it necessary to adapt the use descriptor system currently established under REACH. ECHA is working to make the database usable for such purposes. Therefore, the issue of identifying substances used in installations and/or industrial sectors with regard to their chemical structure moved more and more into the field of attention (cf. Chapter 4.2 and **Error! Reference source not found.**). It is the intention of this report to demonstrate that stakeholders can be supported to interpret the available data for these chemicals they use in many ways, in order to identify relevant substances of concern (cf. the central Chapter 5).

It is a specific objective of the HAZBREF project and this report to establish means to systematically and efficiently provide the crucial substance information to BREFs and ultimately to installation operators (cf. chapters 2.5 and 3.3). The registration dossier for chemicals required

under REACH comprises data such as the identity of manufacturer/importer, information on uses, classification and labelling, guidance on safe use, study summaries on substance properties and hazard properties, and an exposure assessment for identified uses (cf. Chapter 2.2). Data on hazard properties are publicly available to a larger extent than data on uses and exposure, as some of the latter data may be confidential business information. The publicly available REACH and CLP[8] data may be used as a starting point for a characterisation of a substance in the BREF review context.

However, the parameters of concern regarding fate, behaviour and toxicity do not have the same denominations and impacts in wastewater treatment, and can therefore not be compared or offset against each other, and further, from an environmental point of view, toxicity should not be given precedence over fate. Therefore, an 'interactive scheme' developed in HAZBREF WP 2 for interpreting substance data will provide assistance for the identification of target substances (cf. Chapter 5). Of course, the categorisation of concerns is based on the common trigger values (cf. Chapter 5.4).

While abatement techniques for release of substances to water focus on the wastewater treatment, it should be kept in mind that risk management for chemicals draws on preventive measures and is not limited to the end-of-the-pipe, i.e. the industrial WWTP. It may include process-integrated measures such as reduction of amounts of chemicals used in certain process steps, optimised application of substances thus preventing losses, or cleaning of reaction containers and pipes to reduce chemicals losses. Substitution of particularly critical substances is another measure at the source. All risk reduction measures may be part of the BAT conclusions. Nevertheless, risk reduction measures are based on the identification of concerns which result from substance properties.

It is important to keep in mind, that BAT apply only for chemicals used or emitted via process based at industrial installations. The whole field of consumer use and protection, releases during the post-industrial life-cycle, as well as end-of life waste issues might not be considered properly in BREFs for a specific branch. This drastically reduces the relevance of many substances for consideration in BREFs, even if they show a widespread occurrence in the environment that results from professional and consumer use. Nevertheless, substances released during consumer use, service-life or end-of-life treatment have once been applied at industrial sites during the manufacturing of products, e.g. in the case of textile products during the manufacture of textiles, and therefore should not be ignored.

For use in practice, this report includes chapters with assistance to support operators of industrial installations and experts in the Technical working Groups in the identification of relevant environmental concerns by the chemicals used, as well as how to handle information on relevant chemical properties, hazard criteria, technical function, and uses in order to prevent and reduce emissions. This assistance for stakeholders is placed at the end of each chapter (see chapters in italics). However, we refrained to prepare a stand-alone guidance manual, because a lot of background information, which should accompany the guidance, but may not be interesting for every stakeholder, should stay closely by.

[8]) Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006 (Text with EEA relevance), OJ L 353/1, lastly amended by Commission Regulation (EU) 2018/669 of 16 April 2018 amending, OJ L 115/1.

In order to ensure that the findings presented in this report will be useful also in the future when updated information on substances will be available at the ECHA database the procedures to identify the relevant chemicals or chemical groups are provided in form of an interactive scheme for decision-making (cf. Chapter **Error! Reference source not found.**). Updated information on relevant target substances used will also be made available by the industrial branches. The interactive scheme assists identification of substances or chemical groups with specific concerns that are relevant to be managed with care in an installation or should be included in the respective BREF. In addition, a guide that allows operators to identify substances already prioritised in EU legislation is provided in Chapter 3.3, with the purpose that hazardous substances with defined features can be more easily detected and assigned for substitution or for further action (prevention or reduction release). The overall guide and interactive scheme also support operators in the access and handling of the available substance related information, contained e.g. in the safety data sheets and the ECHA database of registered substances (cf. Chapter 4.1).

The objectives and intentions of this report may be summarised by the guiding questions identified during the course of the HAZBREF project (cf. presentation of WP 2 results during the Final Webinar):

- Is the substance used in an installation a relevant target substance for a BAT Conclusion?
- What concerns characterizes a substance as a relevant target substance?

- What can the Chemicals Regulation REACH contribute to the implementation of the Industrial Emissions Directive IED?
- What is the remit or scope of the IED with regard to parameters for evaluating the concern of a substance for environment?
- Which problem areas have we perceived in the relationship between REACH and IED with regard to understanding the respective procedures to identify substances of concern?
- How can knowledge and experiences in the respective IED sectors contribute to the identification of relevant target substances of concern?

- How can the REACH substance data and use information from the registration documents be made available to installation operators more efficiently?
- What data is needed to identify relevant target substances respectively to include substances into BREFs and by whom?
- What can the REACH contribute to the identification of relevant target substances for the IED respectively what data on substances are available?
- What information from regulatory processes under REACH is available?

- Where has HAZBREF delivered concrete building blocks for the bridge between REACH and IED?
- with regard to supporting installation operators
- with regard to the identification of BAT Candidates
- with regard to a better understanding among stakeholders

- Where is the need for action (1) by stakeholders of the IED; (2) by stakeholders of REACH?
- How can REACH processes benefit from the implementation of the IED?

1.5 OVERVIEW on the current approach to identify relevant target substances for BREF review

An overview on the final approach to identify relevant target substances for BREF review is presented in this chapter – this may be used as guidance or assistance for installation operators or other stakeholders.

In Figure 4, the comparison of the parameters of concern with trigger values works in two steps (cf. Chapter 5.4)

1. Step: the potential to be released, or conversely, the ability to be eliminated (in the WWTP) – which qualifies a substance as “target substance”, and
2. Step: in addition, the intrinsic potential toxicity of the substance – which may qualify a substance as “relevant target substance”.

All boxes in Figure 4 are explained in the following chapters.

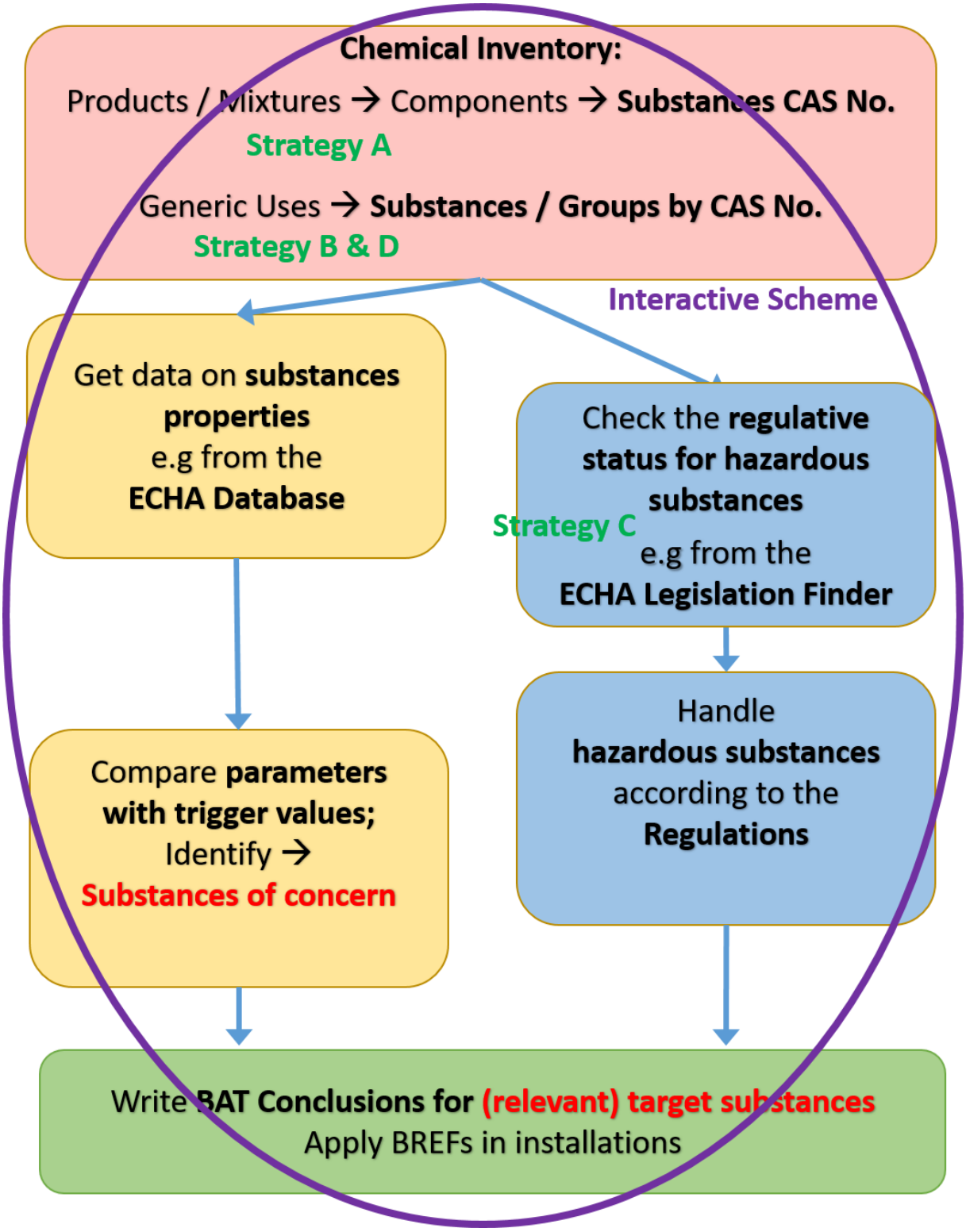

Figure 4: Overview of the current approach to identify (relevant) target substance and assignment of the strategies described in WP 2. For Strategies A-D refer to annex 1.

2 Substances of Concern

2.1 The two-step approach

The HAZBREF project initially refers to “hazardous” substances as those which are "released from industries through discharges to waters, emissions to air and wastes (and which) have a harmful effect on the Baltic Sea environment" (cf. Project Proposal 2017). This covers harmful effects to the environment, as well as to humans via the environment and obviously addresses toxic substances. However, only substances which are released to the environment are of interest. This means that the 2-step approach proposed in WP 2 is already indicated in the project description. The scope of the IED ends at the point of discharge from the installation and BAT refer to the abatement techniques in the industrial WWTP or generally the industrial waste stream. HAZBREF focuses on the waste water stream. Thus, the approaches, especially the interactive scheme (see Chapter **Error! Reference source not found.**) to identify substances of concern focuses on hazards for the aquatic system and man via the aquatic environment.

“Hazardous” in HAZBREF has two aspects (Two-step approach):
1. the potential to be released, or conversely, the ability to be eliminated (in the WWTP) – which qualifies a substance as “target substance”, and
2. in addition, the intrinsic potential (eco)toxicity of the substance – which may qualify a substance as “relevant target substance”.

The term "hazardous" generally refers to eco-toxicological or human toxicological properties of a substance – something like "poisonous". Many listings, such as the WFD list of priority substances refer to these toxicological properties. It should be clear at this point that the term "hazardous substance" is used differently in different areas of law. HAZBREF cannot and will not attempt to create a harmonised definition. Rather, stakeholders from different sectors will be supported in using the substance properties to arrive at an assessment of the hazard potential of chemicals. At the different stages of the processing of chemicals, this results in a different need for action for substances of concern.

Under REACH, substances that may have serious effects on human health and the environment can be identified as substances of very high concern (SVHCs). These are primarily substances which are carcinogenic, mutagenic or toxic to reproduction (CMR substances) as well as substances with persistent and bio-accumulative characteristics (PBT or vPvB substances)[9] Other substances of equivalent concern include, for example, endocrine disrupting chemicals[10]. CMR clearly refers to toxic properties and is and a minimal incorporated amount of the substance may already cause an effect. On the other hand, persistence and bioaccumulation are substance-properties which relate to the fate and behaviour of a substance in the environment

[9]) **C**arcinogenicty, **M**utagenicity, **R**eproductive Toxicity; **P**ersistent, **B**ioaccumulative and **T**oxic, **v**ery **P**ersistent and **v**ery **B**ioaccumulative.

[10]) It should be kept in mind that, according to REACH, there are many more substances that may be considered as hazardous in addition to SVHCs. Not at least, the criteria outlined in the CLP-Regulation should be applied in an appropriate way.

or inside of biota – they are non-toxic properties, but may result in a toxic "body burden". Hazardous with respect to PBT and vPvB substances means that these substances can persist in the environment for a long time and be widely dispersed, causing long-term harm to humans and organisms. Their release should therefore be avoided from the outset.

In consequence, this report addresses substance properties for fate and behaviour (in the WWTP), as well as toxic properties (independently from waste water treatment) in the identification of relevant target substances for consideration in BREFs and for abatement measures.

Starting point for the assessment of chemical hazards are several EU regulations, directives and purpose-specific lists (e.g. SIN-List, NORMAN list), each employing their own set of criteria of concern and combinations thereof, such as the PBT/vPvB-strategy for 'substances of very high concern' (SVHC) under REACH. The identification of the hazard criteria (to identify substances as relevant target substances) in HAZBREF (more details in chapters 2.3.1 and 2.3.2) was done by utilising already existing information, not generating new data, by combining the settings under REACH, the Water Framework Directive (WFD), HELCOM or the Stockholm POPs convention, among others.

Many regulatory frameworks or prioritisation schemes apply a 2nd ranking step for specific purposes, often with regard to uses and occurrence in the environment (e.g. water or biota). The substance finding concept of HAZBREF also applies a twofold identification scheme on a similar data basis. However, HAZBREF is not only looking out for the 'most hazardous' substances, which often conjoin several hazard features and which are often already regulated elsewhere, but also wants to identify less conspicuous substances with a hazardous profile, but which are (or can be) emitted from industrial installations and cause a risk in the environment.

The comparison of regulatory frameworks shows that hazard parameters (and the respective trigger values) do not differ so much between the mentioned regulations. It also seems that there is an interplay between substance lists in various regulatory frameworks, even though they are pursuing different objectives. There is an initial focus on P, B and T for the environment and CMR for human health; and, since a while, endocrine disruption (ED) for environment and human health as well as mobility are gaining attention.

In this report the term "substance of concern" is used for substances that need to be examined more closely. This term is preferred to the term "hazardous substance" for the following reasons:

- The term "hazardous" is used differently in different legislations.". ". The parameters, criteria and test requirements for identification as "hazardous" differ between legislations.
- In addition, "hazardous" is used on different levels. "Hazardous" are substances that have been classified according to CLP. There is a need for regulation for endocrine disrupting substances and substances that in addition to a low long-term no-observed effect concentration (NOEC <0.01 mg/L) for aquatic species have the property of being persistent, bioaccumulative and mobile substance. So far there are no classification criteria available in the CLP regulation for substances with these properties. However, these substances should also be labelled as "hazardous".
- Already identified SVHC according to REACH are labelled for exhibiting "hazardous" properties., The regulatory process of SVHC identification is based on a combination of criteria (REACH Article 57), but it utilizes different criteria for T than the ones

employed in the CLP regulation for the classification and labelling as aquatic toxic. And there are for sure more examples when analysing the different legislations. From this, the ideal conception would be to have an uniform designation for substances that need to be considered in more detail in the various legislations without causing confusion with the choice of the term "hazardous".

A vision for the future is that the identification of substances as "substance of concern" is based on a common set of parameters (e. g. persistence, toxicity, mobility), criteria (e.g. degradability, effect on organisms, K_{oc}) and (OECD) tests regardless of the respective regulation. This is in line with the concept of the EU Commission for the Chemical Sustainable Strategy (here: "one substance, one assessment"). The various legislations then derive their respective need for action based on the identification of "substance of concern". This would ideally avoid misunderstandings between the legislations, the enforcement authorities and the companies / users concerned, as well as loopholes and double regulations.

2.2 Chemicals inventory as prerequisite for the two-step approach

The considerations on the industrial use of a chemical is a relevant starting point to identify substance with a potential to be released. The REACH registration system provides use information on single substances (identified by a CAS or EC number).

This is first of all the use descriptor system which sets out principles for describing the uses of substances. It consists of the following descriptors: Life cycle stage (LCS), Sector of Use (SU), Product Category (PC), Process Category (PROC), Environmental Release Categories (ERC), Article Category (AC) and Technical Function (TF) (see also Chapter 4.1). "In order to support full understanding of the scope of a use, use descriptors alone are not sufficient. Tools like IUCLID and use maps therefore include free text fields for the name of the use and each contributing activity as well as for more specific information on the use process. This more specific information can also be standardised via agreements in the supply chains. The use maps can be used as a vehicle to reach such agreements." (ECHA, 2015: Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.12: Use description).

More specific information was developed by several branch associations with the derivation of special environmental release category (SPERC). Within SPERCs and also within ERCs, generic amounts used are defined and conditions for safe use of the substance are derived. Registrants according to REACH are obliged to derive exposure scenarios for all life cycles stages in which a substance is used for all branches the substance is used. Thus, exposure scenarios are a valuable source of information on uses. The exposure assessment takes into account the substance properties described according to chapters 2.3.1 and 2.3.2.

In contrast, industrial users of chemicals are often only informed about chemical products as a mixture of several substances and the product names for which the composition information in the safety data sheets at best contains the actual active substance or SVHC and labelled hazardous substances according to CLP that are subject to notification. Therefore, the clear identification of the individual components of a chemical product (or as a group of similar substances) is the most important prerequisite for the inclusion of chemicals in the BREFs. Only if plant operators or sector associations know which substances are used in their processes, i.e. chemical inventories exist, it is easy to identify the relevant target substances for inclusion in BREFs.

This information gap exists even though industrial users of chemicals according to REACH must ensure the safe use of a substance. The manufacturer or importer of a chemical sets out the conditions for safe use in their registration of the substance according to REACH. The conditions for safe use are usually made available to the industrial user with the safety data sheet. However, this information can be lost in the supply chain when creating safety data sheets for mixtures.

2.3 Parameters of concern

It is one of the aims of HAZBREF to characterise substances with regard to their properties, which determine their fate in wastewater treatment, i.e. biodegradability, adsorptivity / mobility, water solubility and volatility. The decisive question is whether a substance is eliminated from the wastewater flow by the wastewater treatment plant processes, i.e. whether it is removed or retained and not released from the wastewater treatment plant into the receiving water body. The most important elimination processes are first of all biodegradation (mineralisation) and adsorption to sewage sludge, and secondly abiotic degradation, precipitation and volatilisation (stripping) as well as other end-of-pipe measures. Information regarding fate and behaviour of substances in WWTP can be obtained according to established and commonly used methods as outlined in the REACH Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment (ECHA, 2016). The fate of substances in WWTP can be assessed in the SimpleTreat 4.0 model (cf. HAZBREF Activity 2.2 report, Appelgren et al. 2019).

In addition, substances with an eco-toxicological or human toxicological concern should be flagged by installation operators / branch association for special attention and / or during BREF reviews for additional risk reduction measures based on BAT. These properties underline the relevance of substances for BAT conclusions.

Due to the resources available, the release of substances via air, sludge (e.g. spreading of sewage sludge) or in waste was not considered in this project. If necessary, additional parameters must be considered for this purpose as part of a further development of this approach to identify relevant target substances. Furthermore, the dissemination of pollutants during use and service-life of products and a resulting release into the environment beyond the industrial processing steps – application by professional user (e.g. small-scale business, craftsmen) or consumers - is not a subject of the IED and was not considered in the identification of relevant target substances. However, an inclusion of these life cycle steps in the approach to identify "substances of concern" would be desirable from the perspective of sustainability.

2.3.1 Parameters regarding the “potential to be released”

Under REACH, the transfer from the production process to the waste water stream is referred to as "potential to be released". In this report “potential to be released” is also used to describe the release of substances from the waste water treatment plant into the environment (i.e. the receiving water body).

