

# **Tier 1 and higher tier environmental exposure assessment of substances in articles**

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# 01.

## Introduction



# ECHA project: Substances in Articles (Service Request SR 04)

- Running project: 2012 – 2013 (May)
- Participants: RIVM & DHI. Ad-hoc consultant group:Tecnalia and TNO
- Review of models for consumer exposure assessment
- Review of existing data on migration and releases
- 4 case studies: 3 with focus on consumer exposure and 1 with focus on releases into the environment
- **Ideas/approach/examples presented today have not been approved by ECHA**

# Environmental exposure assessment of substances in articles

- Environmental exposure assessment: Most frequently applied tool: EUSES
  - Continental – regional – local assessments
  - Needs information on:
    - Substance data
    - Use pattern: Wide dispersive use
      - Release estimates – the key issue
        - Abrasive (use, matrix dependent)
        - Molecular (substance, use, matrix dependent)



# 02.

## Tier 1 and higher tier models for release estimates



# Release estimates

- Tier 1: ERC

Note	No	ERC	Default worst case release factors resulting from the conditions of use described in the ERCs. Grey cells indicate release factors which are used for the regional release estimation only (and not for the local one).		
			to air	to water (before STP)	to soil
8	10A	Wide dispersive outdoor use of long-life articles, low release	0.05%	3.2%	3.2% 100%
9,10	10B	Wide dispersive outdoor use of long-life articles, high or intended release	100%	100%	
8	11A	Wide dispersive indoor use of long-life articles, low release	0.05%	0.05%	n.a.
9,10	11B	Wide dispersive indoor use of long-life articles, high or intended release	100%	100%	n.a.
10	12A	Industrial processing of articles with abrasive techniques (low release)	2.5%	2.5%	2.5%
10	12B	Industrial processing of articles with abrasive techniques (high release)	20%	20%	20%

ERC for service life:

- Indoor-outdoor
- High release
- Low release

- Higher tiers:
  - Emission scenario documents

# Higher tier: OECD ESD

An Emission Scenario Document (**ESD**) is a document that describes the sources, production processes, pathways and use patterns **with the aim of quantifying the emissions (or releases) of a chemical into water, air, soil and/or solid waste.**

Some ESDs include service life:

- Plastic additives (3)
- Rubber additives (6)
- Textiles (7)
- Adhesives (20)

# Release estimates

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- Higher tiers:
  - Emission scenario documents
  - Measured data – “read across”

## Relevant measured exposure/migration/release data for substances in articles

### Criteria

- Migration/emission data can be retrieved
- Conditions of use described in data source: duration, dermal area, frequency of use, lifetime, concentration in article...

# Individual sources - example

Main source (Ref.)	No of individual study	Article	Article category	Type of material	Type of substances in article covered <sup>a</sup>			Conditions of use included	Relevance		Migration/emission into air/water/saliva/sweat				Relevance for REACH <sup>b</sup>	Reference	Comments/remarks	
					Heavy metals	Involatile organics	Volatile organics		Consumer	Environment	Air	Water	Saliva	Sweat				
[1]	[1]	Cell phone covers Sleeping mats Gloves Sneakers Clothing	AC13 AC5 AC5 AC6 AC5	Plastic Plastic Wool/synthic Leather Synthetic		x	x							x	High	<a href="http://www2.mst.dk/Udgiv/publications/2012/04/978-87-92903-02-0.pdf">http://www2.mst.dk/Udgiv/publications/2012/04/978-87-92903-02-0.pdf</a>		
[2]	[2]	Products Varnish and paint layers Textiles Foil Paper Carpets Wood Tyres Soles Concrete Various plastic products	AC13 AC5 AC13 AC8 AC5 AC11 AC10 AC10 AC4...	Plastic Various plastic materials, e.g. acrylics, polyamide, polyester, polystyrene, polyurethane Plastic		x	x				x	x	x	x	High. Emissions based on calculations.	<a href="http://www.chemitecs.se/download/18.4a08c3cb1291c3aa80e80001152/CHEMITECS+P4-D4_final_2010-06-24.pdf">http://www.chemitecs.se/download/18.4a08c3cb1291c3aa80e80001152/CHEMITECS+P4-D4_final_2010-06-24.pdf</a>		
[1]	[3]	Jackets (water proof/repels water) Mittens Rubber clogs Wellingtons Pacifier PVC soap packaging material Teddy bears with scent	AC5 AC10 AC11 AC13 AC30	Plastic Wood Synthetic PVC Rubber		x								x	x	High	<a href="http://www.mst.dk/Publikationer/Publikationer/2009/10/978-87-92548-83-2.htm">http://www.mst.dk/Publikationer/Publikationer/2009/10/978-87-92548-83-2.htm</a>	Experimental temperature 37°C Total concentrations in articles could be used for environmental

