HAZBREF WP2:

Selection of relevant target substances in BREF industrial sectors

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Objective: Better use of available data to prevent and reduce releases

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To achieve a reduction of releases of hazardous substances

- Relevant target substances
- Information on hazard properties
- Data on fate and behaviour

- Information needs to be included in BREFs
- Needs to be available for operators of installations.

- Focus on waste water treatment.

Approaches

Interreg Baltic Sea Region — European Regional Development Fund — EUROPEAN UNION — HAZBREF

Strategy A

Substance-based approach:
ECHA database from REACH registrations to identify substances used in specific sector

Strategy B + D

Use-based approach
Information available at specific industrial sector

and case study / installation-based approach
Information from experts

Strategy C

Hazard-based approach
Substance lists from different regulations (REACH, WFD, …)

What data is needed for BAT Candidates?

(chemical groups & substances)

Fate & behaviour
+
Hazard alert
+
decision tree

⬇

Recommendations for risk management in WWT

("Standard phrases")

Strategy A: substance-based approach

Survey in ECHA database on registered chemicals, alignment between modelling exercise (WP 2.2) and case-study substances lists (WP 4)

- Procedure: Select chemicals possibly used in the respective industrial sector by **use categories** or **other descriptors** from the REACH-Registrations (e.g. descriptions containing the string 'textil*').

- As a result for textile sector ~ 940 substances were identified.

- Reality check: The chemical lists from 3 case studies was cross-checked by CAS-number with the 940-list. The overlap was less than one third.

- Conclusion: The registered use categories are to general to match the practice; the use of many substances is too wide-spread to limit it to one sector; communication on real uses in the supply chain is insufficient.

- Benefit: ECHA CHEM database provides access to data on substance properties, data may feed into the characterisation of chemical classes and groups.

Strategy B: used-based approach
Strategy D: installation-based approach

Characterise chemical classes and chemical groups by fate and behaviour in the industrial waste-water treatment

- <u>TXT BREF Questionnaire:</u> around 40 technical functions and 200 chemical groups were identified, but hardly any individual target substances.

Strategy B: use-based approach

Extract from the TXT-BREF Questionnaire (DRAFT June 2018)

Detergents/ wetting agents (surfactants)	Technical function	Fabric softeners	Wetti...
Non-ionic	Alcohol and fatty alcohols ethoxylat	(Ethoxylated) fatty alcohols	
	Fatty acids ethoxylates	(Ethoxylated) fatty acids	
	Alkylphenol ethoxylates (APEOs)	(Ethoxylated) sorbitan esters	
Chemical class	Fatty amines ethoxylates	Alkyl phenol ethoxylates (APEO)	
	Triglyceride ethoxylates	Partial glycerides and ethoxylated	
	Ethylene oxide/propylene oxide add	Fatty amides	Comp...
Anionic	Alkyl sulphonates	Sulphonated and sulphated vegeta	
	Alkyl aryl sulphonates		
	Alkyl sulphates Chemical group	Short-chain alkyl phosphates	
	Dialkylsulphosuccinates	Other	
	Alkyl carboxylates (e.g. sodium palm	Polyamide amines	
	Sulphated alkanolamides	Polyvinylpyrrolidone	
	Alkyl ether phosphates	Bisulphate anion (HSO4)-	
Cationic	Quaternary ammonium compounds	Quaternary ammonium salts with	
		Quaternary ammonium salts with a	
Amphoteric	Betaine derivatives	Amido amines (e.g diethylene trian	
	Imidazolines		

Strategy B: used-based approach
Strategy D: installation-based approach

Characterise chemical classes and chemical groups by fate and behaviour in the industrial waste-water treatment

- <u>TXT BREF Questionnaire:</u> around 40 technical functions and 200 chemical groups were identified, but hardly any individual target substances.

- <u>Next step:</u> assign representative chemicals to these 200 groups; it is assumed that these chemicals are 'similar' (behaviour, properties,..)

- <u>Identification</u> of substances supported by lists from case-studies (WP 4 – **Strategy D**).

