

## Environmental Management

# Environmental risk assessment for relevant ingredients in adhesives and sealants in commonplace industrial uses

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### Abstract

The Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals requires that the risks from the exposure to substances be controlled throughout the life cycle. This includes that conditions of safe use are established via risk assessments, documented and communicated to the downstream users of chemicals. This also applies to the environmental risks originating from downstream uses of chemicals, for instance, those from the industrial uses of adhesives and sealants. Upon application, these products form solid matrices with low emissions to the environment during the application. Hence, it is expected that environmental exposure is low, provided that good industrial practice is followed. To explore this, an environmental risk assessment for industrial uses of adhesives and sealants is performed for the environmentally most hazardous ingredients. These include several solvents, organotin catalysts, fillers, reactive resins, a pigment, and a preservative. Specific environmental release categories (SPERCs) developed by the Association of European Adhesives and Sealants Industries (FEICA) are used to derive emission estimates. In combination with multimedia fate modeling, the environmental risk in water, sediment, soil, and a sewage treatment plant is investigated. The assessment results indicate no environmental risk for any of the ingredients. The discussion evaluates the conservative nature of the assumed values of the use rates, the release factors, the fate modeling, and assessment factors. It concludes that their combination results in a sufficient degree of conservatism. In view of the conservative nature of the assessment and given that the worst-case ingredients of adhesives and sealants are sufficiently controlled under the generically defined use conditions, it is concluded that the SPERCs used represent safe conditions for use, irrespective of the ingredient substances of adhesives and sealants. The essential SPERC information elements are identified for the purpose of communicating the conditions of safe use. The consolidation of this information in safety data sheets for adhesives and sealants is discussed. *Environ Assess Manag* 2022;18:1288–1296. © 2021 FEICA aisbl. *Integrated Environmental Assessment and Management* published by Wiley Periodicals LLC on behalf of Society of Environmental Toxicology & Chemistry (SETAC).

**KEYWORDS:** Downstream user, Environmental release, ERC, Exposure assessment, SPERC

### INTRODUCTION

The Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) is a European Union regulation that entered into force in June 2007 (EC, 2006). Its main objective is to ensure a high level of protection of human health and the environment from the risks posed by

the use of and exposure to hazardous chemicals. To achieve this, manufacturers and importers of chemicals into the EU are responsible for ensuring that information on the safe use of chemicals is available. To that end, they have to conduct chemical safety assessments (CSAs). For substances classified as hazardous, manufactured or imported above a volume of 10 tons per year, REACH requires a chemical safety report (CSR). The CSR documents the CSA. The latter addresses the hazards of the substances and the exposures coming from the use of these substances along the entire value chain of single substances. In addition, the conditions under which chemicals can be used safely are established in the CSA. These conditions are known as exposure scenarios. In addition to being documented in the CSR, they need to be communicated as annexes to the safety data sheets (SDSs) of substances (ECHA, 2018). The suppliers of

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adhesives and sealants are obliged to provide relevant information from the exposure scenarios for the ingredient substances in the SDSs of their products. Currently, two options are available to accomplish this: One is to attach a detailed exposure scenario, and the other is to provide consolidated, safe-use information to the product SDS.

Knowing the conditions under which the products are used in industrial facilities, the Association of the European Adhesives and Sealants Industries (FEICA) has developed specific environmental release categories (SPERCs; Tolls et al., 2016). These SPERCs and their justifications are available at FEICA (FEICA, 2021a) and the European Chemicals Agency (ECHA, 2021a). They support the REACH registrants in the CSAs of substances as ingredients of adhesives and sealants. To that end, they are included in, for example, environmental exposure assessment tools, such as CHESAR (Chemical Safety Assessment and Reporting Tool [ECHA, 2021c]); European Center for Ecotoxicology and Toxicology of Chemicals Targeted Risk Assessment (TRA) tools (ECETOC, 2017); and easyTRA (Jansen-Systems, 2021). The SPERCs define use conditions that represent good industrial practice for using these materials and corresponding factors for quantifying the fraction of substances that may be released into the environment via water, air, soil, or waste. In addition, the FEICA SPERCs define an indicative rate at which adhesive and sealant products are typically used and upper limits of concentration ranges for several generic ingredient types (FEICA, 2018; Tolls et al., 2016). By combining the release factors, the indicative use rates, and the concentration ranges, emission estimates can be obtained for the environmental part of the CSA.