The substance properties that determine the elimination of the substance from the wastewater stream in the treatment plant and thus the potential to be released as defined in this report, are persistence (determined by biodegradability), and mobility (determined by adsorptivity and the partition coefficient). Water solubility and volatility are also important parameters and described in this chapter although they are not used in the two-step approach and the interactive

scheme for the identification of (relevant) target substances. Behind this is the consideration of how these parameters can be employed in the wastewater treatment plant. For an explanation of how sewage treatment plants work, however, reference must be made to the relevant literature (Riffat, 2012; Bauhaus Universität Weimar, 2013).

Table 1 shows how to determine the parameters mentioned above. Chapter 2.4 explains were to find the necessary data. The decision on the concern then follows the interactive scheme (see Chapter **Error! Reference source not found.**). Further explanation to some of the parameters is provided after Table 1.

Table 1: Parameters of concern (fate and behaviour) for the identification of target substances for BREFs

Parameter of concern **Mobility**	Mobility is the property of a substance to remain in the water phase and be further relocated. Mobile substances tend to pass through sewage treatment plants into the environment, which constitutes the concern here. The reverse of mobility is adsorptivity, which means that substances in the wastewater treatment plant are bound to suspended solids and sludge and thus eliminated from the wastewater stream. However, substances that are already bound to suspended matter can still be remobilised together with it. Generally, adsorption in WWT is not limited by the availability of adsorbing surfaces.			
Substance properties for the determination of the parameter of concern				
Denomination	*Unit*	*Guidelines for measurement or determination*	*Trigger values for a hazard identification*	*Remarks*
Adsorptivity log K_{oc}	L/kg or dimensionless	OECD 106 or OECD 121 (HPLC-method) or calculation from log K_{ow}	log $K_{oc} \leq 4$; indicative trigger for mobile substances[a]	Determination of the organic carbon/water partition coefficient may be difficult to measure or to be calculated for ionisable organic chemicals or substances with surface active properties, like for example tenside.
Octanol- water distribution ratio log D_{ow}	dimensionless	No guideline; calculation from log K_{ow} and pK_a	log $D_{ow} \leq 4$; indicative trigger for mobility	The octanol-water distribution ratio (D_{ow}) is a unit of K_{ow} that accounts for the pH dependency of an ionisable organic chemical, and is a unit of the distribution of dissociated and non-dissociated species in octanol and water as a function of pH [b]
Water solubility S_{water} or WS	mg/L	OECD 105	no trigger value for mobility	Medium to high water solubility is a surrogate for low adsorptivity. However, not all water-soluble substances are necessarily mobile.

[a] UBA Report (127/2019) Protecting the sources of our drinking water: The criteria for identifying persistent, mobile and toxic (PMT) substances and very persistent and very mobile (vPvM) substances under EU Regulation REACH (EC) No 1907/2006 (https://www.umweltbundesamt.de/sites/default/files/medien/1410/publikationen/2019-11-29_texte_127-2019_protecting-sources-drinking-water-pmt.pdf)

[b]) ECETOC Technical Report 123 (2014) – Environmental risk assessment of ionisable compounds (https://www.ecetoc.org/publication/tr-123-environmental-risk-assessment-of-ionisable-compounds/), Section "Partition coefficient (KOW) and distribution ratio (DOW)".

Parameter of concern **Volatility**	The solubility of gases depends on temperature and on pressure. To characterise the potential of a substance to be released into air, the vapour pressure as well as the boiling point have to be taken into account. Elimination to air may supported by turbulence.			
Substance properties for the determination of the parameter of concern				
Denomination	*Unit*	*Guidelines for measurement or determination*	*Trigger values for a hazard identification*	*Remarks*
Vapour pressure (at 20 °C)	kPa	OECD 104	highly volatile > 25 kPa medium volatility < 0.5 – 25 kPa low volatility > 0.01 – 0.5 kPa non-volatile < 0.01 kPa	
Boiling point (at 1 bar)	°C	OECD 103	> 150 °C → tendency for volatility is expected to be low < 50 °C → tendency for volatility is expected to be high	
Parameter of concern **Persistence**	Degradability is a key parameter in finding target substances. Many substances can be degraded by microbial activity and this may be enhanced in WWT by adaptation. However, removal of substances during waste water treatment processes cannot be applied for the assessment of persistency in the environment. But it can be utilised to refine the assessment of the emission load into the environment. The less a substance is degradable, the higher is the possibility that the substance could be released from a WWTP and persist in the environment. Biodegradation is a complex process and may not be described like a single physico-chemical parameter.			
Substance properties for the determination of the parameter of concern				
Denomination	*Unit (depending on test system)*	*Guidelines for measurement or determination*	*Trigger values for a hazard identification*	*Remarks*
Ready biodegradability	Mineralisation of the test item within the pre-defined test	OECD 301 a-f [c] OECD 310	A substance is **readily biodegradable**, if	According to the test result, ready bio-degradability is a yes/no decision and more a classification than a statement about the degradation behaviour. If the test criteria are

[c]) Tests that use dissolved organic carbon (DOC) as an endpoint are not listed here because their interpretation is difficult. DOC tests could erroneously exonerate adsorptive and volatile substances.

	criteria (pass levels and time windows)		≥ 60 % O_2 depletion or CO_2 development (pass level) [d] is achieved and the 10-days-window is fulfilled	narrowly missed, it is not possible to conclude on a "possible" or "inherent" degradability.
Inherent biodegradability	Mineralisation of the test item within the pre-defined test criteria	OECD 302 B and C	≥ 70 % O_2 or DOC depletion (pass level) and specific criteria are fulfilled[e]	This series of screening tests creates favourable conditions for degradation in sewage treatment plants, just as they can be achieved in reality.
Degradation half-life dt_{50}	Disappearance of (50 % of) the test item in days	OECD 309 [f]	$dt_{50} \geq 40$ d[g]	Under REACH a substance also fulfils the persistency criteria, in case one of the corresponding trigger values (degradation half-lives) for the water/sediment or soil compartment was exceeded.
Abiotic degradability	Hydrolytic half-life dt_{50}	OECD 111	longest half-life t½ determined within the pH range 4-9 < 16 days [h]	Abiotic degradation usually occurs by hydrolysis and does not lead to mineralisation.

[d]) The 60 % pass level refers to the 'theoretical' oxygen demand (ThO_2) or 'theoretical' CO_2 ($ThCO_2$) evolution for a complete mineralisation of the test item in 28 days. For the theoretical DOC depletion, the pass level is 70 %, but DOC tests are not recommended due to erroneousness results for adsorptive and volatile substances.

[e]) OECD 302 B Zahn-Wellens/EMPA Test: pass level must be reached within 7 days, the log phase should be no longer than 3 days, and the percentage removal in the test before degradation occurs should be below 15%. OECD 302 C MITI (II) Test: pass level must be reached within 14 days, and the log phase should be no longer than 3 days.

[f]) In addition to OECD 309 there are further OECD guidelines on simulation test for other compartments (OECD 307 and OECD 308).

[g]) Cf. Table R.11-1, page 17 (PBT criteria), in the ECHA Guidance on Information Requirements and Chemical Safety Assessment, Chapter R.11: PBT/vPvB assessment, Version 3.0, June 2017.

[h]) Guidance on the application of the CLP Criteria, Guidance to Regulation (EC) No 1272/2008 on classification, labelling and packaging (CLP) of substances and mixtures, Version 5.0, July 2017. This hydrolysis half-life concerns classification purposes only. It also needs to be demonstrated that the hydrolysis products formed do not fulfil the criteria for classification as hazardous for the aquatic environment.

Parameter of concern **Bioaccumulation**	If a substance can be accumulated in a living organism, this is called bioaccumulation. Although this process does not take place in the sewage treatment plant, bioaccumulation is *per se* a hazard indicator from the PBT concept, so that it should in principle be avoided that bioaccumulating substances are released into the environment.			
Substance properties for the determination of the parameter of concern				
Denomination	*Unit*	*Guidelines for measurement or determination*	*Trigger values for a hazard identification*	*Remarks*
Bioconcentration factor BCF	L/kg	OECD 305 I aquatic exposure OECD 305 III dietary exposure	BCF > 2000 BMF and $k_{elimination}$ [i]	Choose this version if the substance is poorly water soluble
Octanol/water partition coefficient log K_{ow}	L/kg	OECD 107 Shake Flask method OECD 117 HPLC method OECD 123 slow stirring method	log $K_{ow} \geq 4.5$	adequate for substances in the range log K_{OW} between -2 and 4; log K_{OW} between 0 and 6; log K_{OW} up to 8.2; choose this guideline if the substance is poorly water soluble

[i]) There is as yet no generally recognised trigger value for biomagnification (accumulation via food intake). Furthermore, such studies are still rare.

Parameter of concern **Human toxicity**	**Related to Chapter 2.3.2** This table does not replace the procedure of classification und Regulation (EC) No 1272/2008. Rather, a relationship to the T-criterion according to REACH Annex XIII should be established (cf. chapter 3.2.3, for further advice please see ECHA Guidance R.11).			
Denomination	*Unit (depending on test system)*	*Guidelines for measurement or determination*	*Decision levels for a hazard identification*	*Remarks*
Carcinogenic (Cat 1A or 1B or 2)		e.g. OECD TG 451, 453	Carcinogenic cat. 1A or 1B or 2	source: CLP Annex VI
Germ cell mutagenic (Cat 1A or 1B or 2)		e.g. OECD TG 483, 478, 488	Germ cell mutagenic cat. 1A or 1B or 2	source: CLP Annex VI
Toxic for reproduction (Cat 1A, 1B, or 2)		e.g. OECD TG 443, 416, 414	Toxic for reproduction cat. 1A or 1B or 2	source: CLP Annex VI
Chronic toxicity (STOT RE Cat 1 or 2)		e.g. OECD TG 452, 453	STOT RE cat 1 or 2	source: CLP Annex VI
Parameter of concern **Ecotoxicity**	The mentioned guidelines are only examples as there are many more possible test guidelines from which the effect concentrations can be derived (see ECHA Guidance R.7b chapter R.7.8.4 and Appendix R.7.8-2).			
Denomination	*Unit (depending on test system)*	*Guidelines for measurement or determination*	*Trigger values for a hazard identification*	*Remarks*
Short-term aquatic toxicity	mg/L	e.g. OECD TG 203, 236, 202, 201, 221	$EC/LC_{50} < 0.1$ mg/L $EC/LC_{50} \leq 1$ mg/L	screening T acc. to REACH Annex XIII; (for further advice please see ECHA Guidance R.11) Aquatic acute 1 (H400) (CLP Regulation)
Long-term aquatic toxicity	mg/L	e.g. OECD TG 211, 210, 234, 201	$NOEC/EC_{10} < 0.01$ mg/L	T-criterion acc. to REACH Annex XIII; (for further advice please see ECHA Guidance R.11)

			NOEC/EC_{10} ≤ 0.1 mg/L	Aquatic chronic 1 (H410) (substance not readily biodegrad.) (CLP regulation) OR Aquatic chronic 2 (H411) (substance readily biodegrad.) (CLP Regulation)

(For OECD Test Guidelines, please refer to the OECD website: https://www.oecd.org/chemicalsafety/testing/oecdguidelinesforthetestingofchemicals.htm)

Mobility

Mobility of chemicals in water has been recently identified as emerging concern next to the classical PBT-criteria (Neumann and Schliebner, 2019). Parameters and criteria for mobility are described in Table 1. All substances classified as PMT are water soluble, but not all water-soluble substances are mobile. Besides that, distribution of substance can also be the result of adsorption to suspended matter, which then carries the substances out of the WWTP into water streams.

Mobile substances are difficult to retain in wastewater treatment plants (e.g. not even by activated carbon), so they should be the focus of BAT. Only reverse osmosis has been shown to be effective in binding mobile substances – a very costly process that can only be used under specific circumstances.

Water solubility

The water solubility of a substance is a supportive parameter for the assessment of wastewater treatment. Water solubility must be distinguished from water miscibility, which is dependent on molecular loadings. Further, water solubility can be pH-dependent, in particular for ionisable organic compounds. The water solubility of the dissociated compound can be orders of magnitude higher than for the neutral species.

Elimination from water by adsorption or precipitation alone is not sufficient as decision parameters for the potential to be released. At this point, however, no further elaboration takes place, as the assumptions made in the interactive scheme are sufficient for the purpose pursued here of identifying relevant target substances, which require a closer look at safe use.

Hydrolysis

The hydrolysis of the test item, which can be abiotic or enzymatic in the test vessel, does not affect the endpoints O_2 demand, CO_2 evolution or DOC depletion. For some molecules, however, it can be nicely shown that this so-called primary degradation subsequently leads to mineralisation of one transformation product, while the other remains completely persistent. In such a case, the original substance is also considered to be persistent. Another example for persistence after primary degradation is for instance molecules with perfluorinated side chains, like 6:2 fluorotelomer alcohol which is biodegraded to persistent and mobile perfluorohexanoic acid.

Ready biodegradability

The tests for ready biodegradability (OECD 301a-f and OECD 310) are a screening tool for the fate of a substance in surface water. Further, this screening uses sum parameters and take into account a fixed period of time (28 days), which does not have to correspond to the time spent in the treatment plant. These tests are not suitable to reproduce or simulate biodegradation in reality. Due to the OECD test design, the significance of these screening tests should therefore not be overestimated. In any case, it must be checked for each test substance whether the appropriate screening test has been used.

The 60 % pass level refers to the ‘theoretical’ oxygen demand (ThO_2) or ‘theoretical’ CO_2 ($ThCO_2$) evolution for a complete mineralisation of the test item in 28 days. For the theoretical

DOC depletion (dissolved organic carbon), the pass level is 70 %, but DOC tests are not recommended due to erroneousness results for adsorptive and/or volatile substances. The 10-days-window describes the degradation kinetic and is fulfilled if the pass level is reached within 10 days. The 10-days-window starts as soon as 10 % of the substance is degraded.

With regard to the identification of substances of concern, persistence is of course important. However, a basic condition of the tests for ready biodegradability is that the inoculum (i.e. bacteria taken mostly from municipal sewage treatment plants) is not adapted to the test items. Conversely, this means that installation operators can adapt their industrial wastewater treatment plants to the chemicals used in the specific plant, or can try to do so. This is an example of BAT where a theoretical concern (i.e. persistence) can be mitigated by adapted measures to ensure safe handling of chemicals.

Inherent biodegradability

The tests for inherent biodegradability (OECD 302 series) create favourable conditions for biodegradation in the test. While this is in line with the development of BAT, inherent biodegradability is not applicable to degradation in surface waters where waste water from wastewater treatment plants enters after treatment. In such cases, the provisions of REACH and the WFD must be respected.

Water/ sediment system, degradation half-life

Tests to simulate the degradation behaviour in the water/sediment system are described in OECD Guidelines 308 and 309; they allow the derivation of a degradation half-life (dt_{50}). However, simulation tests are costly and studies are especially required and provided for plant protection products, biocides and HPVC.

Monitoring in effluent water

Finally, an indication of an alternative, but very direct method for identifying target substances is given. The HAZBREF project proposes to improve the inventory of chemicals used in an installation. Once the chemicals to be expected in the waste water are known, it will be possible to monitor the wastewater flow using targeted analytical methods. Substances that appear in this continuous monitoring are then to be regarded as target substances.

This monitoring follows on from current considerations that trace substances may also be relevant to water protection. By definition, trace substances are found in low concentrations in water bodies, usually below acute effect thresholds. However, their repeated occurrence in monitoring gives cause for concern and measures should be taken to reduce the release of these trace substances at source. This is in line with the objectives of the IED.

2.3.2 Parameters regarding the “potential for eco- and human toxicity”

Substances with an ecotoxicological or human toxicological concern should be flagged for safe handling at installation level and during BREF reviews for additional risk reduction measures based on BAT. These properties determine the relevance of substances for BAT conclusions.

The basis for the definition and transfer of information on the hazardousness of chemicals is the Globally Harmonized System (GHS). It is a globally uniform system for the classification of chemicals and mixtures and their labelling on packaging and in safety data sheets. Therefore, a globally valid classification with H-phrases (hazard phrases) and pictograms has been established. The CLP Regulation (Classification, Labelling and Packaging; (EC) No. 1272/2008) regulates the classification and labelling of substances and mixtures on the basis of GHS in the EU.

An obligation of self-classification according to CLP exists for chemicals since 2010 and for mixtures since 2015. The classification and labelling of chemicals are intended to make handling safer for humans and the environment in all areas (production, transport and use). In addition to the information on hazards within the supply chain, measures for occupational safety, as well as consumer and/or environmental protection are derived on the basis of the hazard classes (e.g. "acute toxicity" or "hazardous to the aquatic environment"). Furthermore, it can be the reason for further risk management measures under the REACH regulation. Many regulations under REACH are linked to specific hazard classifications as well as the unacceptable risks identified.

The relevant endpoints and trigger values in the context of HAZBREF are listed in Table 1 and should be considered by the installation operator following the interactive scheme to determine whether the substances released via the water pathway represent a "substance of concern". The data on (eco-)toxicity for the substance listed in the chemicals inventory of the facility can be taken from the SDS and/or the database entries of ECHA (cf. Chapter 2.4).

Of the many different substance properties used to determine human health concern, carcinogenicity, mutagenicity and reproductive toxicity are the most serious and are listed in Table 1. The respective hazard categories (carcinogenic (Cat. 1A or 1B or 2), germ cell mutagenic (Cat. 1A or 1B or), toxic for reproduction (Cat. 1A, 1B or 2) and chronic toxicity (STOT RE Cat. 1 or 2) and the classification criteria are listed in annex I to the CLP Regulation[20]. This annex also sets out their differentiations and contains additional provisions on how the criteria can be met. It must be noted here that according to REACH Annex XIII, 1.1.3. toxicity (b), for the identification of PBT or vPvB substances, the criteria for carcinogenic and germ cell mutagenic do not include Cat. 2. In this respect, there is a deviation from the CLP Regulation, Annex VI.

The relevant ecotoxicological endpoints, more precisely those ‘hazardous to water’, which are to be considered by the installation operator following the interactive scheme are short-term and long-term aquatic toxicity. In addition to Table 1, a few more trigger values for ecotoxicological hazard identification are given here.

Following the definition in the CLP regulation (annex I, Part 4) ‘acute aquatic toxicity’ means the intrinsic property of a substance to be harmful to an aquatic organism in a short-term aquatic exposure to that substance. ‘Chronic aquatic toxicity’ means the intrinsic property of a substance to cause adverse effects to aquatic organisms during aquatic exposures which are determined in relation to the life-cycle of the organism.

The basic elements used for classification for aquatic environmental hazards are:

[20]) Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006, https://eur-lex.europa.eu/eli/reg/2008/1272/2020-11-14

- short-term (acute) aquatic toxicity,
- long-term (chronic) aquatic toxicity,
- potential for or actual bioaccumulation, and
- degradation (biotic or abiotic) for organic chemicals.

The relevant trigger values for the aquatic environment in terms of classification and labeling under CLP are as follows (with reference to hazard phrases):

For the acute environmental classification, the data from acute tests are used (EC/LC_{50} values) and are shown in Table 2:

Table 2: Criteria for classification and labelling acute toxicity for environment

Aquatic acute 1 (H400)	$EC/LC_{50} \leq 1$ mg/L

For the chronic environmental classification, the results from long-term studies (EC_{10}/NOEC values) are shown in Table 3.

Table 3: Criteria for classification and labelling chronic toxicity for environment, substances readily biodegradable

Aquatic chronic 1 (H410) (substance not readily biodegradable)	$NOEC/EC_{10} \leq 0.1$ mg/L
Aquatic chronic 2 (H411) (substance not readily biodegradable)	$0.1 \text{ mg/L} < NOEC/EC_{10} \leq 1$ mg/L
Aquatic chronic 1 (H410) (substance readily biodegradable)	$NOEC/EC_{10} \leq 0.01$ mg/L
Aquatic chronic 2 (H411) (substance readily biodegradable)	$0.01 \text{ mg/L} < NOEC/EC_{10} \leq 0.1$ mg/L
Aquatic chronic 3 (H412) (substance readily biodegradable)	$0.1 \text{ mg/L} < NOEC/EC_{10} \leq 1$ mg/L

If long-term data are not available for all 3 trophic levels (algae, aquatic invertebrates, fish), then the acute data are used in substitute.

