

HAZBREF WP2: Target Substances

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

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



Three strategies to derive lists of relevant target substances for BREFs:

- A. Identify chemicals possibly used in the industrial sector by use categories or other descriptors, and prioritize them according to hazard and environmental release and fate criteria (**substance-based approach**).
- B. Use information available from specific industrial sectors and processes applied there to identify specific applications or technical functions (e.g. surfactants, bleaching agents etc.); identify several compounds in each sector of **use or technical function** and try to characterize this chemical group with regard to hazard and environmental release and fate criteria (**group-based approach**).
- C. Identify critical hazard or environmental release and fate characteristics (e.g. CMR, high persistence etc.) and derive lists of chemicals, which are *per se* undesired in chemical processes (**substances of concern, hazard-based approach**).

Strategy A



- **A practical example: Chemicals from the textile sector in use at industrial sites and by professional workers**
- The starting point are the roughly **21.000 substances** in the ECHA CHEM database.
- From these **13.907 substances** have an entry for uses at industrial sites.
- If only those which contain the string "**textile**" in the "Sector of Use", are filtered, **1.798 remain**.
- when the string "textile" is also filtered from the "widespread use by professional workers", only **937 substances** remain.
- → This means that **937 substances are used at industrial sites and by professional workers, which may also be used within textile industry.**
- We do not recommend to use these lists of 937 substances directly for inclusion into BREFs for the textile finishing industry.
- This list needs to be filtered according to substance properties (hazard criteria).

Strategy B: group-based approach

Extract from the TXT-BREF Questionnaire (DRAFT June 2018)					
Detergents/ wetting agents (surfactants)		Fabric softeners	Wetting/penetrating/de-aerating agents (surfactants)		
<u>Non-ionic</u>	Alcohol and fatty alcohols ethoxylat	(Ethoxylated) fatty alcohols		Alcohol polyglycol ethers	
	Fatty acids ethoxylates	(Ethoxylated) fatty acids		Alcohol polyglycol esters	
	Alkylphenol ethoxylates (APEOs)	(Ethoxylated) sorbitan esters		Alkane sulphone	
	Fatty amines ethoxylates	Alkyl phenol ethoxylates (APEO)		Ethoxylated amines	
	Triglyceride ethoxylates	Partial glycerides and ethoxylated			
	Ethylene oxide/propylene oxide add	Fatty amides			
<u>Anionic</u>	Alkyl sulphonates	Sulphonated and sulphated vegeta	Complexing/Sequestering/Dispersing agents		
	Alkyl aryl sulphonates			Phosphated alcohols	
	Alkyl sulphates	Short-chain alkyl phosphates		(EDTA) Ethylenediamine tetraacetate	
	Dialkylsulphosuccinates	Other		(NTA) Nitrilotriacetate	
	Alkyl carboxylates (e.g. sodium palm	Polyamide amines		(DTPA) Diethylenetriamine pentaacetate	
	Sulphated alkanolamides	Polyvinylpyrrolidone		Phosphonic acid derivatives (phosphonates)	
	Alkyl ether phosphates	Bisulphate anion (HSO ₄)-		Gluconic acid derivatives (gluconates)	
<u>Cationic</u>	Quaternary ammonium compounds	Quaternary ammonium salts with Q		Polyacrylates	
		Quaternary ammonium salts with a		Other	
<u>Amphoteric</u>	Betaine derivatives	Amido amines (e.g diethylene trian			
	Imidazolines			Condensation products of naphthalene sul	
	Modified fatty amino ethylates			Lignosulphonates	
	Other chemicals (e.g. alkalis)			Naphthalene sulphonates	
Solvents used					
trichloroethylene (TCE)	Perchloroethylene	Perchloroethylene (PERC)			
benzene		Glycol ethers (e.g. dipropylene glycol tertiary-butyl ether)			
white spirit		Liquid silicone (decamethylcyclopentasiloxane or D5)			
solvent naphtha		Liquid CO ₂			
other					

Strategy B

Outcome of consulting with the textile industry

- Consider '**performance chemicals**', which give textiles the desired appearance (are fixed to the fabric) ...
- and '**process chemicals**', which support the production of polymers and the application of performance chemicals (go to waste water in the end);
- Textile processing industry does not use individual chemicals, but **mixtures and formulations** – they don't know the chemical composition!
- Textile chemicals producers will **not disclose their recipes!**
- Besides that, basic chemicals may contain **impurities of toxicological concern;**

Strategy C: hazard-based approach

Water Framework Directive Priority Substances

- Plant Protection products are not considered as target substances
- For other priority substances use information was gathered from ECHA website and from Nordic chemical product register (SPIN)
 - Substances grouped according to the NACE category to 3 sectors
 - Only data from year 2016 was used from SPIN register