Furthermore, REACH requires that each downstream user identifies and applies this information to their products to warrant the safe use of chemicals in their operations. This also relates to the industrial users of adhesives and sealants who apply these products in manufacturing a wide variety of goods, such as packaging, labels and tapes, motor and non-motor vehicles, vehicle parts and tires (except retreading), computers and electronics, and in general assembly (OECD, 2015). Additional industrial applications identified by adhesives and sealants trade associations (FEICA, 2021b) are uses in wood or furniture, bookbinding, and the textile, leather, and shoe industries. The prevalent technologies for applying adhesives and sealants are roll-coating and curtain-coating, followed by dip-coating, syringe and bead applications, and spraying. In syringe and bead applications, lines or beads of adhesives or sealants are applied to a substrate, for example, from a tube or a cartridge (OECD, 2015). As a result of the application of adhesives and sealants, a solid matrix is generated, which bonds two substrates in the case of adhesives, or seals the joint between two solid substrates (for sealants).

The present investigation explores whether the environmental risk of the adhesives and sealants ingredients with the most hazardous properties is sufficiently controlled based on the release factors defined in the FEICA SPERCs. It outlines the relevant information elements from these SPERCs for

inclusion in the SDSs. Finally, the two options available for including these information elements are discussed with a focus on providing fit-for-purpose information on safe use to the Safety Health and Environment (SHE) professionals who are responsible for the dangerous-goods management in the various industries that use adhesives and sealants.

## METHOD

### *Substance selection*

A survey was conducted among FEICA member companies to identify substances for a realistic worst-case scenario. To that end, substances that are classified as hazardous to the aquatic environment were identified and assigned to the adhesives and sealants ingredient classes as defined for the FEICA SPERCs (Tolls et al., 2016). Based on typical concentration ranges of the ingredients in adhesives and sealants (also from the survey) and the indicative use rate, the respective emission amounts were established.

For each substance log  $K_{OW}$ , log  $K_{OC}$ , boiling point, molecular weight, water solubility, vapor pressure, biodegradability, acute (LC50, EC50) and chronic ecotoxicity data (no-observed effect concentrations [NOEC]), and predicted no environmental effect concentrations (PNECs) for each environmental compartment were obtained from ECHA dossiers (ECHA, 2021b; cf. Tables S1 and S2a–c). Physical–chemical property data that are not available at ECHA were modeled by EpiWeb v 4.1 (Syracuse Research Corporation, U.S. Environmental Protection Agency), for example, for the dibutyltin catalysts and dibutyltin oxide.

The substances with the highest quotients of amount used over PNEC were identified as the worst-case substances. Dibutyltin-di(laurate) and -di(acetate) were selected because the demonstration of their environmental safety is of particular interest to FEICA due to the ongoing regulatory discussion. These substances hydrolyze rapidly in water to form dibutyltin oxide (RPA, 2005). Following the recommendation of the REACH Guidance R.16 (ECHA, 2016) dibutyltin oxide is assessed as the hydrolysis product of the dibutyltin catalysts.

### *Environmental exposure assessment*

The environmental risk assessment presented here follows the REACH Guidance R.12 (ECHA, 2015). For the industrial uses of adhesives and sealants, four SPERCs have been defined. The overview in Table 1 demonstrates that these SPERCs distinguish four emission situations for volatile (SPERC 4.x) and nonvolatile (SPERC 5.x) substances, and for solvent and/or solvent-less and water-based product types, respectively. The assignment of the appropriate SPERC exposure scenario is defined by the boiling point of the substance. According to the definition of volatile organic compounds by the World Health Organization (WHO, 1989), a threshold of 250 °C distinguishes volatile and nonvolatile ingredients. Emissions were assessed using the indicative use rates for the industrial uses of adhesives and sealants (3000 kg/day) and the upper limits of concentration ranges specified in Table 2.