Substance not readily biodegradable and/or BCF $\geq$ 500 (if not available: log $K_{ow} \geq 4$) is determined with the criteria shown in Table 4.

Table 4: Criteria for classification and labelling chronic toxicity for environment, substances not readily biodegradable

Aquatic Chronic 1 (H410)	$EC/LC_{50} \leq 1$ mg/L
Aquatic Chronic 2 (H411)	$1 \text{ mg/L} < EC/LC_{50} \leq 10$ mg/L
Aquatic Chronic 3 (H412)	$10 \text{ mg/L} < EC/LC_{50} \leq 100$ mg/L
Aquatic Chronic 4 (H413)	safety net, e.g. substance poorly water soluble without effects in the

	acute toxicity tests, plus not readily biodegradable and/or BCF ≥ 500 (if not available: log K_{ow} ≥ 4) without a complete chronic data set.

The classification is then made in the "strictest" category (in the case of a mixed acute and chronic data set).

If emissions of substances from installations via the water pathway into the environment are not completely excluded and the substances are classified as aquatic acute (H400) or aquatic chronic toxic (H410), they are relevant target substances and require on-site risk management measures. Consequently, they are a matter of verification of the safe use conditions at installation level or of BAT conclusions in the context of the BREF revision. The focus is not on the absolute amount of a substance of concern possibly discharged from the plant (this might be subject to approval), but whether this substance requires special attention in the chemical management and the approval procedure of a plant (i.e. permitting of discharges).

In case of a PBT assessment a screening of the short-term aquatic toxicity in accordance with Section 9.1 of annex VII to REACH and Section 9.1.13 of annex VIII is the first step. But the trigger values are different to that under CLP regulation for classification and labelling (EC/LC_{50} < 0.1 mg/L). Data on the acute aquatic toxicity are only used as an indication that the substance may fulfil the T-criterion. Acute data for aquatic toxicity cannot be used for concluding definitively “not T” within the PBT assessment. If long-term or chronic aquatic toxicity data are available, a definitive assessment can be made. The regulation states that chronic aquatic toxicity testing should be firstly carried out on non-vertebrate species, unless there are indications that fish is the most sensitive group. If NOEC or EC_{10} are found to be < 0.01 mg/L, then the PBT criterion is confirmed. If the NOEC or EC_{10} values are ≥ 0.01 mg/L, then the substance is considered as ‘not T’, and the PBT assessment is stopped.

2.4 Information sources for substance data

There are two main sources for substance information for down-stream users: The ECHA database of registered substances and the Safety Data Sheets (SDS). The usability of these data sources is described in this chapter.

In addition, there are also publicly accessible databases containing relevant information for the operator (these can be consulted, for example, either to search for data that is not otherwise available or to check data supplied by upstream bodies that appear inconsistent or implausible). Other sources for gathering information are information systems like GESTES, the OECD eChem Portal, TOXNET and IPCS INCHEM[21].

2.4.1 ECHA’s registered substances data base and the CLP inventory

Within the European Economic Area, a substance can only be placed on the market if it has been registered according to REACH at the European Chemicals Agency ECHA. The

[21]) Guidance on the compilation of safety data sheets, Version 3.1 November 2015, European Chemical Agency (ECHA), ECHA A-15-G-07.1-EN. https://echa.europa.eu/documents/10162/23036412/sds_en.pdf/01c29e23-2cbe-49c0-aca7-72f22e101e20

obligation for registration comes into force if a substance is manufactured or imported above 1 ton per year and legal entity.

By end of March 2021, there are 25,828 registered unique substances in 99,588 dossiers [22]). For all registered chemicals there is a data set that also contains all substance data relevant for HAZBREF stakeholders; these are summarized in the so-called substance factsheet (for the structure of the factsheets see Chapter 2.5). The sum of all factsheets is the ECHA chemicals database – the "Universe of Registered Substances". ECHA's Chemical Universe is referred to in this study as the "ECHA database": https://echa.europa.eu/information-on-chemicals/registered-substances

ECHA recognises the need to improve the provision of this data. Several projects are already underway to facilitate access. But this cannot be done overnight, longer-term activities are underway.

Aside from that, the Classification and Labelling Inventory contains information on 180,541 substances[22]. Here are some quotes from the ECHA website for understanding CLP[23]:

> "The Classification, Labelling and Packaging (CLP) Regulation ((EC) No 1272/2008) is based on the United Nations' Globally Harmonised System (GHS) and its purpose is to ensure a high level of protection of health and the environment, as well as the free movement of substances, mixtures and articles.
>
> One of the main aims of CLP is to determine whether a substance or mixture displays properties that lead to a hazardous classification. In this context, classification is the starting point for hazard communication.
>
> Once a substance or mixture is classified, the identified hazards must be communicated to other actors in the supply chain, including consumers. Hazard labelling allows the hazard classification, with labels and safety data sheets, to be communicated to the user of a substance or mixture, to alert them about the presence of a hazard and the need to manage the associated risks.
>
> CLP sets detailed criteria for the labelling elements: pictograms, signal words and standard statements for hazard, prevention, response, storage and disposal, for every hazard class and category. It also sets general packaging standards to ensure the safe supply of hazardous substances and mixtures. In addition to the communication of hazards through labelling requirements, CLP is also the basis for many legislative provisions on the risk management of chemicals."

2.4.2 Safety Data Sheets

A safety data sheet must always be provided to the professional customer if the substance or mixture meets the criteria for classification as hazardous, and if the substance is persistent, bioaccumulative and toxic or very persistent and very bioaccumulative in accordance with the criteria set out in annex XIII to the Reach Regulation, or if a substance is included in the Candidate List for Authorisation according to REACH for other reasons. There is a need to revise the SDS if new information on hazards becomes available or new information has an

[22]) Data accessed from the ECHA website on 07.04.2021.

[23]) https://echa.europa.eu/regulations/clp/understanding-clp .

impact on risk management measures. Authorisations or restrictions may also make it necessary to update the safety data sheet. It should be noted that in all cases (including when the information on component substances has been obtained from SDSs of suppliers of these substances) it is the supplier of the SDS that retains responsibility for the accuracy of its content. The basic requirements on the drafting of safety data sheets are set out in Article 31 (Requirements for safety data sheets) in conjunction with annex II (Guidance for the drafting of safety data sheets) of REACH Regulation (EC) No 1907/2006.

In the Regulation (EU) 2020/878 it is stated that[24]:

> "The safety data sheet must enable users to take the necessary measures to protect human health and safety at work and to protect the environment. The producer of the safety data sheet must take account of the fact that a safety data sheet must inform its addressees of the hazards of a substance or mixture and provide information on the safe storage, handling and disposal of the substance or mixture."

For the operator of an industrial plant, the safety data sheet is the first direct access to information on the substance properties of the products used in operation. The SDS consists of 16 sections and informs the user about the potential hazards of the substance or mixture and the classifications of the substance or mixture resulting from the application of the classification criteria according to Regulation (EC) No 1272/2008 (Section 2: Potential hazards). The main adverse physical effects and the main adverse effects on human health and the environment are listed in sections 9 to 12 of the safety data sheet, so that even non-experts can identify the risks associated with a substance or mixture. Section 3 of the safety data sheet must indicate the chemical identity of the constituents of the substance or mixture. The chemical identity of all impurities, all stabilising additives and all individual components which are not the main component must be provided where these substances are themselves classified and contribute to the classification of the substance. In this respect, the SDS is also the basis and starting point for establishing an inventory for the chemicals used in the plant. From this point of view, it helps the operator in all decisions concerning the proper storage of the substance or mixture, its correct use in the relevant technical processes, the choice of the risk reduction measures required to protect human health and the environment, right up to the disposal of waste. Consequently, users of chemicals should make appropriate inquiries to their suppliers to fill information gaps and press for the submission of an updated safety data sheet.

All this information should be used by the plant operators to record the substances used in the installation and to create a chemicals inventory. Especially with regard to identifying substances with high release potential and potential (eco-)toxicological properties ("relevant target substances"), a number of important information is passed on to the user via the safety data sheet. This includes physical chemical properties (water solubility, vapour pressure, partition coefficient), environmental fate and pathways (biodegradation, adsorption/desorption) and (eco-)toxicity are listed and available (cf. Table 1). Especially with regard to the properties that determine the fate and behaviour of substances in the wastewater stream this information are of

[24]) COMMISSION REGULATION (EU) 2020/878 of 18 June 2020 amending annex II to Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)

high priority (cf. Chapter 2.3.1). The HAZBREF Sectoral Guidance on Textiles[25] (Annex 4) gives an example and description of good practice for selected sections of a good MSDS. The selection of the sections covered is based on a technical assessment of their relevance for good chemical management. Where appropriate, the sections also include a brief explanation of the contents and recommendations for operators and competent IED authorities on how to use the information contained.

Nevertheless, reviewing the substance lists from the case studies of the textile industry show that these substance data cannot always be read from the safety data sheets. The short-comings of SDS in terms of their comprehensiveness and quality of information have been addressed in the HAZBREF Sectoral Guidance on Textiles (Chapter 0). For instance, it was found that impurities such as solvents and by-products from previous synthesis or isolation processes contained in technical grade chemicals are usually not listed in the SDS.

Also, the HAZBREF Sectoral Guidance for Chemicals[26] reports that the case study representatives state that the quality of SDS supplied by European chemical companies was generally at a high level, although this quality is not always guaranteed by smaller suppliers. Among other things, it is difficult to obtain detailed data from suppliers on possible impurities or intentionally added ingredients, as this information would go beyond the requirements for supply chain communication under REACH. This concerns both impurities and ingredients in low concentrations that remain below the thresholds (levels of concern) that trigger their designation in section 3 (Composition / Information on Ingredients) of the SDS. Even though the impurity concentrations may be low, the emission can be significant when high quantities of raw materials are used. In particular, if these show small degradation behaviour in the sewage treatment plant and cannot be fully retained.

For the objectives within WP 2 also corresponding information in the safety data sheet on suitable measures to limit emissions is highly important. These can be found in various sections of the SDS and are usually of a general nature and formulated as references. They can be found in section 6 (Accidental release measures) and provide advice on all environmental precautions to be taken in connection with accidental spills. They refer to measures to prevent the release of the substance or mixture, such as keeping away drains, surfaces, soil and water. Measures to protect the environment are also dealt with in section 7 (Handling and Storage) and provide general information such as "Shafts and sewers must be protected from entry of the product". section 8 (Exposure controls and personal protective equipment) lists risk management measures that adequately control the exposure of the environment to the substance. However, this is only the case if there is an obligation to prepare an exposure scenario (ES). In this case, exposure limit values for the respective environmental compartments are also represented there in the form of the Predicted No Effect Concentration (PNEC).

If a registrant or a downstream user, when preparing a CSR (according to Article 14 or 37.4 of REACH), is required to include exposure scenarios in his CSR, he shall also include and communicate the relevant exposure scenarios in the annex to the SDS. This data format is referred to as the “(extended) Safety Data Sheet (eSDS)”. They define the information needed for employers to fulfil their obligations under EU environmental legislation and must include a

[25]) HAZBREF Work Package 4, Activity 4.1: Sectoral Guidance for Chemicals Management in the Textile Industry, September 2020.

[26]) HAZBREF Workpackage 4, Activity 4.1: Management in the Chemical Industry with focus on the production of fertilisers and polymers, Draft 28.09.2020.

summary of risk management measures to adequately control the exposure of the environment to the substance. If exposure scenarios are received from downstream users, they have to check whether their own use of the substance and their conditions of use are covered or take alternative measures.

This approach of the companies was also confirmed in the HAZBREF Sectoral Guidance on Chemicals. But it was also criticized that the ES are often very general and difficult to read. Specific environmental release categories (SPERCs) could be helpful here, although these do not exist for all specific uses. Overall, there was a desire for improved documentation of exposure scenarios and information on environmental hazards derived from them. In this respect, such information deserves special attention when identifying relevant target substances in the context of HAZBREF.

One problem for the smooth interaction between REACH and IED is the lack of availability of the CSR information. CSRs are not publicly available, and only ECHA and competent authorities have access to the CSRs (REACH Art. 36(1)) but e.g. environmental permitting and supervisory authorities do not have access to information.

Generic information on uses and operational conditions resulting from the application of the use descriptor scheme (see Reach Guidance on information requirements and chemical safety assessment, chapter R.11; ECHA, 2015) can be found in CSRs and it is available at the ECHA CHEM database, too. But some registration dossiers might lack sufficient detail level in the generic use description due to inattentive update policies of single registrants. Improvements in ECHA's technical completeness check being introduced for new registrations or dossier updates only. Therefore, this verification process will not catch those dossiers with incomplete use information and the information gap at ECHA CHEM database remains.

More detailed information about the conditions of application for a specific substance might be retrieved in case the exposure estimates are based on sector Specific Environmental Release Categories (SpERCs). For those, the relevant industry sectors responsible for SpERC development are requested to document their assumptions for common operational conditions, together with release rates derived from sector specific knowledge and make this set of information available in background documents for the different actors (industry and authorities). In case SpERCs are used but no background documentation is available, the applicability of these SpERCs should be rejected and generic considerations should be made (i.e. conservative release rates and absence of any abatement technology).

Thus, more transparent information is needed e.g. related to use of chemicals in order to improve the situation. However, some of the information filled within a registration has to be considered as confidential business information, that should not become publicly available - such as amounts of substance used per year on-site or details effecting specific operational conditions.

Information included in both SDS and ES can be used as a basis for identifying techniques to be considered in the determination of BAT, although there are potential technical constraints or limitations on their applicability. Ultimately, the use of the information obtained from the SDS could help to further support the development of BAT conclusions and help to better regulate the safe use of the hazardous substances in industrial installations. Nevertheless, the data included in the SDS is also confidential business information, i.e. information provided by the supplier of the substance. Permitting Authorities in charge of permitting industrial installations do not generally revise SDS. Thus, before processing this data during the elaboration and

review of BAT conclusions, the data needs to be validated or reality-checked by the parties involved in the Sevilla process (HAZBREF Activity 3.1: Report, Chapt. 3.2; Suhr et al. 2020)[27].

2.5 ASSISTANCE for the access to substance data and the assessment to derive substances of concern

This chapter shall assist installation operators in the identification of substances used in the installation, and finding the appropriate data for an assessment.

a) What is the source and base of all substance data?

- All relevant data for the Chemical Universe – including those for parameters of concern in Chapter 2.3 – can be found in ECHA's database of registered substances and the Classification and Labelling Inventory.
- The ECHA factsheets for registered substances are the primary source of information: https://echa.europa.eu/information-on-chemicals/registered-substances ;
  The CLP Inventory may be accessed through:
  https://echa.europa.eu/information-on-chemicals/cl-inventory-database
- For each substance there is a factsheet; it is structured as explained in this PDF: https://echa.europa.eu/documents/10162/22177693/registered_substance_factsheet_en.pdf/4ce42d65-58bb-d829-2cee-f803579b13d5 [28].
- The EU Chemicals Legislation Finder (EUCLEF) gives an overview on any chemicals legislation – aside from REACH and CLP – for a substance via the substance infocard: https://echa.europa.eu/legislation-finder ;
  In addition, there is information on cross-regulation activities, other data, and data from previous legislation here: https://echa.europa.eu/information-on-chemicals .

b) What are "chemical mixtures" and "chemical substances"?

- In the case of chemical mixtures), the composition should be known (determination of the components of the mixture and its substance identities, e.g. CAS No.) so that the properties of the respective components (i.e. the individual substances) can be accessed via ECHA database.
- The need to draw up an inventory of chemicals used for each industrial installation is substantiated in Chapter **Error! Reference source not found.** and in Report on WP 3.2. There, guidance is also given on how such an inventory of chemicals could be structured.

c) Which substance properties (of concern) should be included in the assessment?

- According to the evaluation approach chosen in this report, those properties that influence the occurrence and distribution of substances in sewage treatment plant (potential

[27]) HAZBREF Work Package 3, Activity 3.1: Analysis of the interfaces, possible synergies or gaps between Industrial Emission Directive, REACH Regulation, Water Framework Directive, Marine Strategy Framework Directive and the POP Regulation concerning hazardous substances, 07.08.2020.

[28]) More information on chemical infocards may be found here: https://echa.europa.eu/documents/10162/22177693/ what_is_an_infocard_en.pdf/4960b3a4-a84f-461d-926c-b4a683b2f98f .

to be released), as well as (eco-)toxicological properties, determine the relevance for a removal from the waste stream and/or an elimination in the wastewater treatment. Not all of these parameters are needed for the interactive scheme described in chapter 5.

- For fate and behaviour, at least the following database entries from the ECHA fact-sheet must be assessed:
  - General information: IUPAC name, CAS number, constituents, impurities, PBT assessment;
  - Physical and chemical properties: vapour pressure, partition coefficient, water solubility, dissociation constant;
  - Environmental fate & pathways: abiotic stability, biodegradation in water and soil, bioaccumulation, adsorption K_{oc}, K_{ow}, distribution modelling, monitoring data (if available).
- Ecotoxicological information: aquatic toxicity (fish, invertebrates, algae), sediment toxicity, terrestrial toxicity (in particular earthworms).
- Toxicological information: acute toxicity to vertebrates, sensitisation, repeated dose toxicity, carcinogenicity, mutagenicity, toxicity to reproduction (CMR), endocrine disruption.
- The evaluation (i.e. the comparison with trigger values) is carried out using the interactive scheme.

d) For which parameters (substance properties) is a more detailed interpretation of the study results from the data source (factsheet) necessary?

- Mobility of a substance in water is not yet a standard parameter under REACH. However, a procedure for the assessment, taking adsorptivity and dissociation into consideration, is provided in the so-called PMT concept (Hale et a., 2020)
- Biodegradation is a complex process and interpretation of the study results (e.g. for ready biodegradability) depends on the study design and the endpoint (cf. Table 1). Degradation half-lives are often not available, and therefore preference should be given to **persistence**.

e) Alternative sources for substance information are:

- Safety Data Sheets (SDS) – cf. Chapter 2.4.2.

f) How shall the results of the substance data search in the ECHA database (and possibly other sources) be processed?

- For the documentation of the substance data search, installation operators, branch associations or the TWG should develop a meaningful template that also can be used to set up a chemicals inventory. The data collected can be used to operate the interactive scheme. A suggestion to structure the chemicals inventory can be found in chapter 5.3.1. Further examples to structure such an inventory is for example the ECHA Infocard or the suggestion for a chemicals inventory provided by ECHA, compare figure 6

g) Can established substance evaluation tools such as EUSES and SimpleTreat 4.0 support substance evaluation for BREFs?

- Yes, but the handling of these tools requires expert knowledge.
- SimpleTreat 4.0 in particular is designed for wastewater treatment plants and considers the above-mentioned physico-chemical properties and biodegradation. As a result SimpleTreat 4.0 shows a distribution of the substance in the environmental compartments water, soil/solid, air, from which the degree of elimination from the wastewater stream can be determined.
- Some substances were evaluated in HAZBREF with the SimpleTreat 4.0 model (cf. Appelgren 2019). It should be noted that the distribution model is generic and does not consider specific elimination mechanisms, e.g. micro-organisms adapted for biodegradation. On the other hand, SimpleTreat 4.0 may indicate a "concern" to which BAT can be applied.

3 Substances for which regulations of different legal contexts are already in place

The assessment of the regulated substances (this chapter) and the (non-regulated) substances of concern (SoCs; Chapter 2) from the chemical universe are complementing each other in identifying those substances that should be addressed during BREF reviews.

Some regulated substance groups such as some SVHCs and WFD priority substances are still used in EU area (Annex 2 of this report, WFD substances used in Finland (Kangas 2018)) and should be assessed during BREF reviews.

The regulated substance groups that should be assessed during BREF reviews are e.g. the following (see full substance group list in HAZBREF Activity 3.2 report (Suhr et al. 2021 draft)):

- CMR 1a and 1b substances
- WFD Annex X - Priority substances
- Biocides such as disinfectants, preservatives and other products
- SVHCs on the Candidate list
- SVHCs subject to authorisation and listed in Annex XIV REACH
- Substances with restrictions on use listed in Annex XVII REACH
- Persistent, Bioaccumulative and Toxic substances (PBT) and Very Persistent and Very Bioaccumulative substances (vPvB)
- POPs Regulation substances

Substance groups of REACH SVHCs and WFD Annex X Priority substances were selected for more detailed assessment on (possible) uses in selected four industrial sectors (see chapter 3.1) and in several other BREF sectors presented in Excel file available in HAZBREF websites[29].