# Release estimates

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- Higher tiers:
  - Emission scenario documents
  - Measured data – “read across”
  - Modelling of releases

# Modelling of the releases

- Several emission tools exist, e.g.:
  - RIVM Emission tool: Models the release from articles into air
    - Diffusion inside article
    - Binding to matrix
    - Transfer of substances from surface into air
    - Could be extrapolated to model the releases into water
- Evaporation: concentration in air above article surface cannot exceed saturated vapor concentration
- Solubility limitations: molecular release from article into water cannot exceed solubility (pure water/water with detergents)

# 03.

## Case study



# Substance data

Property name	IUCLID data	Input parameter for
CAS-RN	103-23-1	
CLP-classification	Aquatic Acute 1	
Physical Form	liquid	TRA Worker
Molecular Weight	370 g/mol	TRA Worker TRA Consumer EUSES 2.1
Melting Point	-67.8 °C at 101,325 Pa	[EUSES 2.1]
Boiling Point	417 °C at 101,325 Pa	
Vapour Pressure	3·10 <sup>-5</sup> Pa at 20 °C	TRA Consumer EUSES 2.1 [TRA Worker]
Partition Coefficient(Log Kow)	8.94 at 25 °C	EUSES 2.1
Water solubility	0.003 mg/L at 22 °C	EUSES 2.1
Henry's Law Constant	5.06 at 25 °C	[EUSES 2.1]
Biodegradation in Water screening tests	readily biodegradable	[EUSES 2.1]
Bioaccumulation BCF (aquatic species)	27 (-)	[EUSES 2.1]
PBT/vPvB	No	
PNEC aqua (freshwater)	0.001 mg/L	
PNEC sediment (freshwater)	15.6 mg/kg sediment dw	
PNEC aqua (marine water)	0.001 mg/L	
PNEC STP	35 mg/L	
PNEC soil	0.865 mg/kg soil dw	
DNEL (general population, oral)	200 mg/kg bw/d	
DNEL (general population, inhalation)	4.4 mg/m <sup>3</sup>	

# Relevant service life uses for substance

## (Only molecular releases)

ID	Use	Substance tonnage (t/yr)	Assigned ERC	Argument for ERC-assignment
1	Indoor use as a plasticizer in PVC and rubber articles, such as flooring, wall-covering and wires/cables	75 000	ERC11b	As the substance is not physically bound and integrated into the article, the release of the substance can be substantial. Therefore, the ERC category ERC11a is considered not to be sufficient conservative. Release will occur during contact with water.
2	Outdoor use as plasticizer in outdoor PVC and rubber articles such as roofing, pipes	10 000	ERC10b	
3	Indoor use of substance as adhesives in articles	20 000	ERC 11a	The substance is integrated into the article. Therefore, the release of the substances is expected to be very low.
4	Outdoor use of substance as adhesive in articles	5 000	ERC 10a	
5	Indoor use of coated articles	20 000	ERC 11a	The substance is integrated into the article. Therefore, the release of the substances is expected to be very low.
6	Outdoor use of coated articles	5 000	ERC 10a	

## Tier 1

### Tier 1 models based on ERC

- ERC 10b: Release factor to water 100%
- ERC 11b: Release factor to water 100%
- ERC 10a: Release factor to water 3.2%
- ERC 11a: Release factor to water 0.05%

Risk not controlled for any of the service life exposure scenarios with RCR above 1 for one or more targets

## Softener

- Indoor vaporisation losses from flooring, wallcovering and wires/cables can be estimated at 0.05% when the assessed substance is used as a plasticizer
- Losses from flooring during cleaning based on the soapy water extraction data has been estimated to be 0.05% for interior-based products.
- Few data are available for emissions from products used outside. But for roofing the annual loss has been estimated to be 0.75%.