**TABLE 1** Background information for four specific environmental release categories (SPERC) used for emission estimation of adhesives and sealants during industrial manufacturing

Ingredient types	Indicative concentration of ingredient (%)	Indicative ingredient use rate (kg/day)	Release factor acc. to SPERC for					
			Air (%)		Water (%)		Soil (%)	
			FEICA SPERC	FEICA SPERC	FEICA SPERC	FEICA SPERC	FEICA SPERC	FEICA SPERC
<b>Industrial use of solvent-borne adhesives and sealants</b>			4.2b <sup>1</sup>	5.1a <sup>2</sup>	4.2b	5.1a	4.2b	FEICA SPERC 5.1a
Solvent (volatile)	80	2400	98.5	98.5	0	0.3	0	0
Fillers: inorganic or polymeric	50	1500						
Reactive resins	50	1500						
Fillers: organic, nonpolymeric	10	300						
Pigments	<1	<30						
Catalysts	<1	<30						
<b>Industrial use water-borne adhesives and sealants</b>			4.1c <sup>3</sup>	5.1c <sup>4</sup>	4.1c	5.1c	4.1c	FEICA SPERC 5.1c
Fillers: Inorganic or polymeric	50	1500	98.5	1.7	0.3	0.3	0	0
Reactive resins	50	1500						
Fillers: organic, nonpolymeric	25	750						
Pigments	1	<30						
Catalysts	1	<30						
Preservatives	0.3	<9						

Note: For each relevant ingredient type, the daily amount of product used at an industrial site (product use rate), the ingredient concentrations (indicative concentration of ingredient), and the amount of each ingredient used at an industrial site (indicative ingredient use rate), as well as the release factors for air, water, and soil, are summarized. An industrial site (product use rate), the ingredient concentrations (indicative concentration of ingredient), and the amount of each ingredient used at an industrial site (indicative ingredient use rate), as well as the release factors to air, water, and soil are specified.

<sup>1</sup>FEICA-SPERCs 4.2b, Industrial use of *volatiles* in solvent-borne and solvent-less adhesives and sealants.

<sup>2</sup>FEICA-SPERCs 5.1a, Industrial use of *non-volatile substances* in solvent-borne and solvent-less adhesives and sealants.

<sup>3</sup>FEICA-SPERCs 4.1c, Industrial use of *volatiles* in water-borne adhesives/sealants.

<sup>4</sup>FEICA-SPERCs 5.1c, Industrial use of *non-volatile substances* in water-borne adhesives/sealants.

The environmental fate was assessed with the simple-box model (Brandes et al., 1996; Den Hollander et al., 2004), because it is implemented in the software tool easyTRA (version 5.0.0.5635; Jansen-Systems, 2021). It yields the predicted environmental concentrations (PECs) in different environmental media (air, water, soil, and sediment) by accounting for degradation and partitioning of the substance in and among the environmental compartments.

#### Risk characterization

In the risk characterization, the PEC obtained from the exposure assessment is compared with the PNEC, that is, the respective threshold value below which adverse environmental effects are not expected. A risk is considered controlled if this risk characterization ratio (RCR = PEC/PNEC) is less than 1.

## RESULTS

### Substance selection

Table 2 shows the list of selected substances, their boiling points, and the typical use concentrations in solvent and solvent-less and water-based adhesives and sealants. Cyclohexane, naphtha, n-hexane, and n-heptane belong to the adhesive and sealant ingredient type “solvents.” They are nonreactive processing aids (ERC4) and typically make up to 50% of the product content of solvent-borne adhesives and less than 15% in water-borne adhesives. Dipropylene glycol dibenzoate is used as an organic filler in concentrations up to 50% in solvent-borne adhesives and sealants and typically up to 6% in water-borne adhesives, and therefore meets the generic ingredient typification by Tolls et al. (2016). Dibutyltin-di(laurate) and dibutyltin-di(acetate) act as catalysts mainly in sealants. These substances hydrolyze in water

**TABLE 2** Overview of the test substances, their functionality in the product, and their respective allocation to the specific environmental release category (SPERC) based on the ingredient boiling point threshold of 250 °C

Substance name (CAS)	Boiling point (°C)	ERC	Ingredient type (primary use)	Solvent-borne products		Water-borne products	
				Typical (mean) value (lowest–highest %)	Calculated max. industr. tonnage (kg/day)	Typical (mean) value (lowest–highest %)	Calculated max. industr. tonnage (kg/day)
Acrylic acid (79-10-7)	141	4	Catalysts	0–0.01	0.3	0–2	60
Dibutyltin di(laurate) (77-58-7)	205	4	Catalysts	0.09–1	30	0–0.2	6
Dibutyltin di(acetate) (1067-33-0)	146	4	Catalysts	0.1–1	30	0–1	30
Dibutyltin oxide (818-08-6)	162 (D)	5	Catalysts	0.1–0.15	4.5	0–1	30
Cyclohexane (110-82-7)	<250	4	Solvent, volatile emulsifier	8–40	1200	0–15	450
Naphtha (64742-82-1)	140	4	Solvent, volatile emulsifier	1–50	1500	0–2	60
n-Heptane (142-82-5)	<250	4	Solvent, volatile emulsifier	1–50	1500	0–5	150
n-Hexane (110-54-3)	<250	4	Solvent, volatile emulsifier	1–30	900	0.1–5	150
Sebacate (52829-07-9)	275 (D)	5	Catalysts	0.1–0.2	6	0–0.01	0.3
Dipropylene glycol dibenzoate (27138-31-4)	270 (D)	5	Fillers: organic, non-polymeric	1–50	1500	0.1–6	180
ZnO (1314-13-2), 7440-66-6	(D)	5	Fillers: inorganic	0.1–5	150	0.4–1.5	45
BHT (128-37-0)	296	5	Reactive resins	0.1–5	150	0.0001–0.1	3
IPDI (4098-71-9)	310 (D)	5	Reactive resins	0–8	240	0.1–0.5	15
Drometrizole (2440-22-4)	397	5	Catalysts	0.02–0.5	15	–	0
Dibenzoylperoxide (94-36-0)	328	5	Catalysts	0–1	30	–	0
MIT (2682-20-4)	130	4	Preservatives	0.01–1	30	0.003–1	30

Note: The realistic concentration ranges of individual substances have been investigated, and typical mean values are reported. The calculated maximum use rate is based on the typical indicative use rate (Table 1) multiplied by the upper concentration reported for each ingredient. Abbreviations: BHT, 2,6-di-tert-butyl-p-cresol; (D), decomposition; IPDI, isophorone diisocyanate; MIT, methyl isothiazolone; ZnO, zinc oxide.

to form dibutyltin oxide with a half-life of less than one day, which is equated to a rate constant of  $0.69 \text{ day}^{-1}$  and used for environmental fate modeling. In the context of the present investigation, this is reflected by employing the EU TGD default degradation rate constant for rapidly degrading substances. Following the REACH Guidance R.12 (ECHA, 2015), the respective hydrolysis product dibutyltin oxide is included in the present analysis.

The chemicals 2,6-di-tert-butyl-*p*-cresol (BHT), drometrizole, and dibenzoylperoxide serve as antioxidant, UV absorber, and polymerization initiator, respectively. These functions are not specifically mentioned in the generic ingredient typification by Tolls et al. (2016). Because of their relatively low concentrations in adhesives and sealants, they are typified as catalysts (Table 2). Acrylic acid and isophorone diisocyanate (IPDI) are monomers. They also occur in end products at low concentrations and are typified as catalysts (Table 2). The UV stabilizer bis (tetramethyl-4-piperidyl)-sebacate is used in solvent-borne adhesives and sealants with concentrations typically ranging up to 0.2% and is considered a catalyst according to the FEICA ingredient types. The pigment zinc oxide is typically used as an inorganic filler in solvent (<5%) as well as in water-borne products (<3%). Finally, we included methyl isothiazolone (MIT) as an example of a preservative. Methyl isothiazolone is not used above 1% in adhesives and sealants. Due to its boiling point, MIT is considered to be a volatile substance and a nonreactive processing aid (ERC4).

Naphtha (EC 919-446-0), an important solvent for adhesives, is a complex (UVCB) substance for which a single substance risk assessment is impractical. For that reason, an existing multisubstance risk assessment for naphtha as an ingredient of coatings (Exxon, 2018) was used as a basis to explore the environmental safety of this substance as a constituent of adhesives and sealants. To that end, the release factors for air ( $RF_{\text{air}}$ ), soil ( $RF_{\text{soil}}$ ), and water ( $RF_{\text{water}}$ ), and the substance use rate for RCR equal to 1 ( $m_{\text{Safe,coatings}}$ ), were obtained from an SDS for naphtha (Exxon, 2021). The release factors to air, water, and soil, and the indicative substance use rates per site ( $Q_{\text{adhesive}}$ , kg/day) for solvents in industrial applications of solvent-borne adhesives and sealants, were retrieved from the FEICA SPERCs (Tolls et al., 2016). The RCR equal to one for adhesives application ( $m_{\text{Safe,adhesives}}$ ) was calculated according to

$$m_{\text{Safe,adhesives}} = m_{\text{Safe,coatings}} \times (RF_{\text{water,coatings}}/RF_{\text{water,adhesives}}) \times (RF_{\text{air,coatings}}/RF_{\text{air,adhesives}}).$$

The use of adhesives is considered safe if  $m_{\text{Safe,adhesives}} > Q_{\text{adhesive}}$ .

### Risk assessment results

Table 3 provides an overview of the results of the risk assessments given as RCRs for each substance in the respective environmental compartment. The highest RCRs in

water are calculated for dibutyltin-di(laurate) ( $RCR = 0.81$ ), and drometrizole ( $RCR = 0.53$ ). The highest RCRs for sediment are obtained for dibutyltin oxide ( $RCR_{\text{sed}} = 0.63$ ), drometrizole ( $RCR = 0.55$ ), and dipropylene glycol dibenzoate ( $RCR = 0.52$ ). The values for the freshwater and marine environment differ only slightly (e.g., for dibutyltin oxide  $RCR_{\text{sed,freshwater}} = 0.63$  and  $RCR_{\text{sed,marine}} = 0.64$ ). In soil, the highest values are obtained for dibutyltin-di(laurate) ( $RCR_{\text{soil}} = 0.83$ ), and for dibutyltin oxide ( $RCR_{\text{soil}} = 0.41$ ). Hence, for all substances and all environmental compartments, an RCR less than 1 is indicated.

Volatile substances evaporate during use, and their emission factors are high for the air compartment. Nevertheless, the highest RCR values for solvents (0.01–0.07) are found in the sediment and water compartments (Table 3). All RCRs are well below 1. Likewise,  $m_{\text{Safe}}$  for naphtha (~270 000 kg/day) is well above the indicative use rate of adhesives and sealants ( $Q_{\text{adhesive}} = 3000 \text{ kg/day}$ ).

## DISCUSSION

### Conservatism of the safety evaluation

As outlined (Tolls et al., 2016), the release factors for water, air, and soil represent worst-case values, that is, they tend to overestimate the emissions and lead to overprediction, that is, protective RCR values. The indicative use rate for adhesives and sealants (Tolls et al., 2016) is used for all substances investigated in this paper. They obtained the substance use rate values by multiplying the adhesives and sealants use rates in industrial sites (kg of adhesives or sealants per day) with the ingredient substance concentration (kg of substance/kg of adhesive or sealant). Before that, an expert poll established the adhesives and sealants use rates in industrial sites and the ingredient concentration ranges. Using the 95<sup>th</sup> percentile value of the adhesives and sealants use rate in industrial sites (3000 kg/day) and the ingredient concentration values (per ingredient type) from the upper end of the concentration range yielded the conservative estimates of the substance use rates (Tolls et al., 2016). The conservative character of the respective value ensures that the generic substance risk assessment for the CSR is adequate, that is, it ensures that safe conditions of use are demonstrated for most use situations.

The current investigation intends to shed light on the evaluation of safe use for concrete situations. To that end, it takes into account that, in specific cases, these indicative use rates may be exceeded in actual products. Similarly, the preservative methyl isothiazolone (MIT) may, in exceptional products, be included at levels of up to 1%, again more than the indicative use rate of 0.3%. Acrylic acid, typically a residual monomer occurring in low concentrations in polyacrylate-based adhesives and sealants, is assumed to be present at 2% in water-based adhesives, and thus twice as high as that for the assigned category catalysts. To establish sufficiently conservative scenarios, the safety assessments for MIT and acrylic acid are based on concentrations that exceed the upper ranges

TABLE 3 Summary of ingredients, their boiling points, and corresponding ERC and SPERC codes

Substance name (CAS)	Boiling point (°C)	ERC	Environmental risk characterization									
			SPERC code	RCR <sub>STP</sub>	RCR <sub>aqua</sub>	RCR <sub>sed</sub>	RCR <sub>soil</sub>	RCR <sub>marine water</sub>	RCR <sub>marine sed.</sub>			
Acrylic acid (79-10-7)	141	4	FEICA SPERC 4.1.c.v3	0.008	0.26	0.26	0.26	0.0035	0.26	0.26	0.26	
			FEICA SPERC 4.2.b.v3	0	0.02	0.02	0.02	0.0009	0.02	0.02	0.02	
Dibutyltin di(laurate) (77-58-7)	205	4	FEICA SPERC 4.1.c.v3	0.000036	0.81	0.14	0.14	0.83	0.81	0.81	0.14	
			FEICA SPERC 4.2.b.v3	0	0.03	0.0061	0.04	0.16	0.04	0.04	0.0062	
Dibutyltin di(acetate) (1067-33-0)	146	4	FEICA SPERC 4.1.c.v3	0.0022	0.27	0.03	0.03	0.02	0.27	0.27	0.03	
			FEICA SPERC 4.2.b.v3	0	0.01	0.0012	0.01	0.02	0.01	0.01	0.0012	
Dibutyltin oxide (818-08-6)	162 (D)	5	FEICA SPERC 5.1.a.v3	0	0.16	0.15	0.15	0.05	0.16	0.16	0.16	
			FEICA SPERC 5.1.c.v3	0.0023	0.64	0.63	0.63	0.41	0.65	0.65	0.64	
Cyclohexane (110-82-7)	<250	4	FEICA SPERC 4.2.b.v3	0	0.000083	0.00038	0.00074	0.0025	0.000074	0.000074	0.0000074	
			FEICA SPERC 4.1.c.v3	0.0056	0.0088	0.04	0.04	0.01	0.0088	0.0088	0.00088	
Naphtha (64742-82-1)	140	4	FEICA SPERC 4.2.b.v3	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
			FEICA SPERC 4.1.c.v3	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
n-Heptane (142-82-5)	<250	4	FEICA SPERC 4.2.b.v3	0	0.00019	4.4E-5	0.00017	0.0003	0.00017	0.00017	0.000037	
			FEICA SPERC 4.1.c.v3	0.27	0.0064	0.0014	0.0063	0.00018	0.0063	0.0063	0.0014	
n-Hexane (110-54-3)	<250	4	FEICA SPERC 4.2.b.v3	0	0.000054	0.00025	0.00046	6.5E-5	0.00046	0.00046	0.00021	
			FEICA SPERC 4.1.c.v3	0.0029	0.02	0.07	0.07	0.01	0.02	0.02	0.07	
Sebacate (52829-07-9)	275 (D)	5	FEICA SPERC 5.1.a.v3	0	0.03	0.03	0.03	0.0028	0.03	0.03	0.03	
			FEICA SPERC 5.1.c.v3	0.00014	0.03	0.03	0.03	0.0031	0.03	0.03	0.03	
Dipropylene glycol dibenzoate (27138-31-4)	270 (D)	5	FEICA SPERC 5.1.a.v3	0	0.08	0.08	0.08	0.01	0.08	0.08	0.08	
			FEICA SPERC 5.1.c.v3	0.0016	0.52	0.52	0.52	0.19	0.52	0.52	0.52	
ZnO (1314-13-2), (7440-66-6)	(D)	5	FEICA SPERC 5.1.a.v3	0	0.07	0.14	0.14	0.14	0.03	0.03	0.03	
			FEICA SPERC 5.1.c.v3	0.05	0.09	0.18	0.18	0.21	0.04	0.04	0.04	

(Continued)

TABLE 3 (Continued)

Substance name (CAS)	Boiling point (°C)	ERC	Environmental risk characterization						
			SPERC code	RCR <sub>STP</sub>	RCR <sub>aqua</sub>	RCR <sub>sed</sub>	RCR <sub>soil</sub>	RCR <sub>marine water</sub>	RCR <sub>marine sed.</sub>
BHT (128-37-0)	296	5	FEICA SPERC 5.1a.v3	0	0.003	0.07	0.02	0.0032	0.08
IPDI (4098-71-9)	310 (D)	5	FEICA SPERC 5.1c.v3	0.04	0.01	0.36	0.24	0.02	0.37
Drometrizole (2440-22-4)	397	5	FEICA SPERC 5.1a.v3	0	0.02	0.000019	0.000016	0.02	0.00002
Dibenzoylperoxide (94-36-0)	328	5	FEICA SPERC 5.1c.v3	0.0021	0.1	0.00011	3.3E-06	0.1	0.00011
MIT (2682-20-4)	130	4	FEICA SPERC 5.1a.v3	0	0.53	0.54	0.00013	0.54	0.55
			FEICA SPERC 5.1a.v3	0	0.0049	0.0048	0.1	0.00048	0.00047
			FEICA SPERC 4.1c.v3	0.02	0.1	0.41	0.05	0.1	0.41
			FEICA SPERC 4.2b.v3	0	0.02	0.07	0.05	0.02	0.07

Note: Risk characterization ratios (RCRs) for the sewage treatment plant (RCR<sub>STP</sub>), local freshwater (RCR<sub>aqua</sub>), sediment (RCR<sub>sed</sub>), terrestrial environment (RCR<sub>soil</sub>), and marine environment (RCR<sub>marine water</sub> and RCR<sub>marine sed</sub>) are calculated with easyTRA and the respective SPERCs for solvents in solvent-borne/solvent-free adhesives/sealants.  
 Abbreviations: n/a, see text for explanation; (D), substance decomposition, that is no boiling point (ERC5 is assumed as default because substance is not volatile); BHT, 2,6-di-tert-butyl-p-cresol; (D), decomposition; IPDI, isophorone diisocyanate; MIT, methyl isothiazolone; ZnO, zinc oxide.

specified for the respective ingredient types in Table 1, thus leading to protective RCR values. This holds true for all compartments.

#### ***Fate modeling assumptions and assessment factors***

For dibutyltin(dilaurate) and dibutyltin oxide, relatively high  $RCR_{Soil}$  values, up to 0.83 and 0.41, respectively, are obtained. As a result of their properties, they adsorb onto sewage sludge, which, according to the model, is subsequently used as fertilizer. The fate model predicts those substances to end up in agricultural soil assuming a sludge application rate of 5 t/ha per application and assuming that sludge is applied each year. In view of actual application rates ranging from 2 to 3 t/ha (Andersen, 2001; INERIS, 2008; Schowanek et al., 2004) and fertilization with sewage sludge occurring at two- or three-year intervals or even less frequently (Schowanek et al., 2004), the modeled soil concentrations tend to overestimate the actual ones.

The highest RCRs in water are obtained for dibutyltin(dilaurate) ( $RCR=0.81$ ), dibutyltin oxide ( $RCR=0.64$ ), and drometrizole ( $RCR=0.53$ ). These RCRs are the result of applying the REACH Guidance (ECHA, 2015), reflecting the conservatism that is imparted in the assessment factors (AF; i.e., 1000 for the organotin compounds and 50 for drometrizole). The conservatism imparted in these factors (AF) carries over to the resulting RCRs. For dibutyltin(dilaurate) and dibutyltin oxide, an AF of 1000 is applied in the absence of chronic ecotox data to obtain the PNEC from acute ecotoxicity data only. For drometrizole, the PNEC derivation is based on two NOECs from daphnia and algae.

#### ***Generalizing the risk assessment results***

The discussion above outlined the conservative nature of the safety assessment and demonstrated that the RCR values obtained for highly environmentally hazardous substances are less than 1. Given that the worst-case ingredients of adhesives and sealants are sufficiently controlled under the conditions outlined in the FEICA SPERCs, it can be deduced that the same holds true for those ingredients with a lower quotient of amount used over PNEC. Because this is the case, the generically defined SPERCs and the conditions of use defined therein are safe for all ingredients of adhesives and sealants, as demonstrated in the risk assessment. Consequently, it is possible to communicate the generic conditions of safe use for adhesives and sealants independently of individual ingredients.

#### ***Implications for suppliers of adhesives and sealants***

This information on safe conditions of use has to outline fundamental prerequisites warranting safe use at the industrial facility. The maximum amount of adhesive or sealant used per day of 3000 kg must be specified. It has to be stated that the effluents of the industrial site are submitted to biological wastewater treatment, be it on-site or at a domestic wastewater treatment plant. For reference purposes, the relevant FEICA SPERCs should be mentioned, that is, FEICA SPERCs 4.1c and 5.1c for water-borne products and FEICA SPERCs

4.2b and 5.1a for solvent-borne products. Furthermore, the consolidated safe-use information should include the instruction to not discard neat adhesives or sealants (or residues thereof) into water, to collect solvent washings of equipment and dispose of them as chemical waste, and to dispose of adhesive or sealant residues as chemical waste according to national law. Releases of solvents into the air are not restricted by the SPERCs, because they are not decisively important with regard to environmental risks. It should be noted, however, that the regulation of volatile organic compounds (VOC directive) may require the industrial users of solvent-containing products to control their emissions and, if necessary, to implement measures for reducing solvent emissions, for example, by installing solvent recovery or combustion installations.

Adhesives and sealants are multimaterial mixtures. The European Chemicals Agency has outlined two options for communicating the relevant information from the exposure scenarios of the ingredient substances with the SDS for the mixture (ECHA, 2021d). One is attaching relevant exposure scenarios for the ingredient substances as an annex to the SDS. This option may be preferred in cases in which the combination of substance use amounts, hazardous properties, parameters of the receiving environment, and release factor for the use processes requires tight emission controls. Under those circumstances, it might be warranted to identify the mixture ingredient substance(s) triggering the need for emissions control. This is typically done by the lead component identification methodology (CEFIC/VCI, 2018). The exposure scenario of the lead component(s) may then be attached to the SDS of the mixture to provide more detailed information on safe conditions of use. Companies exposed to such a situation must be able to interpret and act according to information relevant to the chemical safety assessment. (This information includes daily use rates, release factors for water, air, and soil, dilution factors, PNECs, and efficiency factors for risk management measures.) Companies do so either through qualified staff or through the support of qualified service providers.

The second option for communicating the relevant information is to provide consolidated safe-use information for the mixture either as an annex to the SDS or as part of the main body of the SDS, primarily in Section 8. As demonstrated in the safety assessment above, the environmental risk of the industrial use of adhesives and sealants is adequately controlled under the generally applicable conditions defined by the FEICA SPERCs and regardless of the ingredient substance. In addition, these conditions can be summarized as consolidated safe-use information for adhesives and sealants, which is straightforward to understand and implement by Safety Health and Environment professionals. They handle a broad portfolio of topics such as safety instructions for workplaces, safety and environmental training for co-workers, and acquisition and maintenance of permits. In view of the breadth of this array of tasks, SHE professionals need to focus their efforts. Receiving safe-use information in consolidated form is helpful for them in two ways. They can handle one of



their REACH downstream user tasks in a time-efficient manner and also be effective in establishing safe conditions of use for adhesives and sealants in their companies. From this perspective, consolidating safe-use information in SDSs is the “fit-for-purpose” option for communication of the conditions of safe use to the industrial users of adhesives and sealants.

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## DATA AVAILABILITY STATEMENT

All data required for calculations of the Risk Characterization Ratios (RCR) are openly available from public sites (e.g., ECHA registration webpage). Data calculations were performed with easyTRA, a computerized program that can be purchased from Janssen Systems. Computer files for each risk assessment can be made available upon request from corresponding author Thorsten Wind (thorsten.wind@henkel.com).

## SUPPORTING INFORMATION

The supporting information represent a summary of the status quo of publically available substance data. They were used to calculate the individual environmental risk characterization ratios and are not relevant to understand the relevant outcome of the manuscript.

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