In order to identify all substances of very high concern (SVHC) the European Chemicals Agency (ECHA) has developed ECHA's Integrated Regulatory Strategy that brings together the various REACH regulatory processes and sets the basis for the co-operation between authorities – ECHA, the European Commission and the Member States. SVHCs are listed under REACH with the intention to phase-out their use and to reduce exposure. Therefore, in principal they need to be considered for emission minimisation or substitution under BREFs. On the other hand, there should be a flow of information from the REACH list of SVHC candidate substances as well as other hazardous substances via the SDS to the BREFs and the installation operators, to make sure that appropriate measures are implemented and can easily be supervised by authorities.

The inclusion of a substance in the SVHC Candidate List results in immediate obligations for suppliers of the substance and for articles containing the substance above a concentration of 0.1% (w/w).

The existence of authorisations or restrictions for certain substances under REACH is an indication of a particular concern. If a restricted or authorized substance is relevant for given BREF, it should be somehow highlighted in BREF document in order to ensure that companies do not unintentionally use these substances. Thus, IED via BREFs may promote the phase-out of their use and to reduce related exposure to them. Additionally, BREFs could promote the enforcement of the REACH regulation at installation level if the SVHCs as well as restricted and authorized substances are highlighted in BREFs and subsequently in environmental permits.

In 2018, Directive 2013/39/EU listed 45 substances (or substance groups) to WFD Annex X (Annex of EU priority substances, referred as WFD PS in this report). The European Commission reviews the list of priority substances every six years according to Art. 1 2013/39/EU. In practice, the list has been reviewed twice (in 2008 (2008/105/EC) and in 2013 (Directive 2013/39/EU)) since it was first compiled in 2015. Art. 16 par. 2 of the directive introduces a scientifically based methodology for selecting priority substances based on their significant risk to or via the aquatic environment. Emissions of priority substances (PS) are required to be minimised, and emissions of priority hazardous substances (PHS) have to be phased out.

3.1 HAZBREF study – REACH Substances of Very High Concern (SVHCs) and WFD substances

3.1.1 Approach for identifying the uses of SVHC and WFD priority substances in HAZBREF case study industrial sectors

So far, BAT conclusions do not contain substances that are restricted (Annex XVII of REACH), subject to authorisation (Annex XIV of REACH) or of very high concern (i.e. SVHC) in case

[29] https://www.syke.fi/en-US/Research__Development/Research_and_development_projects/Projects/Hazardous_industrial_chemicals_in_the_IED_BREFs_HAZBREF/Work_packages/Target_chemicals_WP2 (note: the table will not be updated by HAZBREF project)

that they are used in the given industrial sector. For each future BREF review, as a routine, it should be assessed if restricted, authorised or SVHC are still used in a sector for which a BREF review is carried out. The results of this assessment should be part of the BAT conclusions..

In order to identify which SVHCs and WFD priority substances are possibly used in the HAZBREF case study sectors, SYKE made a database search for the information. The list of SVHC substances was downloaded from the ECHA webpage (https://echa.europa.eu/candidate-list-table). At the moment of making the exercise (April 2020), the list included 205 substances or substance groups identified as SVHC. The information on substance uses in EU was compiled from the public ECHA database (https://echa.europa.eu/information-on-chemicals) and in Nordic countries from SPIN register (Substances in Preparation in Nordic countries http://spin2000.net/). The total use volumes in EU were derived from ECHA infocards (public ECHA database) as well. The use information from SPIN database was searched from the categories "Industrial Use (NACE)" and "Use (national)". The use volumes in SPIN database are presented for one particular year. If the use volume value in SPIN database is "0" it means that the volume is below the reporting limit, which is 100 kg.

In case of polymer sector the key words were '"polymer" or "polymers" or "used in polymers" or "used in polymer processing" or "elastomers" etc. If the key words appeared in the section 'uses at industrial sites' of the ECHA infocard, the substance was deemed to be used in the sector of concern. For STM sector the key words were 'manufacture of fabricated metal products' or 'metal surface treatment products' or 'surface treatment' or 'coating products' or 'coating of metals. For textile sector the key word was "textile" and for fertilisers "fertiliser", respectively.

3.1.2 Outcome of the approach to link SVHCs and WFD substances to selected industrial sectors

Detailed information on substances possibly used in the selected four industrial sectors are presented in Annex 2 to this report (Strategy C – hazard based approach). A summary is given in Table 5.

Table 5: The number of priority substances identified per industrial sector in the HAZBREF study.

Sector	Number of identified SVHCs / WFD PS or PHS
Polymer (POL)	66
Fertiliser	5
Surface treatment of metals and plastics (STM)	81
Textile	14

SVHC: Substances of very high concern, WFD: Water framework Directive, PS/PHS: priority substances / priority hazardous substances according to WFD.

Additionally, possible uses of SVHCs and WFD substances in several other BREF sectors are presented in Excel fil location in HAZBREF website.

Altogether 66 substances or substance groups were identified to be probably used in polymer sector (POL) and 14 for the textile sector (Table 5). For example, different phenols and

phthalates, cadmium and lead substances as well as a PFAS substance (PFBS) are most likely used in manufacture of polymers.

Altogether 5 substances or substance groups were identified to fertiliser sector (Table 5). Three of these are boron compounds. Boron is an essential plant micronutrient and added to SVHC list due to concerns related to human health. Two of the identified substances are cobalt salts. Cobalt is needed in nitrogen fixation reactions in legume plants.

81 substances or substance groups were identified to be potentially used in the STM sector (Table 5). For example, several phthalates, cadmium, cobalt, chromium and lead substances as well as PFAS substances (PFBS & PFNA) are most likely used in STM sector. The result was checked with the information from HAZBREF case studies: 13 out of 81 substances were in use in HAZBREF case installations.

There are issues concerning the quality of the data in the public ECHA database. Firstly, the use information in public ECHA database is provided by the manufacturers or importers of a substance in the registration dossiers. It is possible that the manufacturer/importer has indicated multiple uses for the substance even though the substance might not be used in POL sector. This results in false positives in the lists and therefore more it should be checked if SVHCs are actually used in the sector of concern. Secondly, the use volumes in ECHA infocards cover all the possible uses of the substance and not only the used amount in on particular sector (i.e. there is no information on amount of use in POL sector). Thirdly, the information on the industrial uses and volumes in public ECHA might be outdated (the year information is originating/based on is unknown). For these reasons the results may include substances, which are not actually used in the sector.

Additionally, the use information on PFAS substances identified as SVHC in ECHA database is very scarce. It is possible that they really are not used or that the public ECHA database is not a good information source for use of PFAS. Due to lack of use data most PFAS were not possible to link to the industrial sectors.

Additionally, the utilisation of chemical use information in polymer sector from SPIN database turned out to be very difficult, because the polymer sector (or term polymer production or even term polymer) is not available and therefore cannot be searched from SPIN database. The only available possibly POL related terms in SPIN register category “Industrial Use (NACE)” are related to manufacture of rubber and plastics. More precise information, e.g., “raw materials for production of rubber products and plastics“, was found from category “Use (national)” in SPIN register, but only for few substances.

3.2 Transfer of information on regulated substances into the BREF revision process

A proposal on how to more systematically consider and include information on SVHC and other priority substances during BREF reviews is described in the HAZBREF Activity 3.2 report: Suhr et al. (2021): Method to include information on hazardous and other substances of concern more systematically into BREFs.

It is in particular chapter 2.4 of the above mentioned Activity 3.2 report which refers to substances to be addressed in future BREF reviews. The table 1 of that report mentions amongst other things the CLP-Regulation, the Water Framework Directive, the Biocidal Products

Regulation, SVHC and restricted and authorised substances from the REACH Regulation, and finally the POP-Regulation. The report closes this chapter with the remark (p- 27):

HAZBREF recommends as a routine for each future BREF review, that it should be assessed if SVHCs or other prioritized substances posing environmental and / or health hazard listed in table 1 are used in the industrial sector for which the BREF is updated. The results of this assessment should be part of the BAT conclusions in form of a list to ease orientation for inspection and enforcement. If authorised substances or substances from the Candidate List (SVHC) are identified to be in still in use in a given industrial sector (BREF), specific considerations about substitution and minimization of use should be part of the BAT conclusions, in case that risk management measures and substitution driven by REACH refers to the application of BAT.

In addition to the statements in the Activity 3.2 report, it should be noted that a repetition of the requirements of safe handling under REACH in BATs should be avoided in order to avoid duplicate regulation. It should also be taken into account that the list of SVHCs according to REACH is updated every six months.

Therefore, flexible reference should be made to the requirements regarding SVHCs as well as on restricted and authorized substances set out in REACH.

3.3 ASSISTANCE to identify uses of SVHC and other regulated substances

The compiled information in annex 2 on uses of SVHCs and WFD substances may be useful mainly for BREF revision process when identifying substances to be addressed.

The flow of information on SVHC and other regulated substances in the supply chain is mainly driven by the Safety Data Sheets, which are prepared by the producers of chemicals and forwarded to downstream users. The SDS also contain information on the safe handling of hazardous substances (cf. Chapter 2.4.2).

The HAZBREF Activity 3.2 report mentions two ECHA tools to check the regulatory status of a substance, which can be accessed by anybody (cf. page 32):

The Public Activities Coordination Tool (PACT; https://echa.europa.eu/pact) best informs about up-to-date information on activities planned, ongoing or completed by ECHA and/or Member States for a given substance. Therefore, for substances for which the use in a given BREF-sector is known, it makes sense to check the entries in the PACT during the frontloading phase of BREF review process. From this screening, SVHCs or possible restrictions or authorisation decisions can be identified. The most important entries in the PACT table in the context of this report is the overview of regulatory risk management measures: harmonized classification and labelling (CLH), identification as SVHC, restrictions on use. The information on data generation and assessment activities and the activities on regulatory management options analysis might be of interest to have an idea what substances might be of relevance in the next years also. Finally, there is also the Community Rolling Action Plan (CoRAP)[30].

The EU Chemicals Legislation Finder (EUCLEF) gives an overview on any chemicals legislation – aside from REACH and CLP – for a substance via the substance infocard: https://echa.europa.eu/legislation-finder.

[30]) https://echa.europa.eu/information-on-chemicals/evaluation/community-rolling-action-plan/corap-table

For detailed information also check Chapter 5 with the interactive scheme.

4 Sector-specific lists of chemicals – wit and nonsense

The original assumption in the HAZBREF project was that the legislative context of the IED, i.e. REACH, WFD and other substance-related regulations, could generate lists of hazardous substances that could then be processed in the BREF review as "Key Environmental Issues". As outlined in Annex 1, HAZBREF WP 2 has prepared four strategies for this, which should result in such sector-specific substance lists from different information sources:

A. Substance-based approach: Identify chemicals possibly used in the respective industrial sector by use categories in the ECHA database, descriptors defined in the REACH-Guidance, and characterise substances according to hazard and environmental release and fate criteria (cf. Chapter 4.1).

B. Use-based approach: Used information and substance-list available from specific industrial sectors and processes applied there to identify applications, technical functions (e.g. surfactants, bleaching agents etc.), compounds in products used in the specific sector of use (mainly textile sector), try to characterise this chemical group with regard to hazards and environmental release and fate criteria (cf. Chapter 4.2). The approach was developed and documented in a way that it can be transferred to other industries.

C. Hazard-based approach: Identify priority hazardous substances or regulated substances, which are per se undesired in chemical processes or require special safety measures to prevent exposure and release; narrow down the substance list by applying actual sector-specific use information (cf. Chapter 3.1 ff.).

D. Installation-based approach: Case-studies (from industrial sectors investigated in HAZBREF WP 4) provided tables of chemical products and in some cases individual substances contained. This approach might provide a list of the most relevant substances used in an installation for a specific process (reality check, cf. Chapter 4.3).

In the course of the work, however, it has become apparent that the focus should not be only on listing of prioritised substances as such, but on the assessment of individual substances on the basis of the parameters of concern (see Chapter 2). First, those substances are separated for which there are provisions in other regulations or directives (see Strategy C in Chapter 3). Then, substances are identified from databases that have use descriptors, or technical and chemical functions that are relevant to the industrial sector in question (see strategies A and B in chapters 4.1 and 4.2). A method of combining similar substances into groups (see HAZBREF WP2 report on Strategy B (Werschkun 2020) in Chapter 4.2 and annex 4) has proved particularly advantageous for the purposes of the BREF process. Nevertheless, even these lists are not sufficient if the substances are not also assessed individually or as a group on the basis of their fate and behaviour or toxicology properties (for the procedure for this, see Chapter 5).

Finally, the evaluation of the case studies examined in HAZBREF (for strategy D see Chapter 4.3) has shown that substance lists from the installations themselves can only be used for the BREF review to a limited extent, more precisely for the examined process within an industry.

Nevertheless, after the BREF review case studies can examine whether the newly developed BAT conclusions can be implemented in practice.

In order to better understand the procedure for identifying BAT-relevant target substances outlined in Chapter 5, the above-mentioned strategies A-D are explained in more detail in this Chapter 4 - they will be needed later. The associated knowledge base, especially the ECHA database of registered chemicals and the safety data sheets, has already been described in connection with the parameters of concern in Chapter 2.4.

Although all strategies presented for identifying relevant target substances have advantages and disadvantages, they should be considered in the BREF review. For this see the report of HAZBREF Activity 3.2 (Suhr et al. 2021), as well as the explanations in the respective "guidance" chapters in this report (the last chapters in each section).

4.1 Use of ECHA database to derive lists of substances for BREFs (substance-based approach)

This approach is primarily relevant for those who deal with the revision of BREFs. The approach and findings are useful for those in collaboration with ECHA. Industry representatives and installation operator can use this chapter as information, especially about the use descriptor system according to REACH as all stakeholders come into contact with the use descriptor system within the framework of SDS or exposure scenarios.

The ECHA database contains data about approximately 23.000 substances (2021) which were registered according to REACH. To derive lists of substances used in a respective sector it is necessary to query the database based on so called "use descriptors" defined in ECHA guidance R12. The HAZBREF project investigated whether the use descriptors available in REACH represent a manageable way of identifying substances that e. g. are used in the textile sector.

Information on uses is available in ECHA database only on a generic sector level, which is much broader than the scope of the BREF. Therefore, further assessment and filtering of data from ECHA database is needed before relevant substances can be identified for BREF review purposes. HAZBREF recommends that such screening is performed during the preparatory frontloading phase of BREF reviews.

In the following the procedure to generate sector-specific substance lists based on the use descriptors in the ECHA database, specifically for the textile processing sector, is described (Strategy A).

In May 2018, ECHA has provided extracts from this registration database with regard to life-cycle stages e.g. industrial use and professional use to UBA. The ECHA database was filtered according to appearance of the term / string 'textil*' (in a very broad sense, as example for one of the industrial sectors investigated within HAZBREF).

Headers (cf. Annex 3; e.g. "About_this_Substance_6_Uses_Industrial_Sites" or "About_this_Substance_4_Professional_Workers") refer to the original Excel-files extracted from the ECHA database in May 2018, and respective columns therein (e.g. "About industrial … product, process, environment, Sector_of_Use"). The task is to select those use or application categories (use descriptions) which will provide chemicals relevant for the industrial textile sector, in this case. Tables for the life-cycle stage 'manufacture', 'formulation and repacking', 'consumer uses', and 'article service life' are outside of the scope of the IED, and are therefore omitted here.

From a large number of use descriptors, a series of combinations with the string 'textil*' were created, which appeared plausible, and applied to the step-by-step filtering concept of the data sets. A standard database programme was used for the administration of the data records and the individual filter processes. In Annex 3 the approach for selection of substances from ECHA database via queries in ECHA database and the numerical result is presented.

Use descriptor system in ECHA Guidance R12 / R16: Sector of Use, Product Category, Article Category, Technical Function

The ECHA Guidance on Information Requirements and Chemical Safety Assessment, Part D, Chapter R.12: Use description (Version 3.0, December 2015, page 22 ff.) includes information on markets where the substance is used (formulating sectors, industrial sectors, types of products, types of articles), which might allow a more specific approach to chemicals used in the textile industry.

'The sector of use category (SU) describes in which sector of the economy the substance is used (e.g. the textile industry). In the case of uses taking place across many sectors, this element may not be needed as registrants are not expected to provide an exhaustive list of all sectors. However, if provided, this information may be useful both for downstream users in the assessment of whether the exposure scenario (ES) is relevant for his use (this is a matter of BREFs), as well as for authorities to understand/assess the type and number of supply chains concerned by this use' (ibid. 22).

'The chemical product category (PC) describes in which types of chemical products (= substances as such or in mixtures) the substance is finally contained when it is supplied to, and used by, end-users. In the case of uses for which many products are relevant, this element may not be needed as it is not expected to have an exhaustive list of all products' (ibid. 22f.).

'The article category (AC) describes the type of article into which the substance has been processed (e.g. textiles). This also includes mixtures in their dried or cured form (e.g. dried printing ink …; dried coatings on various surfaces)' (ibid. 23).

The contributing activities (CA) cover the description of the different activities contributing to one use. However, the contributing use descriptors – process category (PROC) and environmental release category (ERC)[31] – are important for the assignment of the activity to a BREF, but do not help for the identification of relevant target substances.

The technical function of the substance (TF) describes what the substance actually does in the use (e.g. solvent, pigment) and is therefore focused on substances; it is not meant to convey information on the type of mixture or article. The technical function should be clearly distinguished from the product category (PC).

[31]) **Examples for PROCs** are: PROC 8a Transfer of substance or mixture (charging and discharging) at non-dedicated facilities; PROC 21 Low energy manipulation and handling of substances bound in/on materials or articles. **Examples for ERCs** are: ERC5 Use at industrial site leading to inclusion into/onto article; ERC8f Widespread use leading to inclusion into/onto article (outdoor); ERC12b Processing of articles at industrial sites with high release.

For example, in the HAZBREF project the textile sector was analysed. For this sector the sector of use descriptor SU5 – Manufacture of textiles, leather, fur (NACE code C 13-15[32]) is relevant (ibid. 43f.).

The chemical product category relevant here are PC23 (leather treatment products), PC34 (textile dyes and impregnating products, including bleaches and other processing aids), PC35 (washing and cleaning products, including water and solvent based products) are relevant for the textile industry (ibid. 47f.).

The textile industry certainly uses a large number of other chemicals, which are not specific for this sector (other PCs are e.g. adhesives, sealants, adsorbents, biocidal products, coatings and paints, fuels, surface treatment products, hydraulic fluids, processing aids such as pH-regulators, flocculants, precipitants, neutralization agents, laboratory chemicals, perfumes, fragrances, water softeners, water treatment chemicals). These chemicals might nevertheless be released from the industrial production process in the waste stream. If the ECHA database is to be queried with regard to the substances used in a respective sector, it is important to take this into account.

The article category for the textile sector relevant here are the following descriptors: AC5a-h (fabrics, textiles and apparel) and AC6a-g (leather articles) (ibid. 69 f.).

In the HAZBREF project a close link between the ECHA descriptors for technical functions (TF) and a list of chemical groups available in the context of the textile BREF revision was observed; however, the generic TF descriptors under REACH are not limited to a specific industrial sector, such as textile industry. The difference between the description of technical functions under REACH (ECHA Guidance R 12 contains 121 general descriptors of the technical functions of chemicals (ibid. 74 – 86) and in the industrial sectors for example the textile industry is as follows. However, a comparison of different descriptors reveals some differences in their definition, as shown in the table below.

Table 6: Comparison of TXT-BREF and Reach-Descriptors – Example: Finishing substances

TF according TXT-BREF	**TF according REACH**	**TF Description (REACH)**	**Comment**
4.5 Handle-imparting agents			No equivalent at REACH descriptors
4.6 Anti-Electrostatic agents	Antistatic agent	Any substance that prevents or reduces the tendency of a material to accumulate a static charge or alters the electrical properties of materials by reducing their tendency to acquire an electrical charge.	Terms comparable, however the term under REACH is more general
4.7 Repellents	Waterproofing agent	A water-repellent material functions by lowering the surface energy to	Repellent (TXT-BREF) is not limited

[32]) NACE code (**N**omenclature statistique des **A**ctivités économiques dans la **C**ommunauté **E**uropéenne); cf. http://ec.europa.eu/competition/elojade/isef/index.cfm?policy_area_id=0 .