## Adhesive

- When the assessed substances is used as an adhesive the emission can be estimated to be 0% since coupling agents such as adhesives are intended to react within the compounded plastic and thus are intended to change chemically during the processes of compounding. After coupling none of the original substance is available for loss.

## Coating

- No information

# Chemical safety assessment in Chesar

Usage	Water	Air	Soil
Softener indoor use	0.05%	0.05%	ERC
Softener outdoor use	0.75%	0%	0%
Adhesives indoor use	0%	0%	0%
Adhesives outdoor use	0%	0%	0%
Coatings indoor use	ERC	ERC	ERC
Coating outdoor use	ERC	ERC	ERC

Safe use is proved with all RCR below 1

# Studies

Relevant to check if studies, where releases to the environment are measured or assessed, and which are carried out for the test substance or from a similar substance, and for same or similar article categories and use conditions.

- No relevant studies for actual substance and use conditions
- Read-across to other studies?

## Read-across from measured data

- S: substance a – substance b
- U: Use  $\alpha$  - Use  $\beta$
- M: matrix A – matrix B

Parameter	air	water
Diffusion path-length	M	M
Partitioning (matrix-air/water)	M, S	M, S
Diffusion coefficient	S <sub>(D<sub>Air</sub>)</sub>	S <sub>(D<sub>Water</sub>)</sub>
Mass transfer coefficient	M, U, S <sub>(K<sub>ow</sub>, P<sub>S</sub>)</sub>	M, U, S <sub>(K<sub>ow</sub>, S<sub>w</sub>)</sub>
Concentration	U	U
Duration (service life time)	U	U

# Release factors based on water solubility

$$f_w \leq \frac{Q_{\text{regional}} \left( \frac{\text{m}^3}{\text{d}} \right) \cdot 365 \frac{\text{d}}{\text{year}}}{M \left( \frac{\text{tonnes}}{\text{year}} \right) \cdot 0.8 \cdot f_{\text{regional}} \cdot 10^6 \frac{\text{g}}{\text{tonnes}}} \cdot S_w$$

All non-dissolved substance is removed in the first steps in the treatment plant (grease traps, grating, primary settler).

M	tonnage (tonnes/year)
$Q_{\text{regional}}$	daily flow to regional sewage treatment plant. It can be calculated using definitions in EUSES. The size of a regional WWTP is equal to $2 \cdot 10^7$ inhabitants each discharging 200 L/d, i.e. $= 4 \cdot 10^6 \text{ m}^3/\text{d}$ .
$f_{\text{regional}}$	fraction of the total tonnage in each region. It is set to 0.1.
$S_w$	water solubility of substance
$f_w$	fraction discharged to WWTP

Yearly tonnage (tonnes/yr)	$f_w$ -max (fraction)	$f_w$ -max (%)
$\Sigma = 115000$	4.8E-04	4.8E-02