Strategy C: hazard-based approach

REACH: SVHC candidate, Authorisation and Restriction List Substances

- The lists were downloaded from ECHA website
 - SVHC list updated January 2019
- Use information of chemicals were compiled from ECHA website and the excels provided by ECHA (same as in strategy A)
 - SPIN register was utilized
- Substances grouped to 3 industrial sectors
 - + category 'polymers'

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Strategy C: hazard-based approach

	A	B	C	D	E	N	R	S	T	U	V	W	
1	Candidate List	Grey rows: no info in ECHA website										NACE description	
2	Note: Group entries are split in different rows.				Zero Discharge Hazardous Chemicals of plastics and metals				Data from SPIN register		Blue columns: From the BREFs		
3	Name	identifier ECHA	Desc	EC no.	CAS no.	ZDHC	TEXT	CHEM	STM	polymers	Uses from SPIN	Industrial product	
16	Octamethylcyclsiloxane (D4)				556-67-2		X	X					
17	Decamethylcyclopentasiloxane (D5)				541-02-6		X	X					
18	Cobalt(II) sulphate	100.030.291		233-334-2	10124-43-3		X		X	X		metal surface treatment products	
19	Sodium dichromate	100.031.070		234-190-3	10588-01-9, 7789-12-0		X		X	X		metal surface treatment products	
20	Cobalt(II) diacetate	100.000.687		200-755-8	71-48-7		X		X			metal surface treatment products	
21	Lead chromate molybdate sulphate	100.032.496	-	235-759-9	12656-85-8		X			X	Paints, laquers and varnishes	coating products, polymers	
22	Lead sulfochromate yellow (C.I. Pigment Yellow 17)	100.014.267	-	215-693-7	1344-37-2		X			X	Paints, laquers and varnishes	coating products, polymers	
23	Phenolphthalein	100.000.914		201-004-7	77-09-8		X					laboratory chemicals, pH indicators	
24	Imidazolidine-2-thione (2-imidazolinone)	100.002.280		202-506-9	96-45-7			X	?				
25	Diisopentyl phthalate	100.009.172		210-088-4	605-50-5			?		?			
26	Benzyl butyl phthalate (BBP)	100.001.475	BBP	201-622-7	85-68-7			?		?			
27	Hexahydromethylphthalic anhydride	100.042.798		247-094-1	25550-51-0			X		?			
28	4,4'-oxydianiline	100.002.707		202-977-0	101-80-4	X		X		X		polymers, photo-chemicals	
29	1,2-Benzenedicarboxylic acid, di-C6H4-	100.064.611		271-094-0	68515-51-5			X	?	X		polymers, coating products	
30	1-Methyl-2-pyrrolidone (NMP)	100.011.662		212-828-1	872-50-4			X	?			coating products, adhesives	
31	Chromium trioxide	100.014.189		215-607-8	1333-82-0			X	X	X		pH regulators and water treatment	
32	Tetralead trioxide sulphate	100.032.152		235-380-9	12202-17-4			X	X	X	Paints, laquers and varnishes	polymers, coating products	
33	Diisobutyl phthalate	100.001.412	DIBP	201-553-2	84-69-5	X		X	X	X		coating products, fillers, pigments	
34	Cadmium chloride	100.030.256		233-296-7	10108-64-2			X	X		others, laboratory chemicals	laboratory chemicals, metal surface treatment	
35	Cadmium oxide	100.013.770		215-146-2	1306-19-0			X	X		surface treatment, varnishes	metals, metal surface treatment	
36	Lead di(acetate)	100.005.551		206-104-4	301-04-2			X	X		intermediates, surface treatment	laboratory chemicals, coatings	
37	Diarsenic trioxide	100.014.075		215-481-4	1327-53-3			X	X			metals, semiconductors and electronics	
38	Lead				7439-92-1	X		X	X		welding and soldering agents, Colouring agents		
39	Lead oxide sulfate	100.031.672		234-853-7	12036-76-9			X		X	no data, confidential	coating products, polymers	
40	Orange lead (lead tetroxide)	100.013.851		215-235-6	1314-41-6			X		X	anti-fouling agents, pigments	polymers, adsorbents and catalysts	
41	Pentalead tetraoxide sulphate	100.031.867		235-067-7	12065-90-6			X		X	stabilizers, pharmaceuticals	polymers	