TF according TXT-BREF	TF according REACH	TF Description (REACH)	Comment
		protect surfaces against water by making water bead.	only to water repellency see also next line
	Anti-redeposition agent	Any substance that prevents dirt and grease from resettling on a cleaned surface or that helps keep soils from re-depositing onto clothing in the wash water after they have been removed.	"Antiredeposition agent" (REACH)

TF: technical function

It becomes clear that under REACH a corresponding description for technical functions is not always available. However, there are also comparable descriptions of a technical function in the textile sector, although these are more general under REACH. Sometimes the descriptors under REACH can also be more differentiated, as the example on repellents illustrates. In this respect, the descriptors for the textile sector in the respective BREF are not always identical with those under REACH. In this respect, a correspondence with substance lists generated for a sector and the entries for substances in the ECHA database is not always possible (cf. Chapter 4.3.2). Queries in the ECHA database based on these elements for use description or intelligent combinations thereof {e.g. [SU5 and/or (PC23 or PC34) and/or AC5a-h]} could also be conducted, e.g. in the frontloading process of BREF revision in the future with the support of ECHA's IT team. Combining such results additionally with technical functions could lead to a more appropriate query of ECHA database for "textile activities" (cf. Chapter 4.2).

With a view to the strategy to identify relevant target substances described in Chapter 4.2, it would make sense, for example, to link the technical functions and descriptors for substance groups to each substance data entry in ECHA database (or in chemicals inventory databases respectively). It should then be possible to perform a query of ECHA database regarding hazard and fate and characterize groups of substances with technical functions. For example, during a working group meeting with ECHA in March 2020, such a procedure was considered possible with a certain amount of resources.

Summary for the substance-based approach using the ECHA database as starting point

The benefit of the ECHA database is that it addresses individual chemicals and opens access to their individual uses and properties. However, as demonstrated above, there are two drawbacks: (a) it seems to be difficult to select chemicals used in a specific sector (examples were given for the textile sector (actual uses might not have been allocated with the appropriate descriptor), and (b) there is no way to prove whether all relevant chemicals for a sector can be derived from the database using the use descriptor system and the above described procedure (for the same reason: actual uses might not have been allocated with the appropriate descriptors). A careful comparison of lists with actual substance identifiers from different life-cycle stage queries might help (this could be a task for each future BREF review).

A prerequisite for any survey in the database is that registrants have notified the uses of their substances properly.

The exercises described above will result in a more or less complete list of chemicals for the textile sector. The procedure presented can be transferred to other sectors. However, the lists

derived from this procedure needs a reality check. But at this point of deriving lists, the chemicals are not prioritised with regard to their hazard potential and their potential to be released to the environment. And further, it can at this point not yet be determined which treatment techniques are appropriate with regard to protection of the environment and which specific elimination techniques should be used in the installation's waste/sewage treatment.

In order to improve the mutual usability of available data, an alignment of the use descriptions between REACH and IED could be helpful. In particular, improving information about the real uses of substances and improving information about substance properties in both regulations REACH and IED are prerequisites for preventing potentially harmful emissions into the environment.

For reasons already discussed above, the substance-specific approach based on a query in the ECHA database to select relevant target substances for BREF based on the use descriptor system entries is not particularly specific for an industrial sector.

The main value of these lists is the possibility of a cross check with substance lists from other approaches, e.g. the use-based approach focusing on grouping of substances based on their technical function (cf. Chapter 4.2). Therefore, the next steps might be to check, whether the selected substances can be associated to technical functions or chemical classes and then run a corresponding query in the ECHA database.

Based on the use descriptors in the ECHA database, sector-specific substance lists were created (Strategy A) - specifically for the textile processing sector. However, the examination compared to the case studies (WP 4; Strategy D) revealed a discrepancy - in fact many more substances were suspected than are actually relevant for the sector. However, not all processes existing in textile industry were covered in the case studies of this project.

Therefore, it will be important in the future to establish meaningful chemical inventories (plant or sector specific). However, in order to get an idea of which substances might be of concern in the respective industrial sectors, the technical and chemical functions of the chemicals or groups of chemicals used were analysed (Strategy B). For the substances thus identified, the parameters for fate and behaviour or for hazard potential can be determined from the ECHA database. In addition, the substances can be checked to see whether they are already subject to regulation (Strategy C). Thus, the substances, for which BAT conclusions are to be developed, are determined. At the end there is a table of chemicals with information on the parameters of concern, as well as possible measures to reduce risks or abatement techniques.

4.2 Use of sector knowledge to derive lists of substances (use-based approach)

In the Annex 4 the use-based approach for the identification of representative chemicals for textile activities is shown under consideration of chemical functions and substance groups used for these activities as described in the list provided by the textile industry. This work has been carried out by an external consultant and resulted in the following report: Dr. Barbara Werschkun (Wissenschaftsbüro, Berlin), (March 2020), Identification of chemicals belonging to chemical classes used as textile auxiliaries, ca. 45 pages [33].

This approach is applicable to all stakeholders which are addressed in this report: operators of industrial installations, branch associations, stakeholders reviewing BREFs. The starting point

[33]) Literal quotations from this consultant report are not marked in this chapter of the WP 2 project report.

is knowledge on substances used in the installation or the branch. The aim is to create the basis for various operational decisions through the meaningful grouping of substances used.

The following describes how on the basis of comprehensive information from sectors the identification of relevant target substances can work. The core of this approach is an intelligent grouping of substances based on their technical function. This approach will be explained for the textile industry as a sector selected for the project. The grouping is supported by using the ECHA database using different search methods (generic name, systematic name fragment, SMILES code, etc.).

A list provided by the textile sector contains a list of textile processing activities (TXT BREF process; cf. 11th page 'textile activities') and respective chemical functions and substance groups used for these activities. The link of the "textile activities" with the ECHA "technical functions" is obvious. The chemical groups are structured 3-fold: technical function, chemical characteristic, substance group denomination.

Figure 6 shows an example of a result of the procedure for the substance-based approach by Werschkun (cf. Annex 4). For the technical function (TF) "surfactant" to chemicals in the textile sector, different chemical classes can be formed. Non-ionic and anionic surfactants are listed here as an excerpt under columns 1A and 1B in the table. The respective chemical classes can be further subdivided into different chemical groups, e.g. alkylphenol ethoxylates (1.A.3) for the non-ionic form or alkyl aryl sulphonates for the anionic form. A detailed description of the results for the chemical classes in the textile sector after filtering and processing of the search results can be found in chapter 3 of the HAZBREF WP2 report on Strategy B (Werschkun 2020).

Reference No.	Cross-reference	Technical function
1		Surfactants
1A		Non-ionic (Chemical Class)
1A.1		Fatty alcohol ethoxylates
1A.2		Fatty acid ethoxylates
1A.3		Alkylphenol ethoxylates (APEOs) ← Chemical group
1A.4		Fatty amine ethoxylates
1A.5		Triglyceride ethoxylates
1A.6		Ethylene oxide/propylene oxide adducts
1B		Anionic (Chemical Class)
1B.1		Alkyl sulphonates
1B.2		Alkyl aryl sulphonates ← Chemical group
1B.3		Naphthalenesulphonates
1B.4		Ligninsulphonates
1B.5		Alkyl sulphates
1B.6		Alcohol ethoxysulphates
1B.7		Sulphated alkanolamides

Figure 5: Example from Werschkun Report on how to structure chemicals based on technical function, chemical class, chemical group

Understanding the use of a chemical in industrial processing (technical function) and knowledge of its chemical function can greatly assist in the identification of chemical properties. When technical function and chemical group are known for a substance the formation of groups of similar chemicals is possible. Why and for what purposes it is appropriate to create groups will be explained in Chapter 4.2 (cf. the Werschkun approach). Knowing the technical function and technical processes of use also provides the first decisive indications as to whether a substance from the production process enters the waste stream (water, air and solid waste) and to what extent. Further details on the chemicals inventory are described in Chapter 5.3.1

While the lists do not specify individual chemicals, it may be assumed, that the substance groups given there[34] (e.g. alcohol and fatty alcohols ethoxylates) are sufficiently homogenous with regard to their behaviour in the processes, waste and sewage treatment and environmental fate, and maybe also with regard to their (eco-)toxicological properties, that they can be addressed by a common BAT, e.g. for the need of elimination in wastewater treatment. If this is true, it might not be necessary to derive a list of chemicals from the ECHA database, but rather to address or prioritise substance groups for development of BAT by the TWG.

Summary of the use-based approach using sector information as starting point

The basic idea of HABZREF activity WP 2 was to start with a list of substances used in an industrial sector and then to characterise substances or substance groups with regard to specific concerns. The approach is described with the textile industry as an example sector but the results can be transferred to other sectors. Prerequisite is a list of substances derived in the respective sector. There may be limitations to this approach for sectors that use inorganic substances, for example.

The textile processing industry did not provide lists of individual substances or the composition of chemical products used. Therefore, the described approach took the effort to derive groups of substances predetermined from technical function and chemical use data, for which representative individual substances could be identified. A list of textile substance groups from the textile industry was used as starting point. The following steps were carried out: find a small number of representative chemicals for each group and/or technical function with the support of the TEGEWA sales catalogue and/or the ECHA database (combined survey via 'sector of use', 'chemical product category', 'article category'; cf. above).

Using the substance properties[35] provided by the ECHA database, and based on the assumption that group members are similar with regard to (eco-)toxicological and environmental properties, a chemical profile for each textile activity or technical function was prepared, which provides the basis for a group-specific BAT or a horizontal BREF (e.g. the emission from storage BREF). Support for the characterization of the fate and behaviour of target substances/groups can also be provided by the SDS information from new case studies in the BREF revision process. This

[34]) Certain chemical groups are used in more than one activity (e.g. non-ionic surfactants); therefore the page 'Chemicals' may be condensed.

[35]) Relevant substance properties are generally: human health toxicology, including CMR-properties (may be derived from CLP information); ecotoxicological data, in particular toxicity to aquatic organisms and micro-organisms; (bio-)degradability, mobility, and other physico-chemical data to determine the potential to be released; for a more detailed discussion of substance properties and hazard thresholds see chapter below.

issue was not pursued further in the present approach, but such a procedure is recommended in the course of the revision of the BREFs for other sectors.

This circumvents the need to prepare a full list of chemicals used in the textile industry based on registered uses, which can never be comprehensive anyway. Later on, in the implementation of the Textile BREF, it requires however a profound knowledge of each installation operator about which chemicals are used at his site and to which chemical groups they belong.

A reminder: The technical functions and chemical groups from the list provided by textile industry are "real" for the textile industry, but the individual substances derived by similarities in the study are only representative or theoretical for this group, i.e. there is no proof that substances from this group are actually used in the textile processing industry. This question can only be answered by involving the suppliers for this sector and the relevant industry associations.

The HAZBREF WP2 report on Strategy B (Werschkun 2020) summarises the outcome of Strategy B as follows:

The developed use-based approach for the identification of chemicals that may be potentially relevant for certain technical processes can be applied to lists of individual chemicals if there is a well-established relationship between the chemical structure and the technical function. This could be demonstrated with the help of a case study for an alkyd production site. In other case studies, namely from the surface treatment of metals, the technical functions of the chemicals listed were not clearly described (different and in part conflicting terminologies were used in different case studies within this industry sector). If the definition of technical functions could be unified, better progress might be made with the definition of relevant chemical classes. Application of the structure-based approach for the identification of relevant chemicals is not possible for industries or processes that use inorganic chemicals.

Nevertheless, the structure-based approach has made clear that, if the appropriate information is available (intended use, chemical and technical function), it is possible to move away from the single substance approach and define chemical substance groups for a specific sector. In close cooperation with suppliers and industry associations, members of the TWG could, when developing the BATs, check for relevance to these groupings. After linking the substance properties to the corresponding substance class, appropriate risk reduction measures would then have to be defined for the identified chemical substance class rather than for each individual substance. This procedure is also helpful if, as was noted in the substance lists from the case studies, no details are available on the composition of mixtures. In order to solve this task, an activity of the involved actors similar to that for the creation of specific exposure scenarios (SPERCs) under REACH would be desirable and useful.

4.3 Use of information from case studies in installations to identify relevant target substances for BREFs

In the case-studies and sector guidelines, HAZBREF team examines the possibilities for the companies to carry out their own substance evaluations, and considers real uses and real elimination possibilities in wastewater treatment.

The findings from case studies in textile industry are presented in this report and conclusions are drawn to other sectors.

Four case studies from Germany, Poland and Sweden were analysed, which represent a wide range of processes, raw materials and products in the textile industry. If case studies are carried out e.g. as part of a BREF review, care should be taken to ensure that the studies can be compared with each other. A prerequisite for this is that information is presented at a consistent level of detail, e.g. on the substances and mixtures used, information on uses, on the identity of individual substances in mixtures and information on (eco-)toxicology and their fate and behaviour in the environment.

The case studies from the textile sector included several hundred substances and mixtures, and finally it was ultimately possible to identify about 450 substances via their CAS number. Naming with a CAS no. ensures that it is unambiguously clear which substances is meant. Information from the ECHA database is assigned to this substance via the CAS-no. If substance lists are compiled in companies or industries to create a chemicals inventory, it must be ensured that the unique designation of a substance is made with the CAS-no. instead using a trade name or pseudonym.

In addition, during the revision of the Textile BREF, an extensive list of information on textile processing activities and respective chemical functions as well as substance groups used for these activities were available (cf. Chapter 4.2).

Voluntary case studies within the textile sector are an additional and important instrument to enable a reality check against other substance overviews, as they were generated exemplarily via the ECHA database (cf. Chapter 4.1).

4.3.1 Experiences in listing sector-specific chemicals

The results from the case studies show that the knowledge of the chemicals used in a plant varies among the operators. This may be due to the fact that the suppliers' SDSs are not sufficiently well maintained, or it may also be due to the way in which this information is prepared in the plant. The requirements for the preparation of SDS and the importance of complete information in the safety data sheets have already been referred to in detail (cf. Chapter 2.4.2). This includes the obligation of the installation operator to contact his supplier in case of incomplete information in order to obtain, compile and evaluate complete information on chemicals used. This is especially required when identifying hazardous chemicals to prevent their use, reduce their consumption or minimise their emission by applying abatement techniques consistent with BAT (cf. Sector Guidance on Textile).

In the case studies, only the substance lists were considered here and these already represented a pre-selection of the various parameters for the substances and mixtures used, which are transferred from the SDS. It is not possible to go into all details here, but some points can be highlighted.

The tables contained, for example, internal company data on the annual quantities of the substances concerned, and the lists provided by the companies are mostly confidential. Where sources other than the SDS were used, a corresponding reference was made. In one column a possible reference to certain legal acts (e.g. SVHC substance, PBT-substance) or the ZDHC Gateway - Chemical Module was queried. The information on the content of individual substances in mixtures are also positive, although they are mainly ranges. The inclusion of hazard statements according to GHS in the tables should also be emphasized. Sometimes the publication date of the SDS was also mentioned, but many SDS were outdated (older than 5 years).

Greater uncertainties arose from the mere indication of trade names or ambiguous designations for the products. Sometimes a clear identification of substances based on the EC or CAS number is also missing. Often information on the physical/chemical properties (e.g. water solubility, vapour pressure, partition coefficient) was missing in the substance lists or perhaps was not transferred from the SDS. Often there was no information about the degradation tests used to verify statements like "readily biodegradable" or terms were used which have no significance for the degradation behaviour (e.g. "poorly degradable"). The lack of information on aquatic ecotoxicity (algae, daphnia, fish,) of the components of mixtures was striking. In line with the WP2 objective to identify relevant target substances, this information is essential (cf. Chapter 1.3). Especially with regard to the question whether the substances can pass a sewage treatment plant and will pose a hazard to surface waters (cf. Chapter 2.3.1 and 2.3.2).

Ultimately, however, there is also a demand for a complete chemical register in an electronic format that is to be updated regularly and reflects the current conditions for the use of chemicals in an installation. The focus should not be exclusively on those substances that are classified as hazardous, already subject to restriction or authorisation under REACH, identified as SVHC or listed as priority substances under WFD. For example, even substances that do not meet all three PBT criteria can pose a risk for the environment. For example, if they have a high mobility, meet the criterion of persistence and are toxic to aquatic organisms. This task, of course, constantly requires resources and qualified staff, and in the respective industrial sectors the relevant associations could well support their members. The importance of a well-managed chemicals inventory is also emphasized in the Sectoral Guidance under HAZBREF WP 4.1 (see for example Krupanek et al. 2021).

If the definition of technical functions could be unified, better progress might be made with the definition of relevant chemical classes. Application of the structure-based approach for the identification of relevant chemicals is not possible for industries or processes that use inorganic chemicals (Werschkun, 2020). The latter applies to many processes and chemicals in the coating of metals and plastics, and in particular to the production of fertilizers. Furthermore, it is to be noted that these case study reports mainly list chemicals that have already been identified as hazardous during classification and labelling or have been identified as substances of very high concern under REACH or as priority substances under the Water Framework Directive. However, substances from non-regulatory chemical reference lists were also considered. These results on the case studies in other sectors as well as the positive experiences for the textile sector (early presentation of results, strongly differentiated use patterns, large material diversity and input from the BREF revision) made us decide to focus on this sector. However, STM would be a much less complex and less diverse industry for which concrete inquiries would be possible.

The exercises in the textile sector have revealed essential insights into the difficulties of a blanket query in the ECHA database (c.f. Chapter 4.1). It can be concluded that less complex processes can be specifically queried with ECHA's IT experts. In any case, information from the ECHA database is important for the frontloading process of each future BREF revision as demonstrated recently by the cooperation between EIPPC, TWG and ECHA (cf. HAZBREF Activity WP 3.2, Chapter 6.2). Although not always easy to use, ECHA's database should be used to collect data on the substances used in installations by operators when compiling the chemicals inventory.

4.3.2 Case studies from the textile sector

In the following the procedure under strategy D (installation-based approach) to identify relevant target substances for BREFs is demonstrated for the textile sector. HAZBREF WP 4 collected substance lists from case installations in the project partner countries. Initially this was done for the textile sector by consultants (co-ordination by adelphi consult; cf. separate WP-4 report[36]). From each of these 4 case studies, overviews were available for the HAZBREF project team in the form of an Excel spreadsheet. The chemicals used are predominantly mixtures, whereby the individual substances can largely be identified by a CAS number. Further information relates to the technical function, the content in the preparation, the ecotoxicological potential and the degradation behaviour. Depending on the case study, the information on the substances is detailed in different ways. Often only the product name of the manufacturer can be found and a CAS number is missing. This also has consequences for the comparison with the 940 list for the textile industry from the ECHA database.

For instance, two German companies have provided substance lists based on Safety Data Sheets (SDS) with the following structure (what kind of information was provided?):

1. Excel files were separated in forms related to technical functions[37] (products/substances noted for four case-studies).
2. Among others, the result tables contain a chemical characterisation of the products used by product name and ingredients with CAS Nos., if available. GHS-Hazard classifications are provided, as well as the %-weight content for individual (hazardous) substances. Some general chemical parameters are provided too (COD, BOD5, heavy metal and organic halogen content, total nitrogen and total phosphorous), Waste water relevance classification.
3. With regard to the association of fate and behaviour to substances, the indication of biodegradability (% of the theoretical endpoint in OECD 302/310) and ecotoxicity values are most helpful.

An attempt was made to determine the intersection between the substance lists from the ECHA database and the substance lists of the respective case studies in the textile sector. This procedure is called installation-based approach (strategy D) in the sense of a "reality check". In practice, the substances in the case studies were cross-checked by CAS-number with the ECHA textile database entries (940 chemicals by descriptor: industrial site and professional work). Entries without CAS-numbers were not considered herewith. Multiple hits for one and the same substance within one form or in different forms are observed and not considered.

A comparison of the results of the four case-studies based on the available CAS numbers with the results of Strategy A for the textiles sector (see 940 substances in Figure 2) showed the following findings:

Table 7: Matching rate compared to all textile chemicals extracted from the ECHA database by strategy A (substance-based approach)

Form	**Case study (1)**		**Case study (2)**		**Case study (4)**		**Case study (3)***	
	total	hits	total	hits	total	hits	total	hits

[36]) Available at https://www.syke.fi/en-US/Research__Development/Research_and_development_projects/Projects/Hazardous_industrial_chemicals_in_the_IED_BREFs_HAZBREF/Publications

[37]) Cf. the technical functions in Strategy B.

Pretreatment agents	8	2	-	-	10	3		
Textile auxiliaries for dyeing and printing	14	1	19	3	30	2		
Finishing assistants	6	-	61	15	24	3		
Technical auxiliaries for multipurpose use in the textile industry	11	2	10	3	-	-		
Other "textile auxiliaries"	-	-	42	2	-	-		
Basic textile chemicals	9	3	2		10	1		
Dyestuffs and organic pigments	17	6	14	6	27	10		
No. of Substances	**65**	**14**	**148**	**27**	**101**	**19**	**144**	**47**
Percent	**100**	**21,5**	**100**	**18,2**	**100**	**18.8**	**100**	**32,6**

*) Assignment is not possible here because the study uses other groupings for the substances.

It can be seen that in the industrial plants a different number of substances are assigned to the respective technical functions and that in relatively few cases these substances are also found in the 940 list for the textile industry. In total, only 14 out of 65 chemicals in case study 1 (21.5%) and 27 out of 148 substances in case study 2 (18.2%) are confirmed via the ECHA database list by CAS number. A comparison of all four case studies did not yield significantly different results. The intersection of substances for the third case study was 32.6% (144 substances and 47 hits) and for the fourth case study 18.8% (101 substances and 19 hits). Multiple hits for one and the same substance are observed and not considered. The reasons for these observations lie in the following:

a) The four case studies do not, of course, cover all the substances used in the textile sector. As outlined in the Sector Guidance they cover a wide range of processes, raw materials and products covered by the TXT BREF. However, there are lines of products (processing of wool, carpet production) that are not covered. Therefore, it cannot be confirmed on this basis that the substances in the 940 list are all used in the textile sector. Conversely, the 940 list does not include all substances used in textiles, as the following example shows. The problem lies also in the inconsistent use of the descriptors for use sectors and application forms.

b) For instance, an enzyme preparation from ARCHROMA (BACTOSOL PHC LIG CONC) contains an alpha-amylase (CAS 9000-90-2) with 1 - 10%, which is also registered in the 940 list for the textile sector (among others). The preparation also contains 1,2-benzisothiazol-3(2H)-one (CAS 2634-33-5) with 0.05 - < 5%, which does not appear in the 940 list because neither 'Ind-sector-of-use' nor 'Prof-workers-use-sector' contain 'textile*'. This means that substances are used which are not explicitly registered for the textile sector. They may not have a direct function for textile processing, but are process additives (e.g. biocides). The excipients do not appear to be indicated specifically for sectors.

c) It is noteworthy that the whole preparation contains hazard statements (H317, H319, H334). H317 refers to 1,2-benzisothiazol-3(2H)-ones, while H334 is associated with alpha-amylase. This means that hazard warnings can emanate from the main constituents as well as from co-formulants.

d) Not all substances in the 940 list have a CAS number. More than 200 compounds, mainly reaction masses, are therefore not considered in this cross-checking.

e) Almost all chemicals within the 940 list from the ECHA database are selected according to the character strings "Textile treatment agents and dyes" and "Textile, leather or fur". However, the characteristic "textile" is not a clearly defined criterion in the ECHA database as it appears together with the materials "leather" and "fur". For example, some of the identified substances (940 list) can also be used primarily for the processing of leather and furs and represent false positive results.

f) Another point could be that the registrants of a substance under REACH cannot know its full use in the supply chain, so that a niche application in the textile industry is not recognized. This may be due to delays in communication in the supply chain, also.

g) Well over 400 chemicals have been identified within the case studies on the basis of the CAS numbers, although there is little overlap in the use of the substances. For example, only 26 chemicals are used simultaneously in two or three textile processing plants and only four substances are found in all case studies. On the one hand, this proves the special type of applications and the selection of installations under WP 4.2 and, on the other hand, explains the large number of substances/mixtures as listed in the TXT Questionnaire.

h) It could be observed that some substances or classes of chemicals are used for more than one technical function (e.g. surfactants appear in various forms). The differences in the descriptors (e.g. technical function) within a sector and those under the Reach Guidance on information Requirements R12 have already been discussed under strategy A (table 5).

i) In the various case studies there are also chemicals identified under REACH as SVHC substances like cyclic volatile methyl siloxane (cVMS). These are Oktametylocyclo-tetrasiloxan (D4), Decamethylcyclopentasiloxane (D5), and Dodecamethylcyclo-hexasiloxan (D6,). Only D5 can be found in the 940 ECHA list. D4 meets the criteria in Annex XIII to Regulation (EC) No 1907/2006 for the identification of a persistent, bio-accumulative and toxic ('PBT') substance and a vPvB substance. D5 and D6 were identified as vPvB substances, but were also considered to be PBT substances where the concentration of D4 (as a constituent) exceeded a concentration limit of 0.1 % w/w. Since January 2019 for all 3 substances an Annex XV Restriction Report (Proposal for a Restriction) is available). All 3 substances are already registered or listed under the OEKO-TEX label[38].

j) In one case study Tetrachloroethylene was found to be applied, but not in 940 ECHA list. This substance is toxic to aquatic life with long lasting effects and is suspected of causing cancer. It is worth mentioning that this substance is already listed in various action programs of the textile industry such as the Zero-Discharge of Hazardous Chemicals - ZDHC activity (ZDHC MRSL[39]) and the OEKO-TEX certification process.

[38]) Standard 100 by OEKO-TEX: https://www.oeko-tex.com/en/our-standards/standard-100-by-oeko-tex

[39]) ZDHC Manufacturing Restricted Substance List: https://mrsl.roadmaptozero.com/

k) Also, biocides can be found in the list of the case studies. 1,2-benzisothiazol-3(2H)-one (not addressed in 940 ECHA list) is being reviewed for use as a biocide in the EEA for: disinfection, product preservation, preservation of fibres, leather, rubber, or polymers etc. (ECHA, dissemination site). Among other hazards, the substance is very toxic to aquatic life. Permethrin (not addressed in 940 ECHA list) is also used in textiles and is a substance that has negative effects on the aquatic environment (H 400, H410). Furthermore, Pyrithione zinc (13463-41-7, not included in 940 ECHA list) is also found in one case study. According to the classification provided by companies to ECHA in CLP notifications this substance is very toxic to aquatic life, is very toxic to aquatic life with long lasting effects, causes damage to organs and is suspected of damaging fertility or the unborn child.

l) In one case study the substance Titanium dioxide (13463-67-7); and Cetrimonium chloride (CAS-No. 112-02-7, EC No. 203-928-6), are applied to textiles. The latter was not addressed in the 940 ECHA list. According to the classification provided by companies to ECHA in REACH registrations titanium dioxide is suspected of causing cancer and has a long-term negative impact to the aquatic environment (H 413). This substance is manufactured and/or imported in the European Economic Area in > 1 000 000 tonnes per year and included in the Community Rolling Action Plan (CoRAP).
According to the dissemination website Cetrimonium chloride among others is applied as an antistatic agent (textile spin finishes), softening agent (textile finishes) and in textile treatment products and dyes. As many other quaternary amonium compounds this substance has negative impact to aquatic life (H400, H410).

m) The inventory of substances show, that dyestuffs and organic pigments, textile auxiliaries for dyeing and printing as well as finishing assistants are the most abundant groups of chemicals applied in the installations. Dyestuffs often have negative effects on the aquatic environment and the waste water treatment processes, themselves. When looking at the case studies, dyes and inks are often not documented by a CAS number and therefore cannot be clearly identified. It is therefore quite possible that among the descriptions of these chemicals, such as "disperse dye", "direct dye", "reactive dye" and "pigment dye", there are also dyes that have a sensitising effect or are carcinogenic. For instance, 1-hydroxy-4-[[4-[(methylsulphonyl) oxy] phenyl] amino] anthraquinone (CAS-No.: 216-475-4) is applied in one case study. It is widely used in polymers, plastics, textiles, fabrics, binders in paints and coatings, adhesives, textile treatment agents and paints. The substance is included in the Community Rolling Action Plan (CoRAP). According to the classification provided by companies to ECHA in CLP notifications this substance may cause an allergic skin reaction (H317). It shows negative impact to aquatic life (H400, H410). It is expected that the substance fulfils criteria as PBT/vPvB and suspected PBT/vPvB.
Azo dyes and pigments are colourants that incorporate one or several azo groups (-N=N-) bound with aromatic compounds. Azo dyes represent an abounded group of chemicals, but only those that degrade to form cleavable amines are restricted. Azo dyes that release these amines are regulated and should no longer be used for the dyeing of textiles. A non-exhaustive list of dyes which can form restricted amines can be found in the ZDHC-MRSL.

n) In addition to a comparison of the substances from the case studies with the ECHA list, further information can also be obtained in comparison with other substance lists. The MRSL list from the ZDHC program and the list of the quality standard OEKO-TEX should be mentioned here. In contrast to the Restriction Lists (RSL) of some companies and textile associations, the Manufacturing Restricted Substance List (MRSL) of the ZDHC program lists not only pollutants which may be contained in the end product, but also those which

are used during production and will be released into the environment. These substances are of particular interest here.

Conclusions for Strategy D (case-study-based approach)

It should be noted that filtering substances from the ECHA database (chemical universe) for a given sector is a logical starting point for the purpose of identifying relevant target substances for the revision of BREF TXT ("candidate substances"). Even though this reality check for the textile industry based on the case studies showed only about 30% agreement with the 940 list, valuable information for the sector can be drawn from this approach. It may well be that for other sectors in the course of the revision of BREFs this procedure leads to a greater overlap of the substances used. At a meeting of the HAZBREF partners with ECHA on 10.03.2020, reference was made to the comprehensive investigations of the Plastics Additives Initiative[40]. The target of this project was to characterise the uses of plastic additives and the extent to which the additives may be released from plastic articles. From the large pool of substances extracted from the ECHA database, about 58% were finally identified as relevant (under regulatory review). However, this required the broad participation of experts from the plastics industry to obtain the necessary information on the use of these additives. In this respect, the intersection obtained on the basis of four case studies can be considered a fairly good result.

For the identification of substances in the sense of the reality check (Strategy D), the corresponding descriptors between the information in the ECHA database and that in the respective sector play a decisive role. This became clear in both the substance-based approach (Strategy A, cf. Chapter 4.1) and the use-based approach (Strategy B, cf. Chapter 4.2). Likewise, complete information in the SDS of case studies is a mandatory requirement to achieve a large and reliable intersection with the substances used. In this example of the textile sector, a number of conclusions can be drawn from the reality check.

The chemicals in the case-study lists used are predominantly mixtures, whereby the individual substances cannot always be identified in their entirety by a CAS number. Further information relates to the technical function (forms), the content of a substance in the preparation, the ecotoxicological potential and the release behavior. In many cases a GHS-Hazard Classification and some general chemical parameters are provided (e.g. COD, BOD_5, total nitrogen and phosphorous). Depending on the case-study, the information on the substances is given in varying degrees of detail. Often the degradation rates and (eco-) toxicity for mixtures are only given for the mixture as such, but not for the individual components. However, the degradation behavior and (eco-) toxicological effects of individual substances of concern can be masked or underestimated. The COD test is only a theoretical sum parameter, but an important instrument for controlling the biological degradation stage in wastewater treatment plants. Furthermore, the significance of the BOD_5 test is increased by an existing COD test. But they have no significance for the assessment of the biodegradability of individual substances in an industrial plant, although these data are given in many SDS, for example. Nevertheless: Often only the product name of the manufacturer or a description of the substance can be found whereas the CAS number is missing.

The most interesting substances are those from the case studies which give indications of their concentration in the mixture, biodegradability and ecotoxicity. Nevertheless, the available data

[40] Plastic additives initiative – ECHA: https://echa.europa.eu/de/plastic-additives-initiative

on percentages in mixtures are mostly ranges. Information on biodegradability and ecotoxicity can be checked against the corresponding entries in the ECHA dissemination site. However, for many substances there is no clear information on the degradation behavior in the studies. Furthermore, information on the biodegradation of substances that ultimately originate from the SDBL cannot be confirmed when looking at the ECHA database entries (e.g. claims such as "readily biodegradable" are not supported by the available tests or their significance is questioned).

If the substance information e.g. on aquatic ecotoxicity is considered, there are also deviations from the ECHA entries. The information in the safety data sheets does not always seem to be up to date. So how should the quality of SDS be further improved? ECHA has long recognized the need to improve the quality of SDS. In cooperation with the (Enforcement) Forum a checklist for safety data sheets has been developed[41]. The sectoral associations should support their members in identifying the relevant uses. The results could also be used for training purposes of the responsible staff in the industrial facilities. Additional consistency checks are required.

All of this information is, however, crucial in order to first identify the substances with certainty, to be able to draw conclusions about their emission behaviour on the basis of the data on distribution and degradation, and to record relevant target substances in conjunction with information on the danger to humans and the environment as defined in WP2. The case-studies showed that several "substances of concern under ECHA scrutiny" are still in common use (e.g. SVHC, substances included in CoRAP), and these results are of great importance for the revision of any BREF in a given industrial sector. Although the operators of the evaluated installation have indicated that they will not continue to use these substances in the future. The implementation of case studies in the course of the revision of a BREF is a useful accompanying measure to correctly assess the current status of the use of chemicals within an industry sector. Another observation is that many "general purpose chemicals" with negative environmental impact are not specific for the textile sector and clarification is needed, whether they need to be considered in a BREF revision. The experiences with this approach underpin the fact that the requirement for an exhaustive list of hazardous substances for a given sector is not realistic. Rather than to create fix substance lists for the BREFs in any further revision, it is better to refer dynamically to different sources of "substances of concern", which are more or less regularly updated (e.g. WFD, SVHC Candidate List, ZDHC etc.).

In the context of future revisions of BREFs of other sectors, it is therefore recommended to cooperate with ECHA to ensure that a database query is performed on all substances in the sector concerned and the related ongoing regulatory processes. ECHA was able to provide this support to the EIPPC Bureau for the textile sector and to demonstrate this to other sectors under review (e.g. ceramic BREF, started in 2019).

In principle, a reality check based on case studies can also be carried out against strategy B or C. As part of Strategy B, the individual substances and groups of substances resulting from the revision of the Textile BREF document are clearly classified according to their chemical nomenclature. Ideally, these substance groups can then be assigned the ecotoxicological hazard potential and their degradation behavior in water. It would be interesting not only for this sector to know whether the substances identified in the case studies can then also be assigned to these substance groups.

[41] Safety Data Sheet Check List-ECHA: https://echa.europa.eu/de/regulations/reach/safety-data-sheets/checklist

4.3.3 Case studies from other sectors

In contrast to the case studies from the textile sector, the case studies from the chemical sector (polymers) and the STM sector, as well as the substance lists compiled from them, were only partially evaluated by the HAZBREF approaches to identify hazardous substances (strategies A-D). The findings from the case studies and the particular importance of SDS and ES as essential elements of chemicals management in the chemicals sector (polymers) and in the STM sector have been addressed in the corresponding Sectoral Guidelines[42, 43].

In the polymer sector, the substance lists from the various plants varied greatly in terms of scope and information content. In some cases, critical substances have also been identified that occur unintentionally or as impurities. Most of these hazardous substances are bound in the polymer and their concentration is usually low.

The information from the case studies of the STM sector is not as comprehensive as it could be identified for the textile sector. Although the substance lists also contain information on hazard statements, biodegradability or elimination (BOD/COD ratio), toxicity to microorganisms and toxicity to aquatic organisms, the information content here was significantly lower.

One of the HAZBREF approaches to identify hazardous substances from regulatory lists (Strategy C) was applied for STM sector exemplarily and is described in full detail in Annex 7 of the respective Sector guidance document. In this strategy the starting point was to identify which WFD substances and SVHCs are used in the STM sector (cf. Chapter 3 in this report). Altogether 81 substances or substance groups were identified to be potentially used in the STM sector. The identified substances and information e.g. on their uses are reflected. For example, several phthalates, cadmium, cobalt, chromium and lead substances as well as PFAS substances (PFBS & PFNA) are most likely used in STM sector. The outcome of strategy C was compared with the information from HAZBREF case studies: As a kind of reality check 13 out of 81 substances were found to be in use in HAZBREF case installations. This approach makes clear that the identification of hazardous substances in a specific industrial sector requires a reality check by means of various case studies (strategy D) to review lists of substances from different legal frameworks.

The developed structure-based approach (strategy B) for the identification of chemicals, that may be potentially relevant for certain technical processes, was also applied by Werschkun (2020) to case studies from the polymer sector as well as from the STM sector (cf. Chapter 4.2). It is concluded that the identification of chemicals that may be potentially relevant for certain technical processes can be applied to lists of individual chemicals if there is a well-established relationship between the chemical structure and the technical function. This was demonstrated

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[42]) HAZBREF Workpackage 4, Activity 4.1: Report Sectoral Guidance for Management in the Chemical Industry with focus on the production of fertilisers and polymers, 28.09.2020. Draft report available at: https://www.syke.fi/en-US/Research__Development/Research_and_development_projects/Projects/Hazardous_industrial_chemicals_in_the_IED_BREFs_HAZBREF/Work_packages/Best_practices_in_industry_WP4

[43]) HAZBREF Workpackage 4, Activity 4.1: Report Sectoral Guidance for Chemicals Management in the Surface treatment of metals and plastics Industry, DRAFT 28.09.2020. Draft report available at: https://www.syke.fi/en-US/Research__Development/Research_and_development_projects/Projects/Hazardous_industrial_chemicals_in_the_IED_BREFs_HAZBREF/Work_packages/Best_practices_in_industry_WP4

with the help of a case study for an alkyd production site. In other case studies, namely from the surface treatment of metals, the technical functions of the chemicals listed were not clearly described (different and sometimes contradictory in part conflicting terminologies were used in different case studies within this industry sector). Nevertheless, it is obvious that in many cases the existing SDSs and chemical inventories should be expanded and regularly updated.

4.4 ASSISTANCE on creating inventories of chemicals used in installations

As already discussed in Chapter 2.4.2, the safety data sheets are the first and most important source of information for the operators of an industrial plant about the products used there. Consequently, they also serve for the compilation of a chemicals inventory for the complete recording of all individual substances used in the respective process steps.

Based on the current SDS for the chemical products used at the site, the operator should regularly fill the inventory with the necessary information from the SDS. In this context, it is necessary to assign the substances to the processes in which they are used and to describe the type of emission control measures in place. Any changes in the operational process, whether it is the use of new products or the modification of processes, must be recorded in the chemicals inventory.

The inventory is thus an important instrument of chemicals management for the plant operator in order to limit or, if possible, completely eliminate emissions into the environment. In the context of the question of WP 2, this means that all information shall be available on the substances used, that allows an assessment of their fate and behaviour in the wastewater treatment plant pathway (potential to be released). The identification of target substances (two-step approach) is not primarily concerned with the substances with the most hazardous properties, but also with the question of a possible release of all substances used into the environment. Only, if the respective risk reduction measures for emission control are not sufficient, the question of the hazard potential (intrinsic potential toxicity) of the substances for the aquatic environment arises. At the end of the process is the decision whether the target substances are relevant and whether further measures are mandatory.

Beside information on the identity (substance name, CAS- or EC-number) of the substance under consideration the inventory should contain a clear description of the technical processes used. Where available, information on the chemical function of the substance or mixture should also be provided. It is also useful to indicate to which chemical group a substance can be assigned. Information on the concentration of individual substances in mixtures as well as information on classification and regulatory status should not be missing.

In addition, it is necessary to adopt some essential physical-chemical data from the SDS, which indicate the distribution of the substance in the environmental media. These are e.g. data on water solubility, volatility, partitioning coefficient K_{ow} and adsorptivity log K_{oc}).

Furthermore, information on relevant parameters regarding the “potential to be released” and the “potential for eco- and human toxicity” are mandatory as described above (cf. Chapter 2.3.1 and 2.3.2). Corresponding data on endpoints for fate and behavior as well as for (eco-) toxicity are summarized in Table 1 "Substance properties for the determination of the parameter of concern" in Chapter 2.3.1. This overview also contains the information on the common units, Guidelines for measurement or determination and of trigger value for hazard identification. Additionally, there are remarks to illustrate special features of the different parameters and test results.

Furthermore, operational data on the amount of substances used (possibly differentiated by technical processes), the operation of the wastewater treatment plant (effluent flow rate, concentration in waste water) and the risk reduction measures (abatement technique) already established can complete the chemicals inventory.

In all cases where information cannot be obtained from the SDS, it is recommended to search the ECHA database. If required data in terms of the Safety Data Sheet Directive are missing or no reason is given, the supplier is to be contacted.

An overview on the information requirements for chemical inventories is given in the Sectoral Guidance for Chemicals (Chapter 4.5, p. 26) as well as in the Sectoral Guidance for Textiles (Chapter 3.2.3, p. 28). Examples on how to create a good or well-maintained chemicals inventory is provided in Annex 9 of the Sectoral Guidance for Chemicals (p. 51 ff.) and Annex 6 of the Sectoral Guidance for Textiles (p. 103) respectively. At the same time, a current ECHA proposal for the content of the chemicals inventory exists in the Appendix of a document dealing with a methodology to prioritise chemicals for prevention or control of emissions (ECHA, unpublished). It is mandatory that the inventory contains the information on the parameters of concern as listed in an overview table (c.f. Chapter 2.3.1), so that the plant operator can identify relevant target substances using the "interactive scheme" (cf. Chapter 5).

5 Identification of relevant target substances – Interactive scheme

The aim and intention of WP 2 was to exploit existing information sources on chemicals to bring more chemicals related information into the BREFs.

The expectation is to cover all substances used in an industrial sector. This turned out to be difficult:

- the use information provided by registrants in the ECHA database is for some branches very general
- the case studies in the HAZBREF project have provided only fragmented information on the substances used in the specific industrial sector;
- the composition of products and mixtures (with certain technical functions) often could not be identified;
- it is not satisfactory to limit BREFs only to SVHCs or other priority substances, otherwise many substances released into the environment from industry via wastewater (and other waste streams) would not be covered.

An important finding for the further development of BREFs is that inventories of the chemicals used in specific sectors should be compiled. This can be done specifically for installations and their processes, but also generically for technical and chemical functions and chemical groups on branch level. A very good example of this was dealt with in WP 2, starting from the textile processing sector. WP 2 demonstrated with the "Werschkun approach" (strategy B) how chemical groups (based on technical functions) can be resolved into representative individual substances. With this approach, sector-specific substance groups can be compiled and substance data information in the ECHA database may be applied to chemical groups.

In WP 2 a two-step approach to identify relevant target substances that need to be reflected in BREFs was developed.

1. Step: Target substances for treatment in BREFs are those expected to be released from installations with the waste water stream (WP 2 focuses on industrial wastewater treatment plants). The substance properties that are important for potential to be released refer to physico-chemical properties and degradation behaviour. These data can be extracted from the ECHA database. Target substances that have a high potential to be released are substances of concern.

2. Step: Target substances are of particular relevance for BAT conclusions if, in addition to a high potential to be released, they have ecotoxicological or human toxicological properties of concern or are emitted in large quantities. This then characterises relevant target substances for the development of BAT conclusions.

These two characterisations are dealt with in the "interactive scheme". This scheme may guide those responsible for chemicals management or in charge of revising BREFs to identify relevant target substances for which action is required. There is a need for action on the one hand for the preparation of BAT-conclusions (e.g. by the EIPPCB) and on the other hand for the implementation of measures by installation operators for the elimination of these substances from the waste water stream, or for the approval of their emission into the environment by authorities.

In parallel, as a rule for each substance used, a review of the regulatory status should be carried out, e.g. with regard to the identification of the substance as SVHC or the expectation of regulatory measures for the substance according to REACH or the regulation under WFD as priority substance. This will align chemical management measures in the facilities with other regulations besides the IED (e.g. REACH, CLP, WFD or voluntary quality standards).

Annex 6a contains an overview of the interactive scheme, appendix 6b a detailed description of the individual steps from starting the scheme to the final decision-making. The IT-solution of the interactive scheme can be accessed under https://hazbref.rescol.de. Appendix 6b can be used as a guide when using the IT-solution.

5.1 Objective, scope and target groups of the interactive scheme

As said above one aim was to bring information on (relevant) target substances into BREFs.

Another aim turned out during the project: to support operators of industrial installations in safe handling of chemicals during use and wastewater treatment. Detailed information on chemicals actually employed is sometimes lacking by that stakeholders.

The plant operator knows or should know which chemicals are used in his plant. This knowledge or this information should be known when revising BREFs in order to enable a selection of (relevant) target substances from the entirety of chemicals used in a branch in the BREF process. Enhanced knowledge at site level will again support the BREF revision process.

In addition, it seems meaningful to process information about chemicals at the level of branch associations. This is useful to support operators of industrial installations who do not have their own in-house expertise. In addition, branch associations can compile knowledge about processes and the chemicals used or support in the selection of suitable alternatives to (relevant) target substances.

Thus, considerations to create a chemicals inventory and to identify relevant target substances have been developed for the different stakeholders in the implementation of the IED.

The application of the interactive scheme presented in this report is first described from the perspective of the installation operator. Where appropriate, additional information is provided for branch associations and the Sevilla Process. Thus, the interactive scheme supports the following target groups and these target groups should check if actions for the safe use of identified (relevant) target substances are necessary:

- The interactive scheme primarily addresses the plant operator. Plant operators are supported in initiating (additional) risk management measures (emission prevention and control measures) for (relevant) target substances.
- However, the scheme can also be used by the branch associations. Using the scheme, they can create complete lists of substances employed in the branch, subdivided into processes, supplemented by information on alternative substances and information on safe use. Branch associations can also provide compilations of the regulatory status and expected regulations and thus take that burden off the individual companies. At branch association level one can derive standard phrases for safe handling or make provisions for substitution of substances.
- Use of the interactive scheme is also possible when revising BREFs. Here the TWG could use the scheme to identify the substances that should be addressed in the BREFs and identify (relevant) target substances for which BAT should be derived.

Other interested parties, e.g. NGOs, can also use the interactive scheme to make their own statements about substances that they consider to need regulation.

All decisions in the interactive scheme are applicable to the operators and branch association. The TWG can omit decision D 2.3 to D 2.5. as these decisions represent a safety net for the operator.

Annex 6 (powerpoint presentation) provides an overview of the interactive scheme developed to support the stakeholders mentioned to identify substances where (additional) risk management measures might be necessary.

The entirety of all chemical products, mixtures and substances used in an installation is the starting point for the chemicals inventory and the search for (relevant) target substances. There is no limitation to classified substances, hazardous substances (depending on the regulation) or substances regulated for example under REACH or WFD. This decision was made for the following reasons:

- Approx. 25,000 substances are registered under REACH. The identification of SVHC from all these substances has not yet been completed. Furthermore, a minority of the substances has undergone detailed assessments by authorities. A limitation to SVHC when searching for (relevant) target substances would then be too short-sighted. Furthermore, currently, only around 200 substances are identified as SVHC according to REACH. Efforts to substitute these substances are expected or are already underway. A minimization of the release of these substances into the environment is already prescribed by the REACH regulation. Plant operators, industry associations, as well as the TWG should reflect on the provisions made under REACH. Operators should substitute SVHC and branch associations should support in the search for alternatives. In the process of revising BREFs, the TWG should prescribe substitution by referring to the REACH obligations.

- Harmonised classifications have so far been available in the CLP inventory for effects on human health. For the environment there are only classifications for aquatic toxicity and these classifications are not harmonised for all substances in the classification and labelling register. Furthermore, classification for other effects on the environment, e.g. endocrine disruption, PBT-properties, PMT-properties do not exist at all. The limitation to classified substances as a pool for substances relevant for BREFs might be too short-sighted.

The presented interactive scheme is one solution of many. The open office software was used for the interactive scheme. The scheme can be accessed under https://hazbref.rescol.de.

What is an interactive scheme? The interactive scheme is a kind of decision tree. A decision tree describes a sequence of operations to solve a task. This enables decisions and assessments to be made with simplified means. A sequence of operations is called decision-making process in the following chapters.

The task is to identify substances for which a release into the environment can be expected and which have certain properties of concern. For this task the following decision-making processes were developed:

Block 1: Establish and complete a chemicals inventory.

Block 2: Identify relevant target substances in a two-step approach.

Figure 3 shows the total possible emission pathway from an industrial installation. However, the interactive scheme developed is limited to emissions of chemicals via wastewater and sewage treatment into the environment.

Decisions for the identification of chemicals as (relevant) target substances were defined for this pathway. No decisions have yet been defined for direct emissions into the air or the soil, or for chemicals to remain in waste. That means, chemicals that are released into the environment via air, soil or waste, are not recognized as relevant target substances by this interactive scheme. Decisions on the identification as relevant target substance can, however, be added for these pathways at a later stage. The interactive scheme is structured in such a way that additions as decision-making processes are possible. The same applies to emissions of solid substances into the environment via sewage treatment plants. However, these decisions can also be added later.

The interactive scheme puts the results of WP 2 in connection. The results of WP 2 are:

- The derivation of approaches for the creation of lists of substances used in industry (strategy A to D, see chapter 3 and 4)
- The provision and use of information available about chemicals in different legislation, in particular in REACH. These are above all data on substance properties, information on the regulatory status and, to a limited extent, information on the use of substances in industry (limited because there are large gaps in the completeness of use data provided by industry to REACH and deficits in the transferability of the knowledge from REACH to the IED).

The interactive scheme enables access to the results of WP 2 via short decisions and subsequent actions. The use of the interactive scheme should always be accompanied with more detailed information available in this WP 2 report. That means, the interactive scheme is not seen independently of the report. For example, in the scheme reference is made to the strategies A to D for creating lists of substances. However, these are not worked out step-by-step in the scheme currently (this can be added in the future).

5.2 Structural elements of the interactive scheme

We used the following flowchart elements, based on DIN 66001 (see Annex 6 second slide):

- Yellow oval: This starts or ends a process. The interactive scheme contains two processes elaborated (green circle): block 1 and block 2.
- Blue diamond: In the diamond, questions are asked that can be answered with Yes and No. Yes and No are mandatory outputs out of this element.
- Red rectangle: an action is symbolized with a rectangle. Such an action is, for example, collection of data, review of facts such as the regulatory status, or to evaluate system technology.
- Green circles: a green circle refers to a (subsequent) process. Processes are either elaborated in the scheme (block 1 and block 2), or have yet to be developed, as they are outside of the scope of HAZBREF.
- Rectangles with rounded corners: These rectangles represent conclusions and (intermediate) results. The rectangles are differentiated according to the type of conclusion. Green lines represent "positive" conclusion where no further action for safe handling of the substance is needed. Red lines show conclusions where action is needed. Red rectangles with red lines show (intermediate) results for (relevant) target substances and provide further actions needed.
- Brown book symbol: provide further information, provide a choice of options, refer to documents, or provide links.

The use of the interactive scheme begins with the process start at the yellow oval "Block 1". This is followed by a question, blue diamond, e.g. "Are all substances used in the installation recorded in a chemicals inventory?" A question can be answered with "Yes" or "No". Depending on the answer, the interactive scheme leads to the next question or to an action, red rectangle, e.g. "Apply one or more strategies to complete the list of substances used". If the user clicks on the questions or actions in the interactive IT solution (https://hazbref.rescol.de), he gets background information, e. g. what is the point of a question. In case several options to conduct an action are provided this is symbolised in the interactive scheme provided as an overview picture in annex 6 with a brown book symbol. In the IT solution one can reach this further information by clicking on the action. After deciding on a decision or performing an action, the user is forwarded to the next decision or a further action. The process ends when a yellow oval is reached. A process in this scheme can also end when a green circle is reached which starts a new process. The transition from block 1 to block 2, for example, is marked with a green circle "start two step approach". This scheme can be expanded at the points of a green circle. For example, new processes could be developed to evaluate other environmental compartments.

5.3 Block 1 of the interactive scheme: Establishing a chemicals inventory

Block 1 has five sections: 1.1 Improve list of chemicals used in chemicals inventory, 1.2 Complete data on relevant substance properties, 1.3 Record the regulatory status of substances used, 1.4 Handle substances according to regulation, 1.5. Assess the pathway(s) of release. The interactive scheme will guide the user through the various sections and show which tools or data sources can be used.

Structure of chemicals inventory

The aim of block 1is to improve the structure and complete data the chemicals inventory.

Block 1 proposes to create a chemicals inventory for all substances used in an installation and to collect the data necessary to assess the relevance for additional measure to ensure safe handling of substance. In the inventory, all chemicals-related and process-related information is to be compiled, which is necessary for the assessment as a relevant target substance for the specific industrial plant or (from the point of view of the branch associations or TWG) for the branch. Not all elements suggested for the chemicals inventory are required for assessing the decisions in the interactive scheme. Nevertheless, for reasons of environmental protection or human health protection, it makes sense to collect them in a chemicals inventory.

An inventory is required in order to identify sources of emissions to the environment and to take appropriate measures at the various levels by the IED stakeholders to minimise emissions to the environment.

The chemicals inventory should have the following sections:

Heading / Identifier: Substance name, Unique identifier (CAS-no. and/or EC-no., IUPAC name)

A: Information on substance properties and fate / behaviour in the environment: This block contains data that are required to decide whether the substance is a relevant target substance.

B: Information on substance degradation products and their properties, fate / behaviour: Data on degradation products are important, because it is possible that it is not the substance itself but the degradation product that poses a risk for the environment (e.g. PFAS). When substances are mentioned in the interactive scheme, always parent substances and their degradation products are meant.

C: Information on the processes where the substance is used: A substance is used in one or more processes for a specific purpose. The substance itself is used or the substance is contained in a mixture / in a product that is used in the process. It is important to know if the same substance is contained in different products or if the substance or products are used in several processes. Usually, the quantitative information on safe use in the REACH registration or in the SDS assumes that the substance is used in a single process or in a single product. The use of a substance in different processes or in different products increases emissions into the environment. It may therefore be necessary for a plant operator to carry out a risk calculation, i.e. calculate the PEC / PNEC ratio based on the actual quantities used for a substance in different processes or in different products (scaling). Furthermore, information about the purpose or the technical function of the substance in a process is an important input data for the decision whether the substance is built into or onto matrix, whether it is transformed during the process or whether it is released into wastewater, air or waste. It is obvious that this has an impact on the decision on the risk for the environment.

D: Information on the regulatory status

E: Record outcome of assessments

The following table suggests the fields that a chemicals inventory should contain. The proposal also considers suggestion for some elements based on BAT 13 and 14 (textile BREF) and the

ECHA proposal (ECHA, unpublished). The information on the products used in an installation may already be saved in an IT system at installation site. Corresponding compilations can also be available at branch level or at TWG. The mentioned actors can nevertheless compare their register against the one proposed here and expand theirs if necessary.

Substance name, Unique identifier (CAS-no. and/or EC-no., IUPAC name)
A: Substance properties:
• Solubility
• Vapour pressure
• Degradability >> Persistence
• Adsorption / desorption coefficient (log K_{oc}) >> Mobility
• Bioaccumulation
• Effects on the environment: Eco-toxicity, ED-effects, PNEC
• Effects on human health: at least CMR, ED-effects, skin sensibility
B: Degradation products and their properties: similar to properties for the starting substance
• (same as under A)
C: Information on processes where the substance is used
• Process A:
• Description of process, techniques, …
• Substance used as such, in a mixture / product, name of mixture / product, concentration in mixture / product
• Technical function of the substance in process:
• Characterisation of exposure: Environment: ERC or SPERC (e.g. considerations like: reacting on use, integration into / onto matrix, processing aid, Release factor, conditions of safe use (amounts used, risk management measure, PEC derived)
• Release expected to: air / water / solid waste
• Abatement technique in place
• Information on amounts stored, used, recovered, disposed of, returned to suppliers
• Process B:
• (as under process A)
D: Regulatory status

• Regulation under REACH, WFD, national law, etc.
E: Results of assessment
• Results of assessments: degradability, mobility, PEC / PNEC ratio, PBT assessment
• Further action if necessary: e.g. monitoring, adaptation sewage treatment, substitution
• Substance of concern / Relevant target substance e.g. as a result from interactive scheme for waste water)
• (to be added)….

Table 8: Elements of a chemicals inventory

The figure 6 from ECHA shows the relationship between a part of the proposed entries in the inventory.

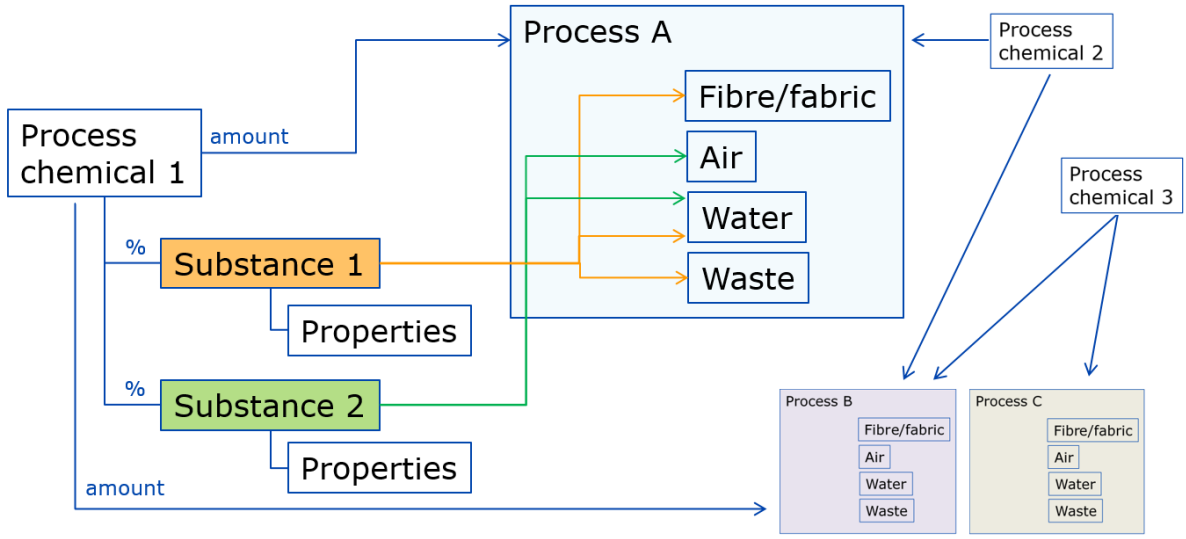

Figure 6: Suggestion to structure a chemicals inventory

(Source: Monique Pillet, ECHA, presentation 04.06.2020 final conference HAZBREF project)

A detailed description of Block 1 step-by-step can be found in Annex 6b.

5.4 Block 2: The two-step approach to identify relevant target substances

Block 2 has 2 sections: Step 1: Check if the substance has potential to be released via WWTP into the environment (identify target substance), Step 2: Check if the substance has (eco)toxicological properties of concern. Result: Identification of (relevant) target substances.

Definitions

The potentially large number of chemicals used in industrial processes, their varying intrinsic properties, the different abatement efficiencies for preventing and reducing releases, and the overall concern they may cause, suggest seeking certain target substances of particular relevance. (Relevant) target substances in HAZBREF project are chemicals or substance groups, which may pose a danger due to their fate and hazard properties, and which occur in industrial activities covered by Annex I of the IED.

Target substances: substances with properties that give rise to concern besides the criteria for identification as "hazardous". This group of substances should be used with caution, as they have a potential to be released and can pose a risk to the environment even without having any yet identified adverse effects on the environment or on human health via the environment. These substances can e.g. in the future be identified as SVHC under REACH based on the "equivalent level of concern" (ELOC) argumentation according to Art. 57 f of REACH. ELOC means that, in the opinion of experts, these substances can have a similar level of concern than substances identified as SVHC according to 57 a – e of REACH. For target substances the operator needs to take (additional) measures for safe use.

Relevant target substance: relevant target substances are released into the environment and have effects on the environment or on humans via environment.

The distinction between target and relevant target substances is necessary and sensible in order to draw attention to substances that may not have been considered in previous prioritisation methods, since the starting point for prioritisation is usually the evidence of an effect on the environment or humans (via the environment). The "prioritisation concept" proposed in this report begins, so to speak, from the other side: it first considers fate and behavior as well as exposure and then the effects. Through the development and discussion of the PMT concept, which puts the properties persistence and mobility in the foreground, the focus in chemicals regulation is increasingly on these substance properties with the aim of identifying these substances as substances of concern and in need of regulation.

The PFAS group is an important example for this. PFAS remain in the environment and can only be removed from the environment with great effort due to their mobility. Due to these properties they are a threat to the resources of our drinking water. Effects on environment or humans have so far only been proven for individual substances in this group. Nevertheless, the focus is on the group as a whole. There is no waiting for hazards to be identified for all representatives of the group. The fact that the substances are emitted into the environment and remain there due to their properties should be assessed as a reason for regulation. The focus is on the need for regulation moving away from hazard-centered to exposure- and hazard-rated regulation.

We suggest to take a closer look on persistent and mobile substances without anticipating that these substances may not be allowed to be used in industrial installations. However, it is recommended that these target substances be examined more closely. This is independent of, but especially if these substances present hazard properties (relevant target substances).

Trigger values are explained in chapter 2 and are based on the values from the REACH Regulation and the CLP Regulation.

A detailed description of Block 2 step-by-step can be found in Annex 6b.

6 Practical conclusions from WP 2

Chapter 6 again takes up the Figure 4 from Chapter 1.5, which provides an overview of the procedure of this report. Some important conclusions are numbered – mainly in the upper part of the figure – and recommendations for stakeholders in the BREF revision process are derived from them – see capital letters mainly in the lower part of the figure.

The procedure for the identification of (relevant) target substances for handling in BAT conclusions starts with the establishment of chemicals inventories for installations and/or, generically, for industrial sectors. Several procedures may be applied to do this, and it is important to break down chemical products and mixtures to their components, individual ingredients and impurities. The outcomes are lists of individual substances or groups of similar substances, for which physico-chemical properties, fate and behaviour in the environment, as well as (eco)toxicological properties may be derived from the ECHA database of registered substances or other sources.

A check of the regulatory status of substances will reveal whether they are already considered to be substances of very high concern under REACH or priority substances under the WFD. Such substances are relevant for BAT conclusions anyway, and this should lead to a substitution of these substances in the industrial production process.

The additional pathway of examination is based on the assessment of certain relevant substance parameters according to the interactive scheme presented in Chapter 5 of this report. These substances of concern might not (all yet) regulated under EU chemicals law or WFD and therefore these substances should be addressed in the BREF process in order to manage their emissions from installations. Therefore, the target is to substitute these substances, next to minimising emissions.

When managing chemicals, the distinction between hazardous substances and substances of concern requires a close collaboration and information exchange between, in particular, authorities and agencies (like ECHA) on the one hand, and installation operators and industrial associations on the other hand.

For further recommendations see HAZBREF Activity 3.2 report (Suhr et al. 2021 draft).

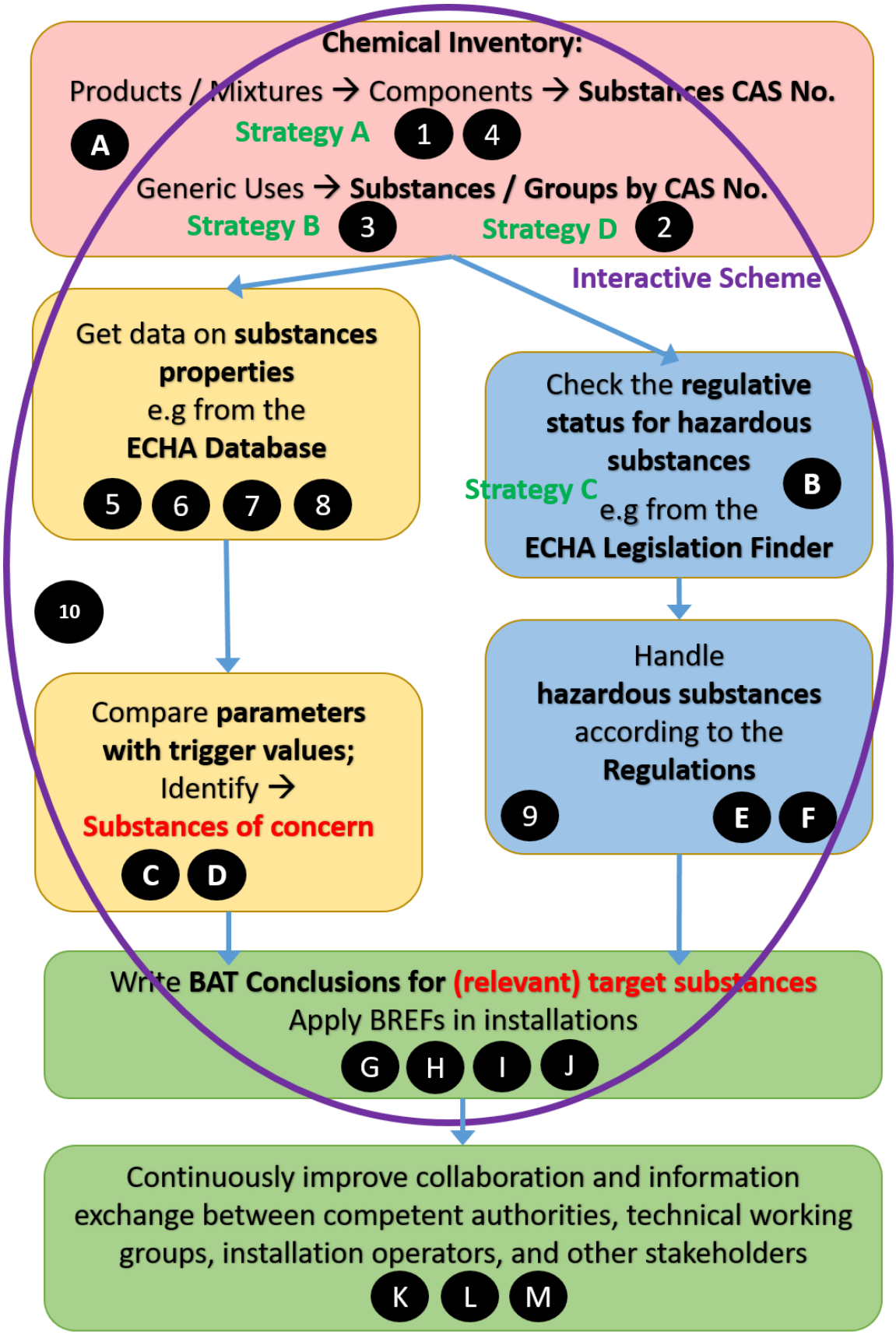

Figure 7: Process steps for the identification of (relevant) target substances and assignment of conclusions (numbers)drawn and recommendations (letters) suggested.

CONCLUSIONS

1. A sector-specific compilation of the substances used requires applying several approaches (refers to the different strategies (A – D) in the context of the WP 2 report) and using various information sources such as SDS, Exposure Scenarios (REACH), ECHA database, non-regulatory lists of chemicals etc. gathering the information needed for decision making purposes. With a broad approach for a meaningful use description[44], the use categories of individual substances can be recorded precisely enough to capture the area of use and thus the possible emission source of the substance. On the other hand, a meaningful use description can also be used to differentiate substances that have broad, cross-sectoral use and are therefore suitable for horizontal BREFs.
2. It is desirable to identify target substances to be considered for BREFs and BAT conclusions based on real site information on production processes and chemicals inventories of industrial installations.
3. Different approaches (utilising use descriptors, technical functions, hazard characteristics) may be applied in parallel and support the grouping of similar substances.
4. The knowledge about individual substances actually used in a sector can be significantly expanded, if the composition of chemical products and mixtures (given by trade names) is disclosed by producers or importers of chemicals e.g. in SDSs. If this is confidential business information an approach descripted in strategy B can be applied to identify chemical classes of substances with similar technical function and similar substance properties. Solid information about substance properties is a prerequisite for identifying target substances and thus release minimisation or substitution.
5. REACH and other prioritisation schemes can provide extensive information on substance properties in order to substantiate hazards and concerns.
6. ECHA is continuously improving access to the public knowledge base on chemicals for stakeholders. However, there is still a lot of room for improvement of the database. This is mainly up to ECHA to check the opportunities for improvement together with sector representatives. Furthermore, it is task of the registrants (according to REACH) to improve information regarding technical functions and uses of the chemicals and update ECHA database regularly. Since the ECHA database was (until now) not designed for overviews of substances used in certain industrial or BREF-sectors, the information on ‘uses’ contained in the database is usually quite general. The information on the ECHA dissemination site is helpful to get a first impression of the use. The conditions of use (exposure scenarios) are usually generic and do not represent one-to-one the specific conditions of use at the industrial site. However, there are currently still gaps in the use description, as some companies do not regularly update their registration dossier of their substance used (see chapter 4.1 and 4.2 WP 2 report).
7. Safety Data Sheets are an important source of information for installation operators because SDSs compile and provide substance information in a use-related way. Nevertheless, it is obvious that existing SDS should be expanded and updated in many cases especially concerning chemical composition of mixtures and exposure scenarios.

[44] Currently the use description under REACH (ECHA guideline R 12 and R 16) is not always compatible with use description under IED or OECD emission scenarios. In addition, it should be considered whether the use or the technical function is the appropriate basis for the description of use (compare conclusion 6).

8. Knowledge on uses and exposure is fragmented, in particular as it relies on industry to provide accurate information. This information need has been stated clearly in European Commission´s Chemicals Strategy for Sustainability[45], which is part of the EU's zero pollution ambition: "… there is much knowledge to be acquired by authorities on the intrinsic properties of a vast majority of chemicals, including polymers and chemicals that are not manufactured in high volumes". This HAZBREF project has also shown the clear need to improve data quality and availability of data when it comes to identifying target substances for BREF revision, which is prerequisite for reducing emissions.
9. In understanding the differentiation between "hazardous" and "of concern", it is appropriate to treat those substances which are *per se* hazardous or priority substances (i.e. regulated in other regulations and directives) differently from those which require action because of their potential for release to the environment.
10. The main outcome of WP2 is that it has been successfully demonstrated how to assess the environmental fate and toxicological relevance of chemicals based on the analysis of substance properties (see the interactive scheme).

RECOMMENDATIONS

The following recommendations are derived from the conclusions described above. It does not make sense to assign the recommendations to the different target stakeholders of the report, as the recommendations are often relevant for different target stakeholders at the same time, who should implement the recommendation from their point of view.

HAZBREF recommends the following:

A. It is helpful that right away or at least during the extended frontloading phase of the BREF revision, sectoral inventories of chemicals be drawn up or made available[46] by operators for their facilities to get an overview of the substances used as a prerequisite to identify target substances, minimise releases or substitute substances of concern. Also, industrial associations could establish chemicals registers for their sectors (see interactive scheme in chapter 5 and Figure 4 and 7). It is also important to derive generic schemes for technical functions and chemical functions for the substances used, so that it is finally known which chemicals or chemical groups are actually used for which purposes (and with which release potentials) (compare strategy B in chapter 4.2). The branch associations and plant operators should have the greatest knowledge of the technical function. Cooperation between ECHA and branches would be an option to make this knowledge available via the ECHA database.
B. The next step following the establishment of an inventory is to identify those substances that are already regulated or regulation is expected in other directives and regulations and to reflect these regulations / obligations for save handling in BREFs (e.g. SVHC or WFD

[45]) European Commission (2020): Chemicals Strategy for Sustainability Towards a Toxic-Free Environment. COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS. Brussels, 14.10.2020, COM (2020) 667 final, 25 pages; https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=COM%3A2020%3A667 %3AFIN .

[46]) It is to be noted that Art. 12 of IED requires that an application for a permit should include, inter alia, a description of […] the substances used by the installation (see par.1, point (b)). This type of information might be readily available (and sometimes organised in the form of preliminary inventories).

priority substances). In this context it should be kept in mind that there is a substitution plan only for substances identified as SVHC and included in Annex XIV of REACH. For SVHC on the candidate list or substances on the registry of intention under REACH no substitution plan is available yet but can be expected in the (near) future. A reflection of these substances at the time of the BREF review is therefore sensible and also necessary due to the significantly different update periods of the REACH annexes and BREFs. In order to ensure the safe use of substances and to enable companies to focus on the future, this recommendation should also be taken up by industry themselves.

C. Different approaches are possible to identify the "substances of concern" which, due to a high potential to be released and potential (eco)toxicological properties, are (relevant) target substances for safe handling or the preparation of BAT conclusions. This report suggests 4 strategies to compile lists of substances used and a two-step approach to identify (relevant) target substances to be addressed in BREF revision process. The developed interactive scheme helps with the identification of target substances.

D. HAZBREF recommends to better identify substances of concern:

- Use the same definitions and trigger values for characterising substances of concern in IED, REACH, WFD etc.;
- align use descriptors (especially in REACH and IED) and unify definitions of technical functions throughout regulations;
- Better linking of various information sources from the different regulations e. g. ECHA database, knowledge from branch associations.

E. For each future BREF review, as a routine, it should be reviewed if restricted, authorised substances, SVHCs on candidate list or WFD substances are still used in a sector for which a BREF review is carried out. The results of this revision should be part of the BREFs. This will align chemical management measures in the facilities with other regulations besides the IED (e.g. REACH, CLP, WFD or voluntary quality standards). Furthermore, make sure decisions on previously used and substituted substances is kept in mind not to invent solutions that already have been discussed twice (history of information should be kept in present).

F. A streamlining of the regulatory frameworks is recommended, in particular with regard to the timeframes for substance evaluation (e. g. within REACH or WFD) and BREF revision. This might accelerate the introduction of recommendations for chemical management from other regulations into BREFs where relevant. Support for the early identification of emerging substances of concern is frequently provided by voluntary, standard-based sectoral programmes (e.g. ZDHC in the textile processing sector), which can often react more quickly than legislation. A link to list of substances of concern in other regulations and voluntary lists make more sense than rigid lists in the BREFs themselves .

G. Data on conditions of use, e.g. amount used in different technical processes, the operation of the wastewater treatment plant (effluent flow rates, concentration in waste water) and the risk reduction measures (abatement techniques) already established can complete the chemicals inventory. These data are necessary to identify sources for emission and to assess if there is a potential to be released to the environment (first step of the recommended two-step approach, see also chapter 5 on interactive scheme).

H. Usage data can support substance-related BAT conclusions. Improvement of use data needs to be done in co-operation with industry (producers / importers of chemical products) and ECHA, IED and REACH authorities and experts at both Member State and EU level. The aim is that ECHA database information such as use information could be more easily linked to IED industrial sectors. The information on the ECHA dissemination site is helpful to get a first impression of the use. The conditions of use (exposure scenarios) are usually generic and do not represent one-to-one the specific conditions of use at the industrial site. However, there are currently still gaps in the use description, as some companies do not regularly update their registration of their substance

I. BAT conclusions can be developed for similar substances (in terms of properties and use) or substance classes - possibly across industrial sectors. After linking the substance properties to the corresponding substance class or group, appropriate risk reduction measures (i.e. abatement techniques) could then be defined for the identified substance class rather than for each individual substance.

J. Clear objectives should be set for the development of BAT conclusions: (a) development of measures to eliminate target substances from the waste stream (water, solids, air) according to the fate & behaviour of the substances; (b) recycling or environmentally sound disposal of chemicals; (c) prevention and replacement of hazardous substances in the production process.

K. An improvement in co-operation between the actors involved is suggested: Exchange of data and information on chemicals (more transparency on substance properties, potential hazards, uses, substance flows, elimination measures) along the value chain; improvement of information on the use of substances in databases; establishment or enhancement of product registers; harmonisation of the objectives and instruments of sustainable chemicals management among the actors and institutions involved; improved use of the specific resources of the actors involved. It should be decided on who is responsible on that. Suggestion: ECHA.

L. During communication of the HAZBREF partners with ECHA with regard to the polymers sector, reference was made to the comprehensive investigations of the Plastics Additives Initiative. The target of this project was to characterise the uses of plastic additives and the extent to which the additives may be released from plastic articles. From the large pool of substances extracted from the ECHA database, about 58% were finally identified as relevant (under regulatory review). However, this required the broad participation of experts from the plastics industry to obtain the necessary information on the use of these additives. This serves as an example for a fruitful co-operation. Make sure that co-operation is established regularly to enhance information on use characterisation. Responsible actor: ECHA and EIPPCB in cooperation.

M. The valuable tool of (extended) Safety Data Sheets should be made more readily usable - with improvements, updates and more realistic emission scenarios. All actors are responsible to introduce the newest and comprehensive data. ECHA as responsible actor to review obligations on eSDS..

R&D SUGGESTIONS

The main finding from WP 2 of this HAZBREF project seems to be that there has been a shift in focus on chemicals relevant to industrial facilities, beyond those chemicals of concern that

are already subject to regulation anyway, to those that give rise to concern because of one property or another. Nevertheless, both assessment of the regulated substances (level of regulation very variable substance by substance; chapter 3) and the non-regulated substances of concern from the chemical universe (chapter 2) are needed because they complement each other in identifying those substances that should be addressed during BREF reviews.

The compilation of these properties in the interactive scheme has revealed the great complexity of this procedure. This is precisely where our recommendations for further work take effect.

Exploiting the knowledge base on chemicals - basically the ECHA database - requires that plant operators and/or industry associations are familiar with the chemicals used in the respective sector. For preparations, mixtures and solutions, the composition, i.e. the individual chemicals used, should be identified. This will then be accessible in sector-specific chemical registers or inventories. Such usage data can also be used for targeted monitoring of emissions from installations, especially the wastewater stream. This can be done by competent authorities or by the plant operators themselves.

Templates for the structure of these chemical registers exist at the regulatory authorities, but also internationally (e.g. at the OECD), which are essentially based on the data already available in the databases. However, there is a certain danger of overloading the chemical registers with detailed information and mixing the two tasks - inventorisation and substance evaluation. The interactive scheme also separates these tasks into two blocks. For this reason, the regulatory authorities (ECHA and national) should agree with stakeholders, especially producers of chemical products and downstream user associations, on a catalogue of necessary entries for the chemical registers. At this point, it is also possible to work with groups of similar chemicals, especially if the chemical functions and environmental behaviour of the substances are similar to each other.

The complexity of the interactive scheme has increased significantly compared to previous assessment schemes that primarily considered degradability. It now takes into account the majority of the entries on substance properties recorded in the databases and has mainly emerged from the working experience of the regulatory authorities involved in HAZBREF. The extent to which the current scheme is practically usable for plant operators or the IPPCB committees remains to be shown.

It therefore makes sense to assess and improve the applicability of the interactive substance evaluation scheme in subsequent research and development projects with the participation of all stakeholders. The current revision of various BREFs can also make a valuable contribution to these efforts.

As a result of these two activities, the quality of safety data sheets (SDS) can also be expected to increase. Improved accessibility and transparency of substance data will benefit the sustainable chemicals management of all installations, but especially of small and medium-sized enterprises.

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Annexes

Annex 1: Approaches to tackle substances of concern in WP 2 of HAZBREF

Annex 2: Table for SVHC and WFD PS identified in Strategy C in Chapter 3

Annex 3: Details on Strategy A: use descriptors in the ECHA Database (Chapter 4.1)

Annex 4: The WP 2 report on Strategy B (cf. Chapter 4.2): Dr. Barbara Werschkun (Wissenschaftsbüro, Berlin), March 2020, Identification of chemicals belonging to chemical classes used as textile auxiliaries, ca. 45 pages.

Annex 5: The report from HAZBREF Activity 2.2 on the usability of SimpleTreat 4.0 (Appelgren et al. 2019) is publicly available under the following link: https://www.syke.fi/download/noname/%7B194D526D-8379-4411-B497-97EC9C591D64%7D/153950

Annex 6a: Interactive scheme (Power point version), see also https://hazbref.rescol.de

Annex 6b: Detailed description of interactive scheme