# 04.

## Conclusions



# Discussion and conclusions

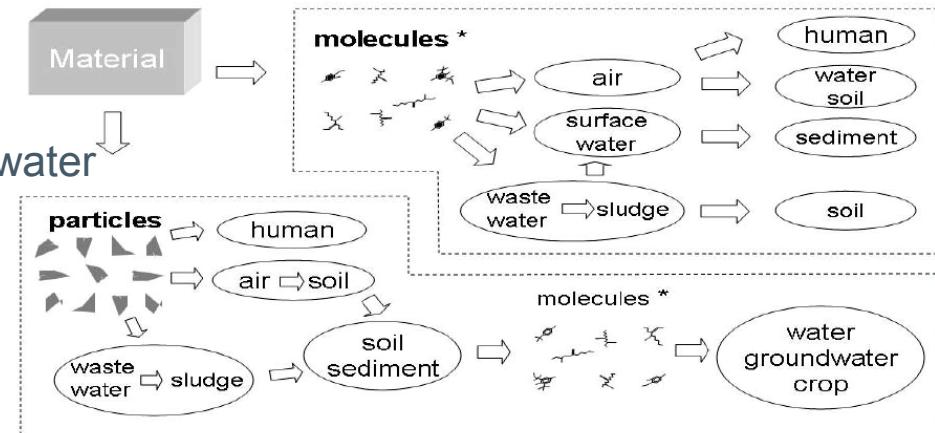
- The releases estimated from ERC 10b/11 b (high releases) are very conservative
- OECD ESD may provide improved release estimates
- Methods/guidelines for "Read-across" of measured data are missing
- Release estimates may be provided by
  - Modelling
  - Considering specific substance properties (water solubility)



# Release considerations

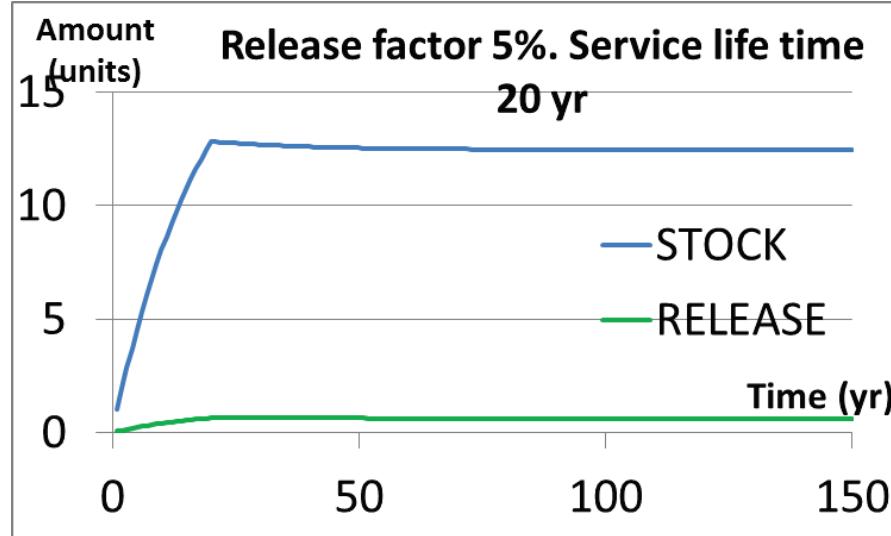
- Type of release:
  - Abrasion
    - Strongly use dependent
    - Independent on substance properties
    - Concentration in particles = concentration in article
  - Molecular

- Diffusion inside the matrix
- Binding to matrix
- Transfer from matrix surface to air/water



# Basic principles

- Articles persist in the society for several years (service life time)
- New articles continuously enter the market
- => articles are accumulated in the society



Release factor (%)	Service life time (yr)	Amount (units/yr)	Stock (units)	Annual release (units)
10	20	1	8.6	0.9
10	10	1	6.1	0.6
10	5	1	3.4	0.3
5	20	1	12.5	0.6
5	10	1	7.4	0.4
5	5	1	3.7	0.2
5	5	2	7.4	0.4

# Overview of use conditions

Parameter	Softener, indoor use	Softener, outdoor use	Adhesives, indoor use	Adhesives, outdoor use	Coatings, indoor use	Coatings, outdoor use
AC	5, 10, 13	5, 10, 13	13	13	13	13
ERC	11b	10b	11a	10a	11a	10a
Yearly tonnage	75,000	10,000	20,000	5,000	20,000	5,000
Indoor-outdoor	Indoor	Outdoor	Indoor	Outdoor	Indoor	Outdoor