SPIN register data

	A	B	C	E	F	G	H	I	J	K	L
1	Note: Data on this sheet is from	SPIN register: http://www.spin2000.net/spinmyphp/									
2	Substance	CAS number	country	Category code	category description	prep	use amount	Industrial use	Chemical	STM	Textile
24	Naphtalene	91-20-3	DK	C19	Manufacture of coke and refined petroleum products	13	4,728.9	X			
25	Naphtalene	91-20-3	FI	C19	Manufacture of coke and refined petroleum products	30	176.0	X			
26	Naphtalene	91-20-3	NO	C19	Manufacture of coke and refined petroleum products	19	39.6	X			
27	Nickel	7440-02-0	FI	C19	Manufacture of coke and refined petroleum products	5	7.0	X			
28	nickel monoxide	1313-99-1	FI	C19	Manufacture of coke and refined petroleum products	44	76.0	X			
29	nickel monoxide	1313-99-1	DK	C19	Manufacture of coke and refined petroleum products	14	12.9	X			
30	nickel monoxide	1313-99-1	NO	C19	Manufacture of coke and refined petroleum products	10	0.8	X			
31	4-Nonylphenol, branched	84852-15-3	DK	C20	Manufacture of chemicals and chemical products	8	0.3	X	X		
32	Benzene	71-43-2	FI	C20	Manufacture of chemicals and chemical products	4	11,350.0	X	X		
33	Benzene	71-43-2	DK	C20	Manufacture of chemicals and chemical products	111	1.2	X	X		
34	Cadmium	7440-43-9	NO	C20	Manufacture of chemicals and chemical products	6	0.0	X	X		
35	DFHP (Bis (2-ethylhexyl)phthalate)	117-81-7	FI	C20	Manufacture of chemicals and chemical products	4	0.0	X	X		
36	Dichloromethane	75-09-2	FI	C20	Manufacture of chemicals and chemical products	5	48.0	X	X		
37	Dichloromethane	75-09-2	NO	C20	Manufacture of chemicals and chemical products	4	25.8	X	X		
38	Dichloromethane	75-09-2	DK	C20	Manufacture of chemicals and chemical products	4	10.0	X	X		
39	Lead	7439-92-1	DK	C20	Manufacture of chemicals and chemical products	5	0.0	X	X		
40	Lead	7439-92-1	NO	C20	Manufacture of chemicals and chemical products	7	0.0	X	X		
41	Lead	7439-92-1	SE	C20	Manufacture of chemicals and chemical products	22	0.0	X	X		
42	Naphtalene	91-20-3	FI	C20	Manufacture of chemicals and chemical products	7	2,601.0	X	X		
43	Naphtalene	91-20-3	NO	C20	Manufacture of chemicals and chemical products	102	2.3	X	X		
44	Naphtalene	91-20-3	DK	C20	Manufacture of chemicals and chemical products	20	2.2	X	X		
45	Nickel	7440-02-0	DK	C20	Manufacture of chemicals and chemical products	9	316.4	X	X		
46	Nickel	7440-02-0	SE	C20	Manufacture of chemicals and chemical products	18	47.0	X	X		
47	nickel monoxide	1313-99-1	SE	C20	Manufacture of chemicals and chemical products	8	15.0	X	X		
48	nickel monoxide	1313-99-1	NO	C20	Manufacture of chemicals and chemical products	4	0.4	X	X		
49	Benzene	71-43-2	DK	C21	Manufacture of basic pharmaceutical products and pharmaceutical	4	0.1	X	X		
50	Dichloromethane	75-09-2	FI	C21	Manufacture of basic pharmaceutical products and pharmaceutical	4	18.0	X	X		
51	4-(1,1,3,3-tetramethylbutyl)phenol	140-66-9	FI	C22	Manufacture of rubber and plastic products	4	0.0	X	X		
52	Benzene	71-43-2	DK	C22	Manufacture of rubber and plastic products	23	0.0	X	X		
53	Lead	7439-92-1	SE	C22	Manufacture of rubber and plastic products	6	0.0	X	X		
54	Benzene	71-43-2	DK	C23	Manufacture of other non-metallic mineral products	10	1,483.9	X			
55	Naphtalene	91-20-3	DK	C23	Manufacture of other non-metallic mineral products	6	85,003.6	X			
56	nickel monoxide	1313-99-1	FI	C23	Manufacture of other non-metallic mineral products	7	76.0	X			
57	Benzene	71-43-2	DK	C24	Manufacture of basic metals	30	0.0	X			

Next Steps (with support from ECHA):

- Strategy A:** Group **textile** substances in the outcome lists;
apply exclusion criteria (i.e. no/low concern);
apply hazard & fate criteria; compare with Strategy B & C.
- Strategy B:** Assign individual chemicals to **textile** groups;
work through the **textile** chemicals handbooks & literature;
characterize groups with regard to hazard & fate
- Strategy C:** Associate substances of hazard concern with industrial uses

Later:

- Strategy A&B for Chemical & STM industry
- Behaviour of selected substances in WWTP (Activity 2.2)