- <u>The ECHA CHEM database</u> can provide data to characterise fate and behaviour (WP 2.2 "reality check" by modelling) of these substances

- <u>Benefit:</u> Overview of chemical groups and individual substances per group. This is starting point to derive generalized descriptions of risk management measures for STP ("standard phrases")

Strategy C: hazard-based approach

Survey in lists of different regulations to identify target substances: REACH Annex XIV: SVHC (Substances of Very High Concern), Substances on the REACH Candidate List, Water Framework Directive Priority Substances, …

- Aim: are known hazardous substances relevant for industrial sectors under consideration in the project and to what extend is the handling already regulated

- Compilation of substances from this list, extraction of use information for these substances from ECHA database (similar as in Strategy A)

- Additionally, the SPIN register was utilized (Substances in Products in the Nordic Countries – only 2016)

- Substances were grouped to the 3 industrial sectors of the project (NACE categories)

- Modelling of fate and behaviour for 20 high volume substances (SVHC and priority substances WFD)

Selection of target substances in BREF industrial sectors (sector-approach)

Objective: Better use of available data to prevent and reduce releases

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Strategy C: hazard-based approach: examples of the tables

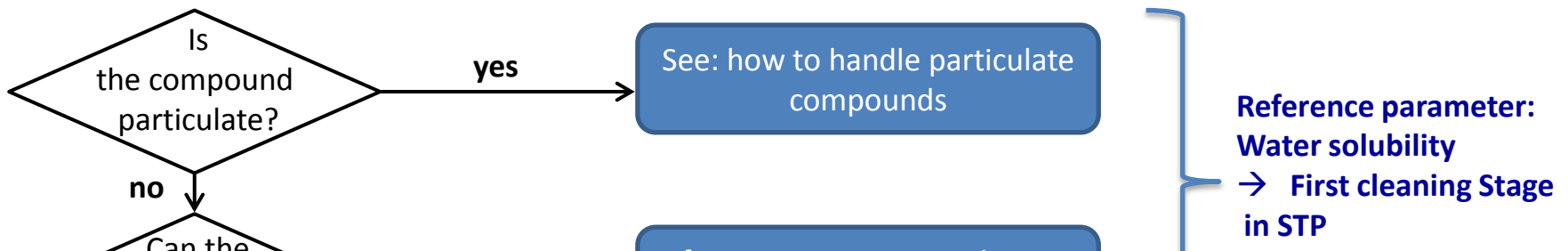|	Name	CAS no.	ZDHC	TEXT	CHEM	STM	polymers	Uses from SPIN	Industrial product	registered uses	Import/manufa
	Candidate List		Zero Discharge Hazardous Che		ST of plastics and met			NACE description Data from SPIN regis	Blue columns: From the	From ECHA website	
	Note: Group entries are split in different rows.										
4	4-aminoazobenzene	60-09-3	X	X	X			not found		intermediate, dye, pigment	intermediate
5	4,4'-bis(dimethylamino)-4"-(methylar	561-41-1		?	X			not found	inks and toners	inks, toners	10-100t.
6	[4-[4,4'-bis(dimethylamino) benzhydr	548-62-9		?	X			manufacture of chem	inks and toners	inks, toners	0-10t.
8	Cobalt dichloride	7646-79-9	X	X	X	X	X	manufacture of chem	metal surface treatment p	metal surface treatment products, laborator	1000-10 000t.
9	Potassium dichromate	7778-50-9	X	X	X	X	X	scientific research ar	metal surface treatment p	metal surface treatment products, pharmac	100-1000t.
10	Diboron trioxide	1303-86-2	X	X	X	X	X	manufacture of basic	laboratory chemicals, wat	laboratory chemicals, water treatment chem	1000-10 000t.
11	Boric acid	10043-35-3	X	X	X	X	X	manufacture of chem	pH regulators and water t	laboratory chemicals, washing & cleaning p	100 000-1000 000
12	Disodium tetraborate, anhydrous	12179-04-3, 1303-96-4,	X	X	X	X	X	Manufacture of fabric	pH regulators and water t	pH regulators and water treatment products	100 000-1000 000
14	N,N-dimethylformamide	68-12-2		X	X		X	Manufacture of cher	laboratory chemicals, adr	manufacture of: chemicals and machinery a	10 000-100 000t.
15	N,N-dimethylacetamide	127-19-5		X	X			manufacture of chem	laboratory chemicals an ir	laboratory chemical, manufacture of: chemi	10 000-100 000t.
16	Octamethylcyclosiloxane (D4)	556-67-2		X	X	X	X	manufacture of chemicals and chemical prode	laboratory chemicals, non-metal-surface tre	100 000 - 1 000 0
17	Decamethylcyclopentasiloxane (D5)	541-02-6		X	X	X	X	Manufacture of chemicals and chemical prode	washing & cleaning products, laboratory ch	10 000 - 100 000
18	Cobalt(II) sulphate	10124-43-3		X	X	X	X	Manufacture of fabric	metal surface treatment p	metal surface treatment products, laborator	10 000-100 000t.
19	Sodium dichromate	10588-01-9, 7789-12-0		X	X	X	X	Manufacture of fabric	metal surface treatment p	manufacture of: chemicals, fabricated metal	100-1000t.
20	Cobalt(II) diacetate	71-48-7		X	X	X		manufacture of fabric	metal surface treatment p	polymers, metal surface treatment products	1000-10 000t.
23	Phenolphthalein	77-09-8		X	X		X	manufacture of rubbe	laboratory chemicals, pH	laboratory chemicals, pH regulators and wa	10-100t.
24	Imidazolidine-2-thione (2-imidazolin	96-45-7		X	X			Manufacture of fabricated metal products, exc	manufacture of: rubber products and metals	100-1000 t.

	Name of priority substance [3]	CAS number [1]	ZDHC list	Identified as priority hazardous substance	Included in current BREFs	Plant protection product	Use categories	Imported/manufactured in EU (tons)	Uses in Finland based on national chemical register (data from years 2001-2014)
12	1,2-dichloroethane	107-06-2	X				polymers, pharm	1 000 000 - 10 000 000	solvent in chemical industry
13	Dichloromethane	75-09-2					washing & clean	100 000 - 1 000 000	solvent, in textile glues, pharmacetical industry
14	Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	X	X			polymers, interm	10 000 - 100 000	softener in rubber and plastics, textile industry, in
15	Diuron	330-54-1				X	polymers, manuf	100 - 1 000	biocide
16	Endosulfan	115-29-7		X		X			
17	Fluoranthene	206-44-0					no data found	no data found	

WP 2.2: Modelling of the fate and behaviour of industrial target substances in typical waste water treatment plants

- The fate of substances in WWTP/STP can be assessed in the SimpleTreat 4.0 model.

- The modelling gives an indication when substance categories/groups or individual substances may be problematic or not problematic in waste-water treatment.

- The modelled substances have been selected based on their use volume (mostly >10 000 tons annually), the uses in sectors (chemical, textile or STM) and with respect to intrinsic properties.

- When is a substance "relevant" in the context of HAZBREF? A trigger value of > 10 % release in the effluent may be used.

- However, it may be recommended that, ideally, any industrial sector may run (model) in SimpleTreat all their substances that they use.

- Examples and results of the modelling are presented in a report (Hazbref WP 2.2 Report May 17, 2019, Swedish EPA).

Decision tree to improve „standard phrases"

- However, the simple treat model provides no answers for:
  - substances that could not be modelled with simple treat (microplastic, substances with very high Kow)
  - whether a specific STP has the technical devices to avoid environmental releases
- Besides that: often mixtures are used, single substances are unknown for industrial operators >> parameters for modelling are missing
- Therefore, a decision tree currently is being developed: relevant parameters of a substance are connected with the single cleaning steps in a STP
- Benefit: improvement of generalized descriptions of risk management measures for STP ("standard phrases")

Is the compound particulate?

yes → See: how to handle particulate compounds

no ↓

Can the

Reference parameter: Water solubility
→ **First cleaning Stage in STP**

Overview of WP 2

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Strategy A

ECHA CHEM database
↓
Registered uses per sector
↓
<Reality check on substances used in sector>
↓
Grouping by chemical similarity
↓
modelling of fate & behaviour

Strategy B + D

Technical functions
Chemical functions
Chemical groups
Individual chemicals
↓
<Reality check on substances used in sector>
↓
Definition of fate & behaviour of chemical groups and representative individual substances

What data is needed for BAT Candidates?
(chemical groups & substances)

Strategy C

Regulated substances
(SVHC, POPs, WFD etc.)
+
C&L Info from MSDS
+
Check uses per sector

Fate & behaviour
+
Hazard alert
+
decision tree
↓
Recommendations for risk management in WWT
("Standard